

The metal-binding sites of glucose phosphates

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Supplementary information

Coupling constants and derived conformations.

		$^3J_{1,2}$	$^3J_{2,3}$	$^3J_{3,4}$	$^3J_{4,5}$
$[\text{Pd}(\text{en})(\alpha\text{-D-Araf5P1,3H}_{-2}\text{-}\kappa\text{O}^{1,3})]^{2-}$	2E	<1	<1	<1	5.2
$[\text{Pd}(\text{en})(\beta\text{-D-Araf5P1,2H}_{-2}\text{-}\kappa\text{O}^{1,2})]^{2-}$	3E to 3T_2	3.3	3.6	4.1	–
$[\text{Pd}(\text{en})(\alpha\text{-D-Ribf5P1,3H}_{-2}\text{-}\kappa\text{O}^{1,3})]^{2-}$	2E	4.4	5.2	5.2	5.0
$[\text{Pd}(\text{en})(\alpha\text{-D-Ribf5P1,2H}_{-2}\text{-}\kappa\text{O}^{1,2})]^{2-}$	2T_3 or 3T_2	3.2	–	–	5.1
$[\text{Pd}(\text{en})(\beta\text{-D-Ribf5P2,3H}_{-2}\text{-}\kappa\text{O}^{2,3})]^{2-}$	ca. 3T_2	5.4	<1	<1	2.5
$[\text{Ga}(\text{tacn})(\alpha\text{-D-Ribf5PH}_{-3}\text{-}\kappa\text{O}^{1,2,3})]^{2-}$	2T_3	3.7	5.1	<1	5.3
$[\text{Ga}(\text{Me}_3\text{tacn})(\alpha\text{-D-Ribf5PH}_{-3}\text{-}\kappa\text{O}^{1,2,3})]^{2-}$	2T_3	3.7	4.9	<1	5.3
$[\text{Co}(\text{tacn})(\alpha\text{-D-Ribf5PH}_{-3}\text{-}\kappa\text{O}^{1,2,3})]^{2-}$	2T_3	3.3	4.1	–	5.5

		$^2J_{1a,1b}$	$^3J_{1a,P}$	$^3J_{1b,P}$	$^3J_{3,4}$	$^3J_{4,5}$
$[\text{Pd}(\text{en})(\beta\text{-D-Fruf1,6P2,3H}_{-2}\text{-}\kappa\text{O}^{2,3})]^{4-}$	4E to 4T_3	10.7	5.0	2.7	6.6	7.2
$[\text{Pd}(\text{en})(\alpha\text{-D-Fruf1,6P2,4H}_{-2}\text{-}\kappa\text{O}^{2,4})]^{4-}$	3E	–	–	–	<1	<1
$[\text{Al}(\text{tacn})(\beta\text{-D-Fru1,6P2,3H}_{-2}\text{-}\kappa\text{O}^{2,3,P})]^{3-}$	4T_3	–	–	–	6.9	9.1

		$^2J_{1a,1b}$	$^3J_{3,4}$	$^3J_{4,5}$	$^3J_{5,6a}$	$^3J_{5,6b}$
$[\text{Pd}_2(\text{en})_2(\alpha\text{-D-Fruf6PH}_{-4}\text{-}\kappa\text{O}^{1,3};\kappa\text{O}^{2,4})]^{2-}$	3E	11.6	<1	<1	6.0	7.7
$[\text{Pd}(\text{en})(\beta\text{-D-Fruf6P2,3H}_{-2}\text{-}\kappa\text{O}^{2,3})]^{2-}$	4E to 4T_3	12.1	6.9	7.7	–	–
$[\text{Pd}(\text{en})(\alpha\text{-D-Fruf6P2,4H}_{-2}\text{-}\kappa\text{O}^{2,4})]^{2-}$	3E	–	<1	<1	4.6	5.0

	$^3J_{1,2}$	$^3J_{2,3}$	$^3J_{3,4}$	$^3J_{4,5}$	$^3J_{5,6a}$	$^3J_{5,6b}$
$[\text{Pd}_2(\text{en})_2(\alpha\text{-D-Glcp6PH}_{-4}\text{-}\kappa\text{O}^{1,2};\kappa\text{O}^{3,4})]^{2-}$	3.9	9.0	–	–	–	–
$[\text{Pd}_2(\text{en})_2(\beta\text{-D-Glcp6PH}_{-4}\text{-}\kappa\text{O}^{1,2};\kappa\text{O}^{3,4})]^{2-}$	<1	9.1	9.1	–	–	–
$[\text{Pd}(\text{en})(\beta\text{-D-Manp6P1,2H}_{-2}\text{-}\kappa\text{O}^{1,2})]^{2-}$	<1	9.9	3.6	–	–	–
$[\text{Pd}_2(\text{en})_2(\beta\text{-D-Manp6PH}_{-4}\text{-}\kappa\text{O}^{1,2};\kappa\text{O}^{3,4})]^{2-}$	<1	9.6	9.6	9.6	–	–