

SUPPORTING INFORMATION

**Analysis of the aromaticity of five-
membered heterometallacycles
containing Os, Ru, Rh, and Ir**

Rafael Islas*^{1,2}, Jordi Poater and Miquel Solà*¹

¹Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Campus Montilivi, 17071 Girona, Catalonia, Spain.

²Departamento de Química, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta s/n, Guanajuato, C.P. 36050, México

Email: rafael.islas.colina@gmail.com, miquel.sola@udg.edu

Contents

Figure S1. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 2.

Figure S2. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 3.

Figure S3. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 4.

Figure S4. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 5.

Figure S5. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 6.

Cartesian coordinates in Å of **1, 2, 11, 12, 13, 14, 15, 21, 22, 23, 24, 25, 31, 32, 33, 34, 35, 41, 42, 43, 44, 45, 51, 52, 53, 54, 55, 61, 62, 63, 64** and **65**.

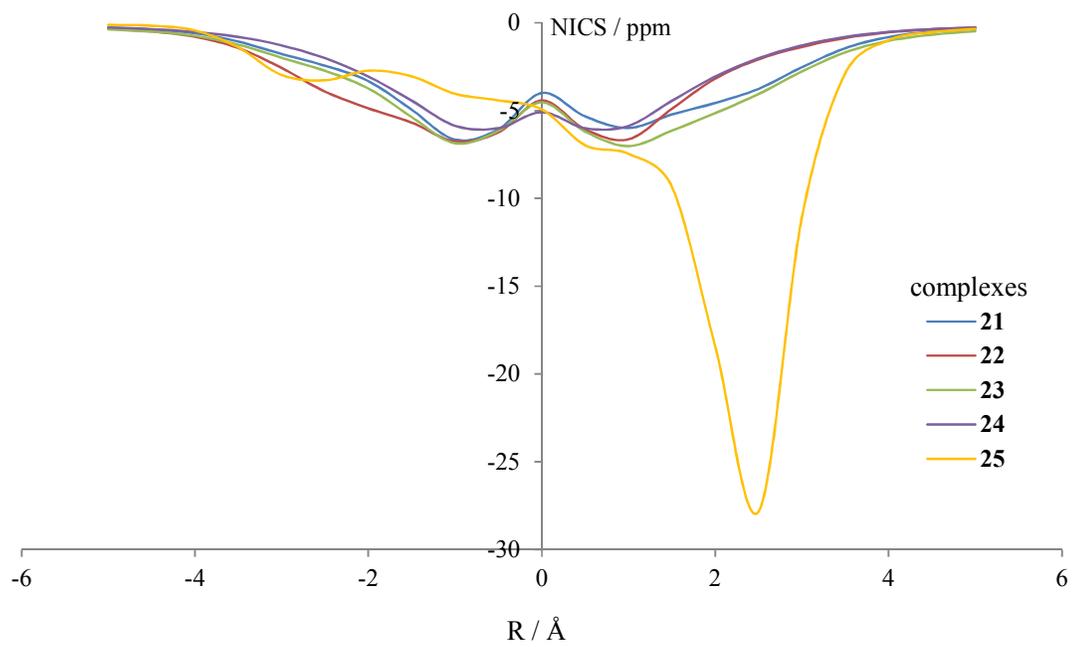


Figure S1. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 2.

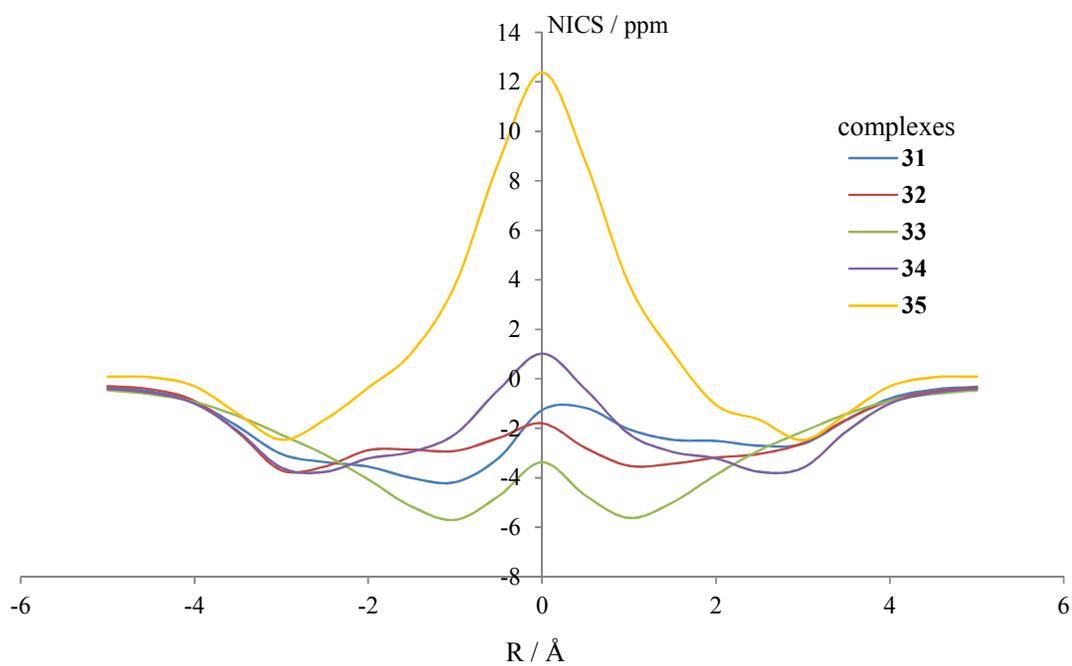


Figure S2. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 3.

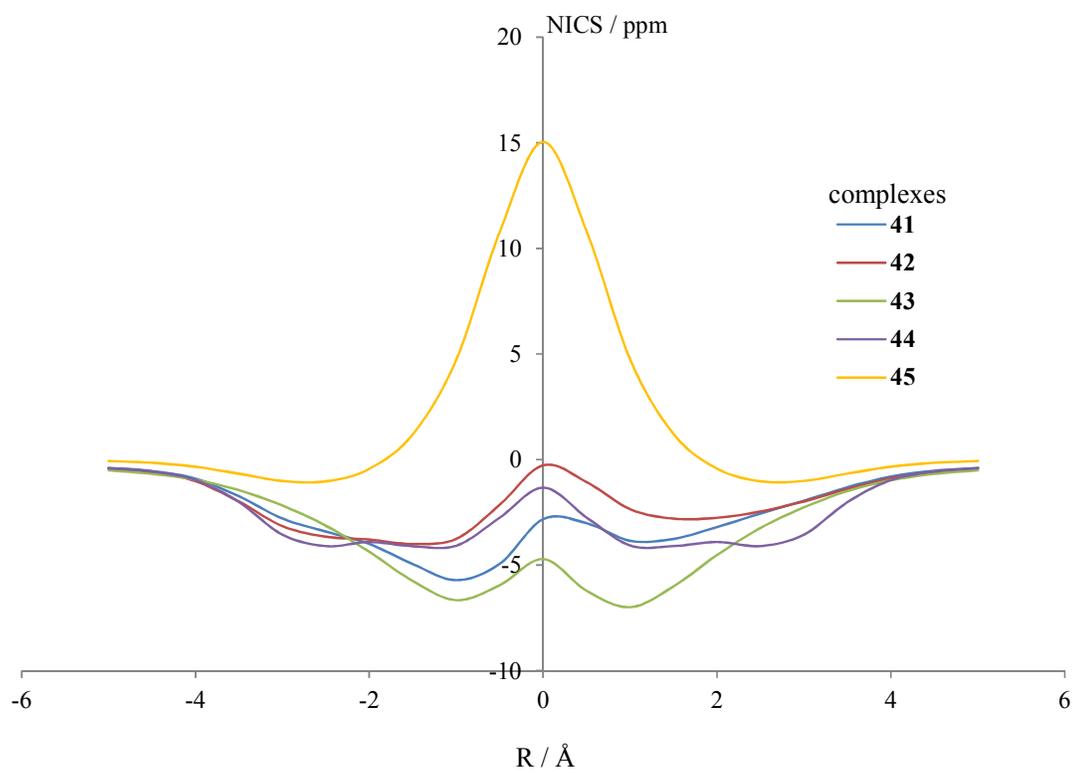


Figure S3. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 4.

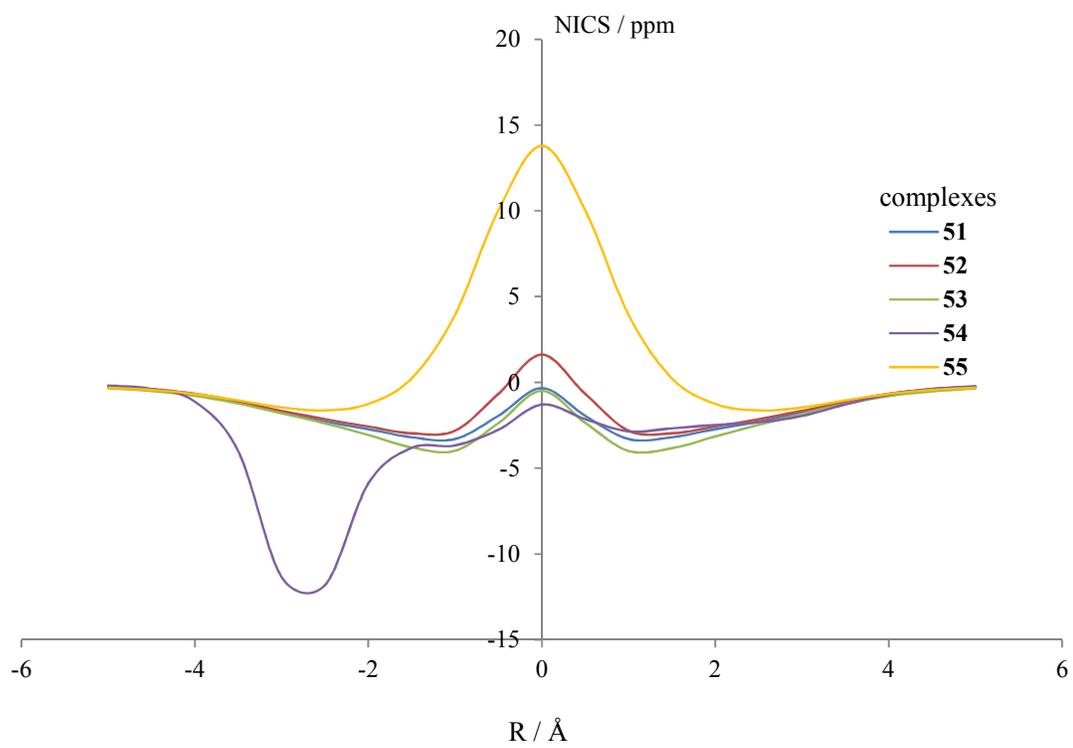


Figure S4. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 5.

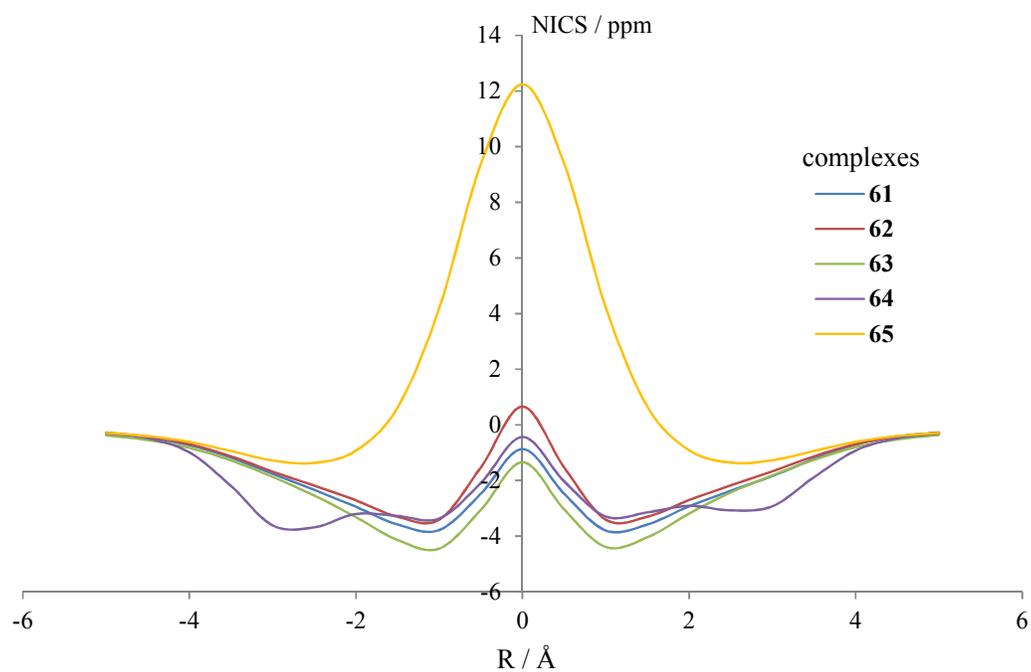


Figure S5. NICS profiles computed in the axis perpendicular to the five-membered rings of the molecules of Set 6.

Cartesian Coordinates in Å of all optimized structures at B3PW91/def2-TZVP are placed in a single file named *coordinates-complexes.xyz* for convenient visualization.