Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2014

## Electronic excited states of chromium and vanadium bisarene complexes revisited: Interpretation of the absorption spectra on the basis of TD DFT calculations

Sergey Ketkov,\* Nikolai Isachenkov, Elena Rychagova and Wen-Bih Tzeng

## **Supporting Information**

15

20

25

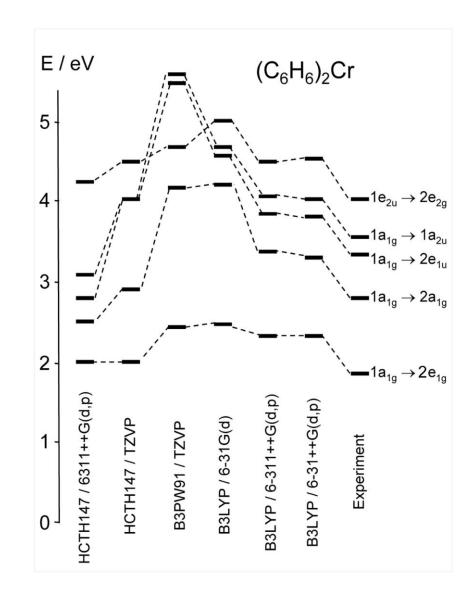


Fig. S1. TD DFT energies of the excited states in the  $(\eta^6-C_6H_6)_2$ Cr molecules calculated at various levels of theory. The MO notation is given in Fig. 1. The experimental values correspond to those in Table 2.