Inter-Atomic Magnetizability: a QTAIM-Based Approach Toward Magnetic Aromaticity

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Table S-1. The σ-framework magnetizabilities of aromatic, nonaromatic and antiaromatic hydrocarbons.

(σ-Framework)		$\chi(C)^{intra}$	$\chi(H)^{intra}$	$\chi(C\|C')$	$\chi(C\|H)$	$\chi_{zz}(C)^{intra}$	$\chi_{zz}(H)^{intra}$	$\chi_{zz}(C\|C')$	$\chi_{zz}(C\|H)$
$C_3H_3^+$		-0.182	-0.855	-0.838	-0.676	-4.213	-1.026	-1.796	-1.452
$C_4H_4^{2+}$		-0.051	-0.662	-0.984	-0.616	-3.228	-0.732	-1.901	-0.948
$C_5H_5^-$		-0.724	-1.537	-1.132	-0.803	-1.976	-1.572	-1.918	-1.383
C_6H_6		-0.009	-1.215	-0.821	-0.667	-2.025	-1.179	-1.499	-1.121
$C_7H_7^+$		+0.538	-1.007	-0.672	-0.593	-2.070	-0.964	-1.536	-1.039
$C_8H_8^{2+}$		+0.989	-0.855	-0.574	-0.516	-2.235	-0.824	-1.727	-0.979
$C_8H_8^{2-}$		-1.451	-1.420	-0.873	-0.576	-1.326	-1.179	-1.332	-0.777
$C_9H_9^-$		+0.328	-1.188	-0.695	-0.498	-1.524	-0.970	-1.307	-0.723
Ethene		-0.365	-1.248	-0.780	-0.688	-2.485	-1.268	-1.334	-1.235
C_4H_4									
	C=C	-0.240	-1.204	-0.566	-0.656	-1.702	-1.204	-0.543	-1.092
	C–C	--------	--------	-0.619	--------	--------	--------	-0.751	--------
$C_5H_5^+$									
	(C_1^+)–C_2	+2.000	-0.912	-0.779[a]	-0.588	-2.347	-1.014	-1.749[a]	-1.262
	(C_2)=C_3	-0.381	-1.063	-0.802[a]	-0.760	-2.299	-1.112	-1.644[a]	-1.335
	(C_3)–C_4	-0.379	-0.994	-0.823	-0.681	-2.201	-1.060	-1.882	-1.278

How a WFX file should be modified for measuring pure π-contribution in magnetizability?

A WFX file contains different types of information about electronic structure of a molecule; modifying these data can help to measure the contribution of a particular orbital to a particular electronic property.

The first part that should be modified is "net charge" this part represents the summation over the number of all protons and electrons. By removing a number of electrons from an orbital(s) the net charge of molecule changes; so, for each electron that is removed one positive charge should be introduced to the net charge. For instance if the net charge of a molecule is –4 and 6 electrons are removed from 3 MOs, the net charge part should change to +2.

"Number of electrons" in a molecule also is presented in every WFX file; this number must also change in order to represent the number of electrons in the new electronic configuration.

Again the "number of alpha electrons" and "number of beta electrons" must change to conform the new electronic configuration and present the *new* number of electrons.

For example benzene contains 42 electrons; if one removes 6π electrons of the molecule the "number of electrons" must change to 36 (instead of 42). Similarly, "number of alpha electrons" as well as "number of beta electrons" must change to 18 and 18 respectively.

The last part that is necessary to be modified is "molecular orbital occupation numbers"; in this part the numbers of electrons in each MO is represented. For a single determinant restricted method (HF or DFT) occupation number of each MO is 2. One can remove electrons from each orbital by changing the occupation number of that orbital into 0 (instead of 2). For instance, in benzene MO 21, MO 20 and MO 17 are π-MOs; by changing the molecular orbital occupation numbers" for each of these orbitals to 0, one removes their contribution to any molecular property such as magnetizability. It is worth noting that removing core electrons BADLY affects the molecular graph and the position of zero-flux-surfaces so

one CANNOT remove core electrons and claim that the remaining part represents the valence properties.