

## Supplementary Information:

### Aromaticity of substituted fulvene derivatives: substituent-dependent ring currents

T. M. Krygowski, W. P. Oziminski, M. Palusiak, P. W. Fowler and A.D. McKenzie

Table 1. HOMA and *p*EDA values for substituted pentafulvene derivatives sorted according to diminishing values of HOMA. These data were used to construct the plot in Figure 4 of the paper.

Substituent	HOMA	<i>p</i> EDA(5F)
CH <sub>2</sub> <sup>-</sup>	0.7427	0.69501
NH <sup>-</sup>	0.7081	0.64108
O <sup>-</sup>	0.6717	0.59841
CC <sup>-</sup>	0.3696	0.33172
NMe <sub>2</sub>	0.26	0.3084
NH <sub>2</sub>	0.2521	0.27378
COO <sup>-</sup>	0.1019	0.23063
OCH <sub>3</sub>	0.0728	0.16465
OH	0.0391	0.15658
F	-0.1169	0.08371
Li	-0.1606	0.14143
CHCH <sub>2</sub>	-0.1617	0.04295
CH <sub>3</sub>	-0.1724	0.05946
Cl	-0.1874	0.02053
CCH	-0.1902	-0.02188
CMe <sub>3</sub>	-0.2111	0.0511
H	-0.2773	0
CONH <sub>2</sub>	-0.3145	-0.0025
SiMe <sub>3</sub>	-0.3203	-0.01181
2xCN	-0.3272	-0.10442
SiH <sub>3</sub>	-0.3504	-0.03628
COCH <sub>3</sub>	-0.3693	-0.07098
CHO	-0.3776	-0.09948
B(OH) <sub>2</sub>	-0.3885	-0.06803
NO	-0.4029	-0.16167
CF <sub>3</sub>	-0.4288	-0.08787
COOH	-0.4297	-0.11451
BH <sub>2</sub>	-0.4614	-0.15779
NO <sub>2</sub>	-0.4801	-0.14994
NH <sub>3</sub> <sup>+</sup>	-0.5104	-0.18649