Supplementary Material for New Journal of Chemistry

Supplementary data

One-electron oxidation-induced dimerizing C-C coupling of a 2,5-diamino-1,4-benzoquinonediimine: a chemical and electrochemical investigation†

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Extended Hückel calculations

Table S1: Atomic parameters used for the extended Hückel calculations[a]

Atom	s shell		p shell	
	H_{ii} (eV)	Exponent ζ	H_{ii} (eV)	Exponent ζ
H	-13.4	1.3		
C	-21.4	1.625	-11.4	1.625
N	-26.0	1.95	-13.4	1.95

[a] from a) R. Hoffmann, W. N. Lipscomb, *J. Chem. Phys.* **1962**, *36*, 2179; b) R. Hoffmann, W. N. Lipscomb, *J. Chem. Phys.* **1962**, *37*, 2872; (c) R. Hoffmann, *J. Chem. Phys.* **1963**, *39*, 1397.

Table S2: Mulliken orbital populations obtained [a] for **[3]** and **[3]**$^{+\bullet}$.

Atom/Orbitals	[3]	$[3]^{+\bullet}$
C(1)		
s	1.163	1.163
p_x	0.968	0.956
p_y	1.220	0.986
p_z	0.944	0.944
net charge	**-0.296**	**-0.049**
C(2)		
s	1.095	1.095
p_x	0.781	0.781
p_y	0.755	0.746
p_z	0.902	0.902
net charge	**0.467**	**0.477**
C(3)		
s	1.106	1.106
p_x	0.795	0.795
p_y	0.802	0.781
p_z	0.903	0.903
net charge	**0.394**	**0.415**
C(4)		
s	1.163	1.163
p_x	0.968	0.956
p_y	1.220	0.986
p_z	0.944	0.944
net charge	**-0.296**	**-0.049**
C(5)		
s	1.095	1.095
p_x	0.781	0.781
p_y	0.755	0.746
p_z	0.902	0.902
net charge	**0.467**	**0.477**
C(6)		
s	1.106	1.106
p_x	0.795	0.795
p_y	0.802	0.781
p_z	0.903	0.903
net charge	**0.394**	**0.415**
N(1)		
s	1.362	1.362
p_x	1.185	1.184
p_y	1.670	1.546
p_z	1.141	1.141
net charge	**-0.358**	**-0.232**
N(2)		
s	1.456	1.456
p_x	1.591	1.591
p_y	1.549	1.484

p_z	1.394	1.394
net charge	**-0.990**	**-0.925**
N(3)		
s	1.362	1.362
p_x	1.185	1.184
p_y	1.670	1.546
p_z	1.141	1.141
net charge	**-0.358**	**-0.232**
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p_x	1.591	1.591
p_y	1.549	1.484
p_z	1.394	1.394
net charge	**-0.990**	**-0.925**

[a] in electron, from extended Hückel (EHT) calculations. The z axis is colinear with C(1)-C(4) and xz corresponds approximately to the plane of the C_6 ring.

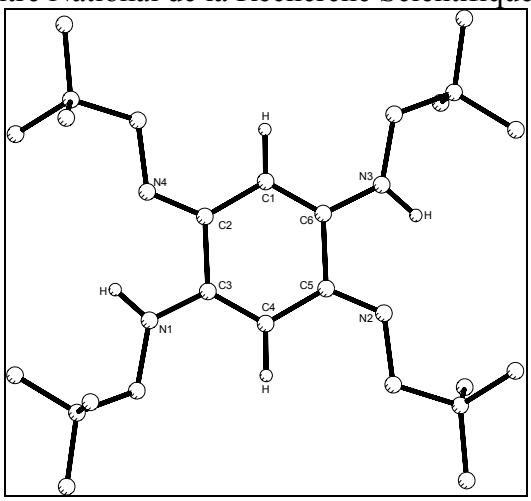

Figure S1: Atom numbering in compound **3**

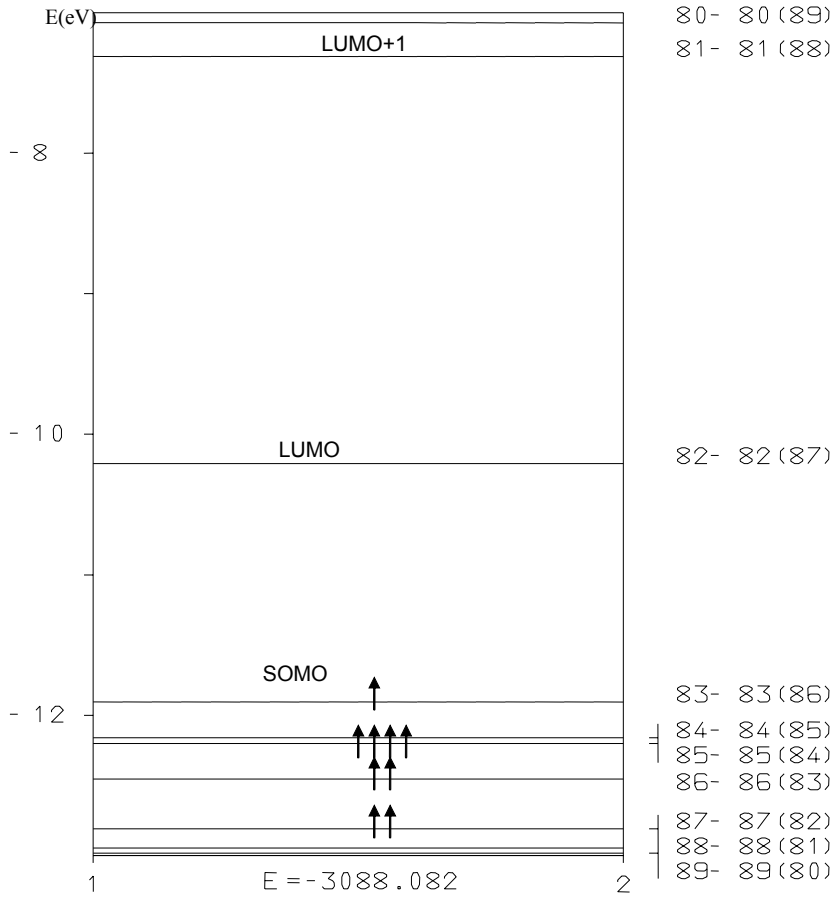

Figure S2: MO diagrams of the frontier orbitals for the **[3]**$^{+\cdot}$

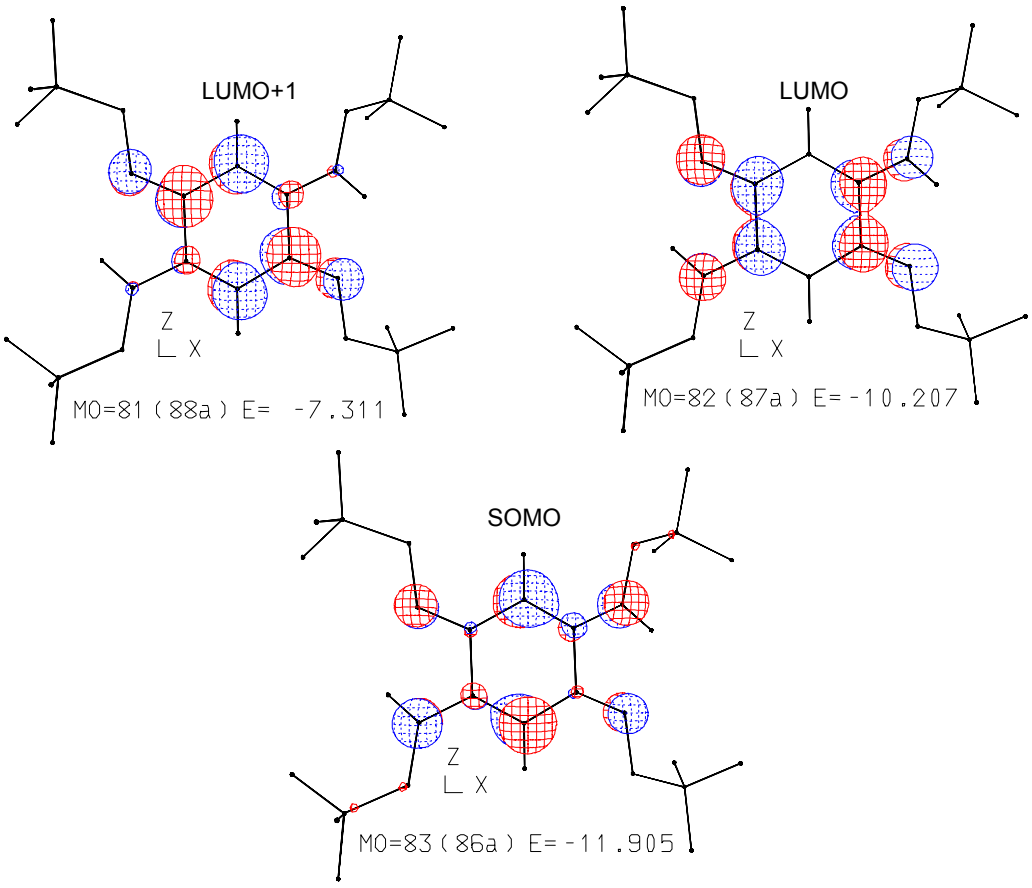

Figure S3: MO representation of the LUMO+x (x = 0-1) and SOMO for $[\mathbf{3}]^{+\cdot}$