

FALDI-Based Criterion for and the Origin of an Electron Density Bridge with an Associated (3,-1) Critical Point on Bader's Molecular Graph

*Jurgens H. de Lange, Daniël M.E. van Niekerk, Ignacy Cukrowski**

Correspondence to: Ignacy Cukrowski (E-mail: ignacy.cukrowski@up.ac.za)

Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Lynnwood Road, Hatfield, Pretoria 0002, South Africa

Supplementary Information

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SECTION 1

Cartesian coordinates of structures (1) – (6) and *cis*-2-butene

Table S1 Cartesian coordinates of structure (1), neutral ethylenediamine.

Atom	X	Y	Z
C	-0.722257	0.575759	-0.311737
H	-0.625778	0.582191	-1.405059
H	-1.250819	1.496903	-0.045971
C	0.683545	0.602724	0.305268
H	1.178606	1.550098	0.035444
H	0.594023	0.584065	1.396961
N	1.435501	-0.591547	-0.104167
H	1.704954	-0.532169	-1.081405
H	2.285144	-0.703899	0.436865
N	-1.553848	-0.567318	0.062894
H	-1.016456	-1.422031	-0.053634
H	-1.808968	-0.514002	1.044528

Table S2 Cartesian coordinates of structure (2), protonated ethylenediamine.

Atom	X	Y	Z
C	-0.687369	0.738379	-0.241313
H	-0.734592	0.826560	-1.327364
H	-1.258182	1.547712	0.210567
C	0.768915	0.666066	0.250148
H	1.321441	1.516193	-0.158570
H	0.796024	0.753680	1.339275
N	1.302221	-0.650041	-0.131055
H	1.714724	-0.645863	-1.059366
H	2.012957	-0.979045	0.513020
N	-1.316961	-0.593183	0.109861
H	-0.505224	-1.258375	-0.004957
H	-1.637996	-0.630857	1.079803
H	-2.095251	-0.854104	-0.497066

Table S3 Cartesian coordinates of structure (3).

Atom	X	Y	Z
C	0.873964	0.155040	0.000000
F	2.133346	-0.418688	0.000000
C	-0.134877	-0.894123	0.000002
C	-1.460747	-0.666427	0.000001
H	-2.147280	-1.510112	0.000002
O	0.768370	1.337072	-0.000001
H	0.207643	-1.918504	0.000003
O	-2.013029	0.555357	-0.000001
H	-2.973241	0.490440	-0.000001

Table S4 Cartesian coordinates of structure (4).

Atom	X	Y	Z
C	1.343190	0.276929	0.000000
H	2.244789	0.927767	0.000002
C	0.082075	1.023325	-0.000001
C	-1.158703	0.498645	-0.000001
H	-2.026005	1.156531	-0.000001
O	1.465604	-0.931300	0.000001
H	0.151958	2.105175	-0.000001
O	-1.416095	-0.819967	0.000000
H	-2.366184	-0.972733	0.000000

Table S5 Cartesian coordinates of structure (5), eclipsed C₂H₄Cl₂.

Atom	X	Y	Z
C	0.000000	0.776056	-1.049034
C	0.000000	-0.776056	-1.049034
H	0.884849	-1.140159	-1.567480
Cl	0.000000	-1.607091	0.554657
H	-0.884849	-1.140159	-1.567480
Cl	0.000000	1.607091	0.554657
H	-0.884849	1.140159	-1.567480
H	0.884849	1.140159	-1.567480

Table S6 Cartesian coordinates of structure (6), eclipsed C₂Cl₆.

Atom	X	Y	Z
C	-0.000015	-0.000012	0.849864
C	-0.000015	-0.000012	-0.849864
Cl	-0.834304	-1.445049	-1.509802
Cl	-0.834304	1.445055	-1.509793
Cl	1.668614	-0.000002	-1.509851
Cl	-0.834304	1.445055	1.509793
Cl	1.668614	-0.000002	1.509851
Cl	-0.834304	-1.445049	1.509802

Table S7 Cartesian coordinates of *cis*-2-butene.

Atom	X	Y	Z
H	0.000000	1.057480	-1.475520
C	0.000000	1.588653	-0.522652
C	0.000000	0.667913	0.664593
C	0.000000	-0.667913	0.664593
C	0.000000	-1.588653	-0.522652
H	0.000000	-1.057480	-1.475520
H	-0.878628	2.243318	-0.503946
H	0.878628	2.243318	-0.503946
H	-0.878628	-2.243318	-0.503946
H	0.878628	-2.243318	-0.503946
H	0.000000	-1.167102	1.631771
H	0.000000	1.167102	1.631771

End of SECTION 1

SECTION 2

Full lists of all computed FALDI components of structures (1) – (6)

Table S8 All contributions made to MDP(N7,H11) in structure (1), expressed as percentages.

Component	$\rho_{\text{Bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Bonding}}(\mathbf{r}^*)$	Component	$\rho_{\text{Non-bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Non-bonding}}(\mathbf{r}^*)$
N10,H11	20.7	1.0	C4,N7	8.8	15.2
N7,H9	7.3	1.8	C1,N10	7.1	27.9
N7,H8	5.5	0.3	C1,C4	1.9	13.7
N10,H12	4.9	4.6	H3,N10	1.0	0.9
N7,H11	4.8	0.5	H2,N10	0.9	1.5
C1,N7	3.9	0.7	C1,H3	0.7	4.2
H5,N7	3.3	2.4	C4,H6	0.7	1.0
N7,N10	2.7	1.6	C1,H2	0.6	2.4
C4,N10	2.3	1.4	C1,H5	0.6	0.9
H6,N7	2.3	0.5	C4,H5	0.5	2.7
H3,N7	1.4	0.9	C1,H12	0.5	0.8
H5,N10	1.0	0.6	H3,C4	0.5	1.1
H2,N7	0.9	0.2	C1,H6	0.3	0.9
C1,H11	0.9	1.1	H2,C4	0.3	0.6
H6,N10	0.9	1.1	H5,H6	0.2	0.3
C4,H9	0.8	0.8	H2,H3	0.1	0.4
H11,H12	0.8	0.2	H2,H5	0.1	0.1
N7,H12	0.8	0.0	H3,H6	0.1	0.1
C4,H11	0.8	0.5	H2,H6	0.1	0.2
C4,H8	0.6	0.5	C4 loc	0.0	0.0
H3,H11	0.6	0.9	C1 loc	0.0	0.0
H8,N10	0.5	0.3	H2 loc	0.0	0.0
H9,N10	0.5	0.2	H3 loc	0.0	0.0
H9,H11	0.5	0.1	H5 loc	0.0	0.0
H8,H9	0.5	0.0	H6 loc	0.0	0.0
H5,H11	0.4	0.1	H8 loc	0.0	0.0
C1,H8	0.4	0.1	H9 loc	0.0	0.0
H2,H12	0.3	0.4	H11 loc	0.0	0.0
H5,H9	0.3	0.1	H12 loc	0.0	0.0
C4,H12	0.3	0.5			
H8,H11	0.3	0.0			
H2,H11	0.3	0.1			
C1,H9	0.3	0.3			
H5,H8	0.3	0.0			
H6,H9	0.3	0.0			
H3,H12	0.3	0.2			
H6,H11	0.2	0.1			
H6,H8	0.2	0.2			
H6,H12	0.2	0.2			
H2,H8	0.2	0.1			
H3,H5	0.2	0.1			
H3,H9	0.2	0.1			
H8,H12	0.2	0.1			
H9,H12	0.1	0.1			
H3,H8	0.1	0.1			
H5,H12	0.1	0.1			
H2,H9	0.1	0.1			
N10 loc	0.0	0.0			
N7 loc	0.0	0.0			

Table S9 All contributions made to (3,-1) CP(N7,H11) in structure (2), expressed as percentages.

Component	$\rho_{\text{Bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Bonding}}(\mathbf{r}^*)$	Component	$\rho_{\text{Non-bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Non-bonding}}(\mathbf{r}^*)$
N10,H11	16.5	13.5	C1,C4	1.1	0.2
N7,H11	14.1	10.5	C4,H5	0.4	0.8
C4,N7	8.3	8.1	C4 loc	0.0	0.0
N7,H9	6.8	3.8	N10 loc	0.0	0.0
N7,H8	6.4	5.5	C1 loc	0.0	0.0
C1,N7	4.6	5.3	N7 loc	0.0	0.0
N7,N10	3.6	3.7	H2 loc	0.0	0.0
C1,N10	3.0	10.1	H3 loc	0.0	0.0
H5,N7	2.8	5.9	H5 loc	0.0	0.0
N10,H13	2.5	6.2	H6 loc	0.0	0.0
N10,H12	2.2	3.6	H8 loc	0.0	0.0
H6,N7	1.6	1.1	H9 loc	0.0	0.0
C4,N10	1.5	0.7	H11 loc	0.0	0.0
H3,N7	1.4	1.4	H12 loc	0.0	0.0
C1,H11	1.3	2.1	H13 loc	0.0	0.0
C4,H11	1.1	1.6			
N7,H13	1.0	1.2			
N7,H12	1.0	1.0			
H11,H13	0.8	0.1			
H2,N7	0.8	0.6			
H9,H11	0.7	0.3			
H11,H12	0.7	0.1			
C4,H9	0.7	0.2			
H3,H11	0.7	0.9			
H5,H11	0.7	1.0			
H8,H11	0.7	0.4			
H5,N10	0.7	0.5			
H3,N10	0.6	0.1			
C4,H8	0.6	0.1			
H9,N10	0.5	0.4			
H2,N10	0.5	0.8			
H8,N10	0.5	0.3			
C1,H5	0.4	0.3			
C1,H3	0.4	1.1			
H3,C4	0.4	0.3			
H6,N10	0.4	0.3			
C4,H6	0.4	0.2			
C1,H8	0.4	0.3			
H8,H9	0.4	0.4			
C1,H2	0.4	0.1			
C1,H9	0.4	0.3			
H5,H9	0.3	0.4			
C4,H13	0.3	0.1			
H6,H8	0.3	0.1			
H6,H9	0.3	0.3			
C1,H12	0.3	0.4			
C1,H13	0.3	0.6			
H2,H11	0.3	0.1			
H2,C4	0.3	0.1			
H5,H8	0.2	0.3			
C1,H6	0.2	0.1			
C4,H12	0.2	0.0			
H6,H11	0.2	0.1			
H3,H9	0.2	0.2			

H2,H8	0.2	0.2
H8,H12	0.2	0.1
H9,H13	0.2	0.1
H2,H12	0.1	0.3
H5,H6	0.1	0.1
H3,H12	0.1	0.1
H2,H13	0.1	0.2
H5,H13	0.1	0.1
H3,H8	0.1	0.1
H3,H5	0.1	0.1
H2,H5	0.1	0.1
H8,H13	0.1	0.0
H12,H13	0.1	0.1
H6,H12	0.1	0.1
H9,H12	0.1	0.0
H2,H3	0.1	0.0
H3,H6	0.1	0.0
H2,H9	0.1	0.0
H6,H13	0.1	0.1
H5,H12	0.1	0.0
H3,H13	0.1	0.1
H2,H6	0.1	0.0

Table S10 All contributions made to MDP (O6,O8) in structure (**3**), expressed as percentages.

Component	$\rho_{\text{Bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Bonding}}(\mathbf{r}^*)$	Component	$\rho_{\text{Non-bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Non-bonding}}(\mathbf{r}^*)$
C1,O6	15.2	9.8	C1,C3	2.5	14.7
O8,H9	10.9	1.1	C3,C4	2.4	12.9
C4,O8	10.4	5.8	F2,C3	1.4	0.2
F2,O6	8.7	6.5	C3,H7	1.0	4.6
O6,O8	7.1	4.1	C1,H7	0.9	1.4
C3,O6	5.5	4.1	C4,H7	0.8	1.4
C3,O8	4.9	3.4	C4,H5	0.7	2.9
H5,O8	3.5	3.9	C3,H5	0.6	0.4
C4,O6	2.7	2.4	F2 loc	0.0	0.1
C1,O8	2.5	1.0	C1 loc	0.0	0.0
O6,H7	2.4	2.2	C4 loc	0.0	0.0
C1,F2	2.4	1.7	C3 loc	0.0	0.0
O6 loc	2.3	9.4	H5 loc	0.0	0.0
F2,O8	2.1	1.2	H7 loc	0.0	0.0
H7,O8	1.5	0.8	H9 loc	0.0	0.0
C1,C4	1.1	1.1			
O6,H9	1.0	0.5			
C4,H9	1.0	0.4			
F2,C4	0.7	0.1			
H5,O6	0.7	0.4			
C3,H9	0.5	0.6			
H5,H9	0.4	0.3			
F2,H7	0.4	0.1			
C1,H9	0.4	0.2			
F2,H5	0.4	0.1			
F2,H9	0.4	0.1			
C1,H5	0.3	0.0			
H7,H9	0.3	0.1			
H5,H7	0.2	0.1			
O8 loc	0.0	0.0			

Table S11 All contributions made to (3,-1) CP(O6,O8) in structure (4), expressed as percentages.

Component	$\rho_{\text{Bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Bonding}}(\mathbf{r}^*)$	Component	$\rho_{\text{Non-bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Non-bonding}}(\mathbf{r}^*)$
C1,O6	13.4	8.8	C1,C3	2.4	12.8
O8,H9	11.3	2.8	C3,C4	2.4	12.0
C4,O8	11.0	3.5	C3,H7	0.9	4.5
C3,O6	7.7	7.0	C4,H7	0.8	1.3
O6,O8	7.7	5.2	C4,H5	0.8	2.9
H2,O6	7.0	6.4	C1,H7	0.7	1.0
C3,O8	4.9	4.2	C3,H5	0.7	0.1
H5,O8	3.8	4.8	C1,H2	0.7	1.4
O6,H7	3.0	2.5	C1 loc	0.0	0.0
C4,O6	3.0	2.2	C4 loc	0.0	0.0
C1,O8	2.3	1.3	C3 loc	0.0	0.0
O6 loc	2.3	8.5	H2 loc	0.0	0.0
H7,O8	1.7	1.2	H5 loc	0.0	0.0
H2,O8	1.5	1.0	H7 loc	0.0	0.0
H5,O6	1.5	0.6	H9 loc	0.0	0.0
O6,H9	1.3	0.7			
H2,C3	1.2	0.4			
C1,C4	1.1	0.6			
C4,H9	1.0	0.3			
H2,C4	0.6	0.0			
C3,H9	0.5	0.7			
H5,H9	0.5	0.4			
C1,H5	0.4	0.2			
C1,H9	0.4	0.2			
H2,H5	0.4	0.0			
H2,H7	0.3	0.0			
H7,H9	0.3	0.2			
H5,H7	0.3	0.0			
H2,H9	0.3	0.1			
O8 loc	0.0	0.0			

Table S12 All contributions made to MDP(Cl4,Cl6) in structure (5), expressed as percentages.

Component	$\rho_{\text{Bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Bonding}}(\mathbf{r}^*)$	Component	$\rho_{\text{Non-bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{Non-bonding}}(\mathbf{r}^*)$
C14,Cl6	14.9	10.9	C2,Cl4	14.4	15.1
C1,Cl4	6.9	6.9	C1,Cl6	14.4	15.0
C2,Cl6	6.9	6.9	C1,C2	4.3	17.6
C14,H5	3.6	1.7	C2,H5	1.6	2.1
H3,Cl4	3.6	1.7	C2,H3	1.6	2.1
Cl6,H8	3.6	1.7	C1,H8	1.6	2.1
Cl6,H7	3.6	1.7	C1,H7	1.6	2.1
C14,H8	2.1	1.5	C2,H8	1.2	0.5
C14,H7	2.1	1.5	C1,H5	1.2	0.5
H5,Cl6	2.1	1.5	C2,H7	1.2	0.5
H3,Cl6	2.1	1.5	C1,H3	1.2	0.5
Cl4 loc	1.0	1.9	H3,H5	0.3	0.0
Cl6 loc	1.0	1.9	H7,H8	0.3	0.0
			H3,H7	0.3	0.1
			H5,H8	0.3	0.1
			H5,H7	0.2	0.1

H3,H8	0.2	0.1
C2 loc	0.0	0.0
C1 loc	0.0	0.0
H3 loc	0.0	0.0
H5 loc	0.0	0.0
H7 loc	0.0	0.0
H8 loc	0.0	0.0

Table S13 All contributions made to (3,-1) CP(C14,C16) in structure (6), expressed as percentages.

Component	$\rho_{\text{Bonding}}(\mathbf{r}^*)$	$\hat{\partial}\rho_{\text{Bonding}}(\mathbf{r}^*)$	Component	$\rho_{\text{Non-bonding}}(\mathbf{r}^*)$	$\hat{\partial}\rho_{\text{Non-bonding}}(\mathbf{r}^*)$
C14,C16	12.3	7.4	C1,C2	2.3	6.6
C1,C16	11.6	17.9	C1,C18	1.7	1.7
C2,C14	10.9	18.4	C2,C15	1.6	1.8
C14,C15	5.6	3.7	C1,C17	1.5	1.4
C13,C14	5.6	3.7	C2,C13	1.5	1.5
C16,C18	5.5	3.6	C15 loc	0.0	0.0
C16,C17	5.5	3.6	C13 loc	0.0	0.0
C1,C14	5.4	6.6	C17 loc	0.0	0.0
C2,C16	5.3	6.5	C18 loc	0.0	0.0
C14,C18	3.1	2.5	C2 loc	0.0	0.0
C14,C17	3.1	2.6	C1 loc	0.0	0.0
C15,C16	3.1	2.5			
C13,C16	3.1	2.5			
C2,C18	1.3	0.2			
C2,C17	1.3	0.2			
C1,C13	1.3	0.2			
C1,C15	1.3	0.2			
C13,C15	1.0	0.2			
C17,C18	1.0	0.2			
C13,C18	0.8	0.3			
C15,C17	0.8	0.3			
C14 loc	0.7	1.8			
C16 loc	0.7	1.7			
C15,C18	0.6	0.1			
C13,C17	0.6	0.2			

End of SECTION 2

SECTION 3

Discussion of structure 4 geometry optimised with basis set aug-cc-pvqz

As mentioned in the main text, geometry optimised organic structure (4) has a DB linking atoms O6 and O8 when using the 6-311++g** basis set, but does not have one when using aug-cc-pvqz, Figure S1. With the latter basis set, the Tognetti and Joubert^{1,2} (TJ) defined β -value obtained is 1.43 (DB absent) which is larger in magnitude than was obtained with the former basis set, 1.41 (DB present), and places even more doubt in the reliability of their interpretation with regards to what factors may govern the presence of a DB.

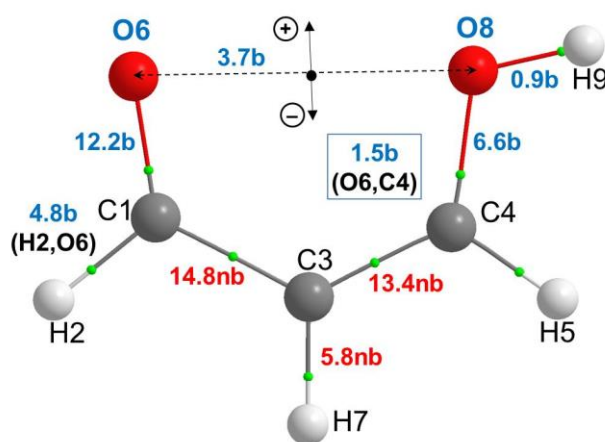


Figure S1. Molecular graph of equilibrium organic structure (4) in the gas phase using the aug-cc-pvqz basis set, including the λ_2 -eigenvector. Blue and red colourings indicate selected individual atom-pairs that facilitate and hinder, respectively, formation of a DB linking atoms O6 and O8 as well as their percentage-slope contributions.

Figure S2 shows the trends of the total *bonding*- and total *nonbonding*-ED, and gradients thereof, along the λ_2 -eigenvector passing through the MDP of the structure in Figure S1. After putting the $CP(\mathbf{r})$ function to the test, we note that it is successful in explaining the absence of a DB(O6,O8). Along the entire vector passing through the MDP only negative values for the $CP(\mathbf{r})$ function are obtained, thus explaining that no DB is present. Importantly, the performance of the $CP(\mathbf{r})$ function does not rely on the basis set used to compute this organic structure, unlike the TJ^{1,2} indicator. We expect that the $CP(\mathbf{r})$ function will explain DB presence/absence regardless of one's choice of level of theory at which to compute a structure.

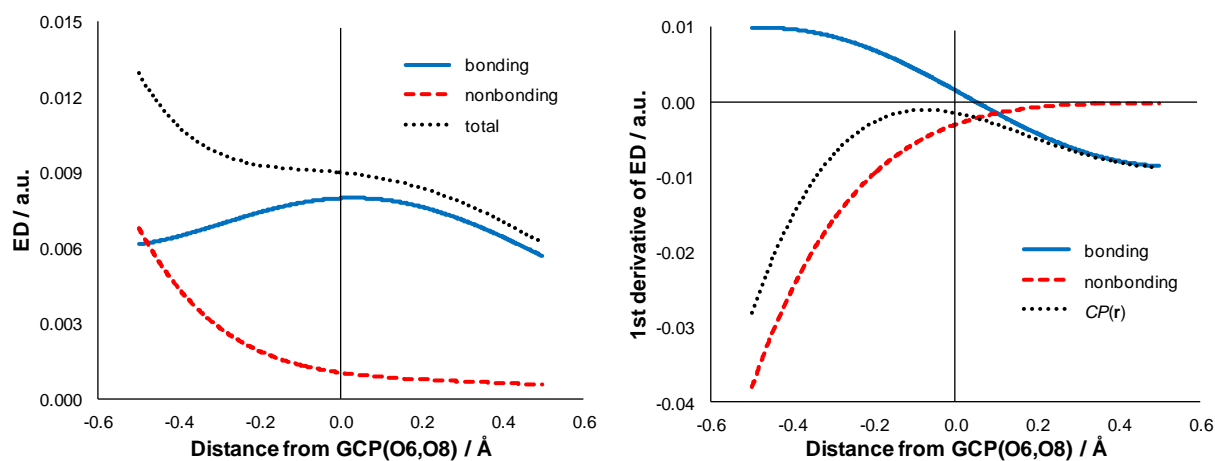


Figure S2. Comparison of the total *bonding* and total *nonbonding*-ED (left), and their 1st derivative curves (right), along the λ_2 -eigenvector passing through MDP(O6,O8) of structure (**4**) computed using the aug-cc-pvqz basis set.

References

1. O. A. Syzgantseva, V. Tognetti, L. Joubert, *J. Phys. Chem. A* **2013**, *117*, 8969–8980.
2. V. Tognetti, L. Joubert, *J. Chem. Phys.* **2013**, *138*, 024102–024111.

End of SECTION 3

SECTION 4

Analysis of (3,-1) CP between C atoms in hexachloroethane

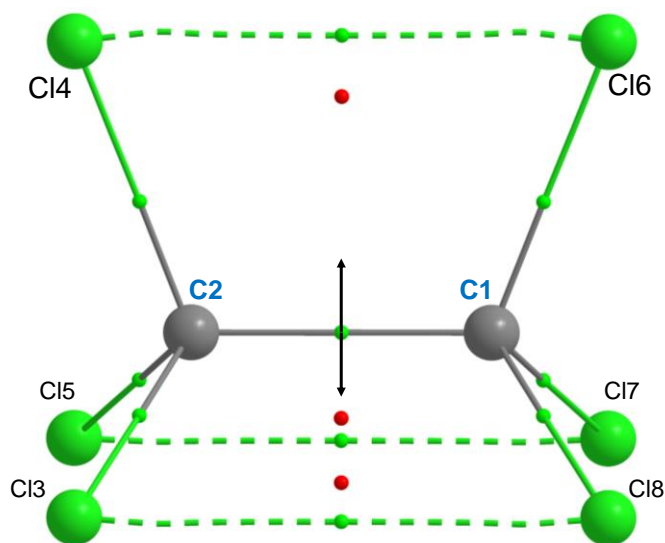


Figure S3. Molecular graph of hexachloroethane (**6**) also showing the direction of λ_2 -eigenvector crossing the (3,-1) CP on density bridge (green small sphere) between nuclei C1 and C2.

Figure S3 shows the molecular graph of hexachloroethane (**6**) as well as the direction of the λ_2 -eigenvector passing through the (3,-1) CP(C1,C2). The *tot*-ED, *bonding*- and *nonbonding*-ED contributions as well as their 1st directional derivative along the λ_2 -eigenvector are shown in Figure S4, illustrating the application of our method to a classic covalent C-C bond.

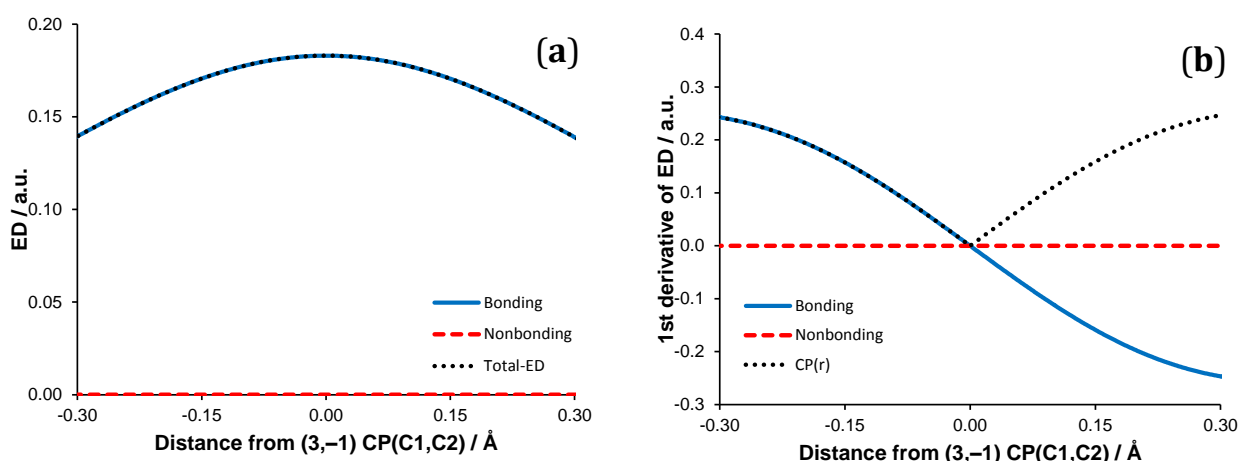


Figure S4. (a) Comparison of total *bonding*- and *nonbonding*-ED along the λ_2 -eigenvector passing through (3,-1) CP(C1,C2) of hexachloroethane (**6**). (b) Comparison of the directional first derivatives along the λ_2 -eigenvector for *bonding*- and *nonbonding*-ED, as well as the $CP(r)$ function.

Interestingly, no FALDI component is of a nonbonding nature relative to the (3,-1) CP(C1,C2), and the *tot*-ED is equal to the *bonding*-ED distribution. As a result, the $CP(\mathbf{r})$ function (shown in Figure S4(b)) is positive throughout, confirming that our approach works equally well for strong, covalent interactions as it does for the weaker non-covalent interactions shown in the main body.

The largest contributor to the total ED arises from the ED delocalized between the atoms of the primary contribution – atom-pair C1,C2 contributes 47.6% to the total ED at the (3,-1) CP(C1,C2), as shown in Table S14. This observation is expected for a classical covalent interaction, and is quite unlike what we observed for the weaker non-covalent interactions.

Table S14. Selected contributions made to the (3,-1) CP(C1,C2) in structure (6). Percentages refer to contributions towards the *tot*-ED and its slope.

Component	$\rho_{\text{bonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{bonding}}(\mathbf{r}^*)^a$	$\rho_{\text{nonbonding}}(\mathbf{r}^*)$	$\partial\rho_{\text{nonbonding}}(\mathbf{r}^*)^a$
C1,C2	0.08714 (47.6%)	0.00000 (0.0%)	-	-
C1,C14	0.00601 (3.3%)	0.00490 (19.6%)	-	-
C1,C16	0.00777 (4.2%)	0.00022 (0.90%)	-	-
C1, C15	0.00601 (3.3%)	-0.00314 (12.8%)		
C14, C16	0.00088 (0.5%)	0.00025 (1.02%)	-	-
Total	0.18300	0.00000	0.00000	0.00000

However, we note with interest that ~52 % of the ED at the CP is contributed by other atom-pairs in the molecule, suggesting that the ED concentrated within the C1,C2 internuclear region is considerably multi-centric in nature. The various C,C1 interactions contribute between ~3 and ~4 % each to a combined sum of 44.4 % of the ED at the CP. The various C1,C1 atom-pairs contribute the remainder of the ED, to a combined sum of 8.0%. All of these factors facilitate the presence of the DB(C1,C2) by concentrating ED along the λ_2 -eigenvector. Finally, the analysis of the contributions to the slope of the ED shows that, at the (3,-1) CP the directional derivative is zero as a result of various *bonding*-ED components with opposite slope. The distribution of the *deloc*-ED for atom-pair C1,C2 is itself a local maximum at exactly the (3,-1) CP, hence it's contribution to the total derivative is zero. The relative contributions to the slope can also be measured at ~0.1 Å away from the CP in order to provide a quantitative description of the rates of changes of the components relative to atom-pair C1,C2's contribution.

End of SECTION 4