Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Density Functional Theory and Bader's Atoms-in-molecules Theory: Towards a vivid dialogue

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TABLE S1. Interatomic interaction energies (in kcal/mol) for the **X*j*** and **XMe*j*** compounds.

	E_{OX}^{IQA}	$E_{OC_2}^{IQA}$	$E_{XC_1}^{IQA}$	E_{OX}^{elec}	$E_{OC_2}^{elec}$	$E_{XC_1}^{elec}$	E_{OX}^{x}	$E_{OC_2}^{x}$	$E_{XC_1}^{x}$
F5	69.1	-71.6	-74.0	74.1	-67.2	-72.7	-5.0	-4.4	-1.2
F6	71.1	-72.7	-73.4	76.4	-68.8	-72.3	-5.3	-3.9	-1.1
F7	71.7	-69.4	-74.7	77.6	-65.6	-73.6	-5.9	-3.7	-1.1
F8	71.9	-76.8	-103.6	76.5	-73.2	-102.3	-4.6	-3.5	-1.4
F9	74.2	-75.9	-102.7	79.0	-72.8	-101.5	-4.8	-3.1	-1.2
F10	74.4	-75.3	-96.6	79.4	-72.5	-95.7	-5.0	-2.8	-1.0
F11	70.2	-75.9	-81.9	75.2	-72.3	-80.4	-5.0	-3.7	-1.4
F12	75.4	-71.7	-103.9	80.8	-68.8	-102.6	-5.4	-2.9	-1.3
F13	75.3	-71.2	-97.7	80.9	-68.6	-96.7	-5.6	-2.6	-1.0
F14	71.4	-71.6	-83.2	76.9	-68.1	-81.7	-5.5	-3.5	-1.5
FMe5	64.5	-65.8	-64.6	65.3	-63.1	-64.0	-0.8	-2.7	-0.6
FMe6	67.2	-68.8	-65.1	68.3	-65.3	-64.4	-1.1	-3.5	-0.6
FMe7	67.4	-66.2	-66.3	68.6	-62.7	-65.5	-1.2	-3.5	-0.8
FMe8	67.7	-70.0	-94.6	68.8	-67.4	-93.9	-1.1	-2.6	-0.7
FMe9	74.2	-75.9	-102.7	70.6	-68.0	-93.6	-1.1	3.0	-0.7
FMe10	74.4	-75.3	-96.6	68.4	-64.8	-89.5	-0.7	-2.8	-1.0
FMe11	70.2	-75.9	-81.9	68.4	-67.2	-73.0	-1.3	-3.0	-0.8
FMe12	75.4	-71.7	-103.9	71.6	-65.5	-95.5	-1.3	-3.0	-0.9
FMe13	75.3	-71.4	-97.2	69.7	-62.3	-91.9	-0.9	-2.7	-1.3
FMe14	71.4	-71.6	-83.2	70.1	-65.2	-75.2	-1.7	-3.0	-1.1
Cl5	3.4	-14.6	-11.3	11.2	-9.9	-9.9	-7.8	-4.7	-1.4
Cl6	3.5	-14.3	-11.7	11.8	-10.1	-10.4	-8.3	-4.3	-1.2
Cl7	5.1	-12.7	-14.3	14.4	-8.7	-13.0	-9.3	-4.0	-1.3
Cl8	3.1	-16.6	-14.3	10.3	-12.8	-12.8	-7.2	-3.8	-1.5
Cl9	4.7	-15.3	-15.8	15.3	-15.3	-15.8	-7.6	-3.4	-1.3
Cl10	4.8	-14.8	-15.0	12.7	-14.8	-15.0	-7.9	-3.1	-1.1
Cl11	2.1	-16.5	-11.3	9.6	-16.5	-11.3	-7.5	-3.9	-1.6
Cl12	6.6	-13.5	-19.6	15.1	-13.5	-19.6	-8.5	-3.2	-1.3
Cl13	6.6	-12.9	-18.4	15.4	-12.9	-18.4	-8.8	-2.9	-1.1
Cl14	4.3	-14.7	-14.6	12.7	-14.7	-14.6	-8.4	-3.7	-1.6
ClMe5	18.7	-17.1	-20.4	20.1	-14.1	-19.6	-1.4	-3.0	-0.7
ClMe6	19.4	-18.6	-21.4	21.1	-14.7	-20.5	-1.6	-2.8	-0.8
ClMe7	21.7	-18.4	-23.5	23.3	-14.6	-22.5	-1.6	-3.8	-1.0
ClMe8	18.8	-18.6	-29.5	20.5	-15.6	-28.6	-1.7	-3.0	-0.9
ClMe9	20.3	-19.0	-30.8	21.9	-15.6	-30.0	-1.6	-3.3	-0.8
ClMe10	21.3	-17.8	-31.3	22.3	-14.7	-30.1	-1.0	-3.1	-1.2
ClMe11	18.0	-19.2	-22.6	19.8	-15.8	-21.6	-1.8	-3.4	-0.9
ClMe12	22.5	-19.1	-34.3	24.2	-15.8	-33.3	-1.7	-3.3	-1.0
ClMe13	24.3	-17.3	-37.2	25.5	-16.0	-35.3	-1.1	-1.2	-2.0
ClMe14	20.2	-19.3	-25.4	22.1	-15.9	-24.2	-2.0	-3.4	-1.1
Br5	-17.2	4.1	7.6	-8.6	8.9	9.1	-8.6	-4.8	-1.5
Br6	-17.6	4.7	7.0	-8.5	9.2	8.2	-9.1	-4.5	-1.3
Br7	-15.3	5.1	3.5	-5.1	9.2	4.8	-10.2	-4.2	-1.3
Br8	-19.3	2.9	12.8	-11.5	6.8	14.3	-7.9	-3.9	-1.5
Br9	-17.2	4.5	10.6	-9.1	8.1	11.9	-8.1	-3.6	-1.3
Br10	-17.2	5.0	9.8	-8.5	8.3	10.9	-8.7	-3.3	-1.1
Br11	-19.3	3.1	10.2	-11.2	7.2	11.8	-8.1	-4.1	-1.6
Br12	-14.7	4.8	5.4	-5.4	8.1	6.7	-9.3	-3.3	-1.3
Br13	-14.7	5.3	5.1	-4.9	8.3	6.3	-9.8	-3.0	-1.1
Br14	-16.3	3.3	5.7	-7.3	7.1	7.3	-9.0	-3.8	-1.6
BrMe5	5.8	-4.9	-8.5	7.1	-1.3	-7.7	-1.3	-3.1	-0.7
BrMe6	6.9	-5.3	-9.6	8.6	-1.3	-8.8	-1.6	-4.0	-0.8
BrMe7	9.5	-6.6	-12.9	11.3	-2.7	-11.8	-1.7	-3.9	-1.0
BrMe8	5.4	-5.1	-11.9	7.1	-3.0	-11.1	-1.6	-3.0	-0.9
BrMe9	7.1	-5.3	-13.9	8.7	-5.3	-13.0	-1.6	-3.4	-0.9
BrMe10	8.5	-4.8	-15.6	9.6	-4.8	-14.4	-1.0	-3.2	-1.2
BrMe11	4.9	-5.7	-8.9	6.7	-5.7	-7.9	-1.8	-3.5	-1.0
BrMe12	10.0	-6.7	-18.6	11.7	-6.7	-17.5	-1.8	-3.3	-1.0
BrMe13	11.3	-6.2	-20.6	12.6	-6.2	-19.0	-1.3	-3.1	-1.6
BrMe14	7.7	-7.0	-12.7	9.7	-7.0	-11.5	-2.0	-3.4	-1.2

TABLE S2. Interatomic interaction energies (in kcal/mol) for the **O*i*** and **S*i*** compounds.

	E_{OY}^{IQA}	$E_{OC_2}^{IQA}$	$E_{YC_1}^{IQA}$	E_{OY}^{elec}	$E_{OC_2}^{elec}$	$E_{YC_1}^{elec}$	E_{OY}^{x}	$E_{OC_2}^{x}$	$E_{YC_1}^{x}$
O1	119.7	-73.4	-119.6	125.5	-69.1	-118.0	-5.9	-4.3	-1.6
O8	125.0	-78.3	-168.9	130.4	-74.9	-167.1	-5.4	-3.4	-1.7
O9	127.8	-130.6	-174.1	133.0	-127.2	-172.6	-5.2	-3.4	-1.5
O10	121.3	-77.3	-127.2	127.1	-73.7	-127.2	-5.8	-3.6	-1.9
O11	122.9	-72.3	-130.1	129.2	-68.7	-128.3	-6.3	-3.6	-1.8
O12	123.7	-84.9	-137.3	129.9	-81.3	-135.6	-6.2	-3.5	-1.7
O13	122.8	-74.0	-118.9	129.8	-70.4	-117.4	-7.0	-3.6	-1.4
O14	124.3	-73.1	-120.2	131.2	-69.4	-118.8	-6.9	-3.6	-1.4
O15	129.8	-75.7	-168.3	136.0	-72.8	-166.8	-6.2	-2.9	-1.5
O16	126.2	-74.0	-146.6	133.1	-70.1	-145.0	-6.9	-3.9	-1.6
O17	124.1	-75.9	-136.0	130.5	-72.5	-134.1	-6.4	-3.4	-1.9
O18	124.1	-104.7	-120.1	131.1	-101.1	-118.7	-7.0	-3.7	-1.4
S1	-50.9	11.9	30.7	-36.2	17.8	32.9	-14.7	-5.8	-2.2
S8	-46.3	11.7	42.5	-35.4	16.3	44.5	-11.0	-4.6	-2.0
S9	-51.8	-37.4	50.0	-40.9	-32.8	51.6	-10.9	-4.6	-1.6
S10	-46.5	11.6	31.0	-35.1	16.4	33.2	-11.3	-4.8	-2.2
S11	-52.5	20.6	34.8	-40.0	35.2	36.9	-12.5	-4.6	-2.0
S12	-52.6	7.7	37.8	-39.9	12.4	39.8	-12.7	-4.6	-1.9
S13	-56.0	11.4	27.8	-37.7	16.7	29.8	-18.3	-5.3	-2.0
S14	-51.7	11.4	27.8	-51.7	16.6	29.8	-17.3	-5.2	-1.9
S15	-46.2	11.6	37.3	-46.2	15.6	39.1	-13.7	-4.1	-1.7
S16	-49.6	11.8	36.7	-49.6	15.7	38.2	-15.6	-4.0	-1.5
S17	-45.5	10.3	30.0	-45.5	14.8	32.1	-13.0	-4.5	-2.1
S18	-59.1	-30.7	32.5	-59.1	-25.7	34.2	-18.7	-5.0	-1.7

TABLE S3. Interatomic interaction energies (in kcal/mol) for the **Oph** and **Sph** compounds.

	E_{OY}^{IQA}	$E_{OC_2}^{IQA}$	$E_{YC_1}^{IQA}$	E_{OY}^{elec}	$E_{OC_2}^{elec}$	$E_{YC_1}^{elec}$	E_{OY}^{x}	$E_{OC_2}^{x}$	$E_{YC_1}^{x}$
Oph1	130.6	-78.4	-172.6	138.5	-76.8	-171.4	-7.9	-1.6	-1.2
Oph2	129.8	25.3	-173.8	137.6	27.0	-172.6	-7.9	-1.6	-1.2
Oph3	130.9	-85.4	-177.3	138.8	-83.8	-176.1	-8.0	-1.6	-1.2
Oph4	119.8	-73.2	-192.9	121.1	-72.1	-190.1	-1.3	-1.2	-2.8
Oph5	130.5	-77.8	-172.2	138.4	-76.2	-171.0	-7.9	-1.6	-1.2
Oph6	131.6	-76.9	-173.7	139.8	-75.2	-172.5	-8.1	-1.6	-1.2
Oph7	113.8	-60.5	-184.4	114.4	-59.3	-181.9	-0.5	-1.2	-2.4
Sph1	-48.0	11.4	37.1	-47.9	14.3	38.4	-15.4	-2.9	-1.3
Sph2	-49.4	10.8	38.9	-34.0	13.7	40.2	-15.4	-2.9	-1.3
Sph3	-50.1	9.7	39.4	-34.2	12.4	40.8	-15.9	-2.7	-1.4
Sph4	-24.7	6.2	24.8	-20.4	7.8	28.1	-4.3	-1.5	-3.2
Sph5	-47.0	11.4	36.1	-31.9	14.3	37.4	-15.1	-2.9	-1.3
Sph6	-47.0	11.6	34.3	-30.8	14.3	35.7	-16.3	-2.7	-1.4
Sph7	-15.4	9.4	11.1	-11.8	10.9	15.1	-3.6	-1.5	-4.0

TABLE S4. Interatomic interaction energies (in kcal/mol) for the **Xph** compounds.

	E_{OX}^{IQA}	$E_{OC_2}^{IQA}$	$E_{XC_1}^{IQA}$	E_{OX}^{elec}	$E_{OC_2}^{elec}$	$E_{XC_1}^{elec}$	E_{OX}^{x}	$E_{OC_2}^{x}$	$E_{XC_1}^{x}$
Fph1a	71.1	-68.1	-100.1	78.2	-66.9	-99.4	-7.2	-1.1	-0.6
Fph1b	76.5	-75.2	-104.4	82.9	-73.6	-103.4	-6.4	-1.7	-0.9
Fph1c	71.4	-66.1	-101.1	79.0	-65.1	-100.4	-7.6	-1.1	-0.7
Fph1d	77.2	-73.4	-105.5	84.0	-71.8	-104.5	-6.7	-1.6	-1.0
Fph1e	70.5	-73.1	-100.5	77.9	-71.9	-99.8	-7.4	-1.2	-0.7
Fph1f	75.9	-80.5	-104.8	82.4	-78.8	-103.8	-6.6	-1.7	-1.0
Clph1a	6.2	-11.4	-20.4	16.4	-10.2	-19.7	-10.2	-1.3	-0.7
Clph1b	5.3	-13.8	-20.2	15.3	-11.9	-19.2	-10.0	-1.9	-1.0
Clph1c	7.2	-10.7	-23.1	17.6	-9.5	-22.2	-10.4	-1.2	-0.9
Clph1d	5.9	-12.9	-22.4	16.4	-11.2	-21.2	-10.5	-1.8	-1.2
Clph1e	2.2	-14.3	-16.9	12.7	-13.0	-16.1	-10.5	-1.2	-0.8
Clph1f	0.8	-16.6	-16.0	11.3	-14.8	-14.8	-10.5	-1.8	-1.1
Brph1a	-13.7	6.0	3.1	-2.9	7.5	3.8	-10.8	-1.5	-0.6
Brph1b	-16.8	5.2	5.3	-6.1	7.4	6.2	-10.7	-2.2	-1.0
Brph1c	-10.9	6.0	-0.9	-0.7	7.4	0.2	-10.2	-1.4	-1.1
Brph1d	-15.3	5.4	2.2	-4.3	7.4	3.5	-11.0	-2.0	-1.3
Brph1e	-17.2	4.0	7.2	-6.7	5.4	8.2	-10.5	-1.4	-0.9
Brph1f	-21.7	3.2	10.4	-10.6	5.2	11.5	-11.0	-2.0	-1.2

TABLE S5. Interatomic interaction energies (in kcal/mol) for the compounds with an intramolecular hydrogen bond.

	E_{OH}^{IQA}	E_{OY}^{IQA}	$E_{HC_1}^{IQA}$	E_{OH}^{elec}	E_{OY}^{elec}	$E_{HC_1}^{elec}$	E_{OH}^{x}	E_{OY}^{x}	$E_{HC_1}^{x}$
Oh1	-144.0	147.6	93.0	-125.6	159.8	93.3	-18.4	-12.2	-0.4
Oh2	-147.4	150.9	91.5	-128.4	163.3	91.9	-19.1	-12.3	-0.3
Oh3	-132.0	149.6	126.1	-119.4	158.8	126.4	-12.6	-9.3	-0.3
Oh4	-129.5	146.0	97.9	-116.9	155.5	98.2	-12.7	-9.4	-0.3
Oh5	-127.2	144.8	91.3	-115.0	154.0	91.6	-12.1	-9.2	-0.3
Oh6	-140.8	154.9	126.0	-125.8	165.1	126.3	-15.0	-10.2	-0.3
Oh7	-148.9	156.7	121.6	-130.8	168.0	121.9	-18.1	-11.3	-0.3
Oh8	-152.0	151.5	90.6	-131.6	164.6	90.9	-20.4	-13.1	-0.3
Sh1	-40.2	-34.1	17.7	-24.5	-26.9	18.1	-15.7	-7.2	-0.3
Sh2	-42.6	-32.5	18.3	-26.2	-25.3	18.6	-16.5	-7.2	-0.3
Sh3	-28.6	-38.4	16.9	-17.0	-33.0	17.2	-11.6	-5.4	-0.3
Sh4	-27.7	-38.9	13.0	-16.2	-33.4	13.3	-11.5	-5.5	-0.3
Sh5	-26.3	-39.1	11.5	-15.1	-33.7	11.8	-11.2	-5.3	-0.3
Sh6	-34.5	-34.8	20.0	-21.0	-29.1	0.7	-13.5	-5.7	19.3
Sh7	-43.7	-30.6	24.5	-27.3	-24.1	24.8	-16.3	-6.5	-0.3
Sh8	-45.4	-33.3	19.0	-28.2	-25.7	19.3	-17.2	-7.6	-0.3
OphH1	-134.4	146.7	92.1	-119.3	156.5	92.4	-15.1	-9.8	-0.3
OphH2	-144.1	151.2	92.2	-126.1	162.7	92.5	-18.0	-11.5	-0.3
OphH3	-131.2	147.6	100.1	-117.7	157.2	100.4	-13.5	-9.6	-0.3
OphH4a	-139.8	155.2	127.1	-124.9	165.0	127.3	-14.9	-9.8	-0.3
OphH4b	-139.4	154.3	128.3	-124.7	164.1	128.6	-14.7	-9.8	-0.3
OphH4c	-141.4	153.8	130.8	-126.2	163.8	131.1	-15.2	-9.9	-0.3
OphH5	-149.4	157.2	123.4	-131.1	168.6	123.7	-18.4	-11.4	-0.3
SphH1	-39.4	-26.7	16.8	-23.1	-20.4	17.2	-16.3	-6.3	-0.4
SphH2	-46.4	-25.7	19.3	-27.7	-18.3	19.6	-18.7	-7.4	-0.3
SphH3	-32.0	-31.6	14.0	-17.7	-25.6	14.3	-14.3	-6.0	-0.3
SphH4a	-38.8	-27.9	21.6	-22.9	-21.7	21.9	-15.9	-6.2	-0.3
SphH4b	-38.7	-29.4	21.8	-22.9	-23.3	22.1	-15.8	-6.2	-0.3
SphH4c	-41.6	-33.4	23.3	-24.5	-27.2	23.7	-17.1	-6.2	-0.4
SphH5	-36.4	-25.5	19.3	-21.5	-19.8	19.8	-14.9	-5.7	-0.4
	$E_{N_2H}^{IQA}$	$E_{N_1N_2}^{IQA}$	$E_{HC_1}^{IQA}$	$E_{N_2H}^{elec}$	$E_{N_1N_2}^{elec}$	$E_{HC_1}^{elec}$	$E_{N_2H}^{x}$	$E_{N_1N_2}^{x}$	$E_{HC_1}^{x}$
NNh	-125.2	159.9	68.5	-106.0	169.8	68.8	-19.2	-9.9	-0.3

TABLE S6. Selected O…X bond critical points properties (in atomic units) for the **X*j*** and **XMe*j*** compounds.

	ρ_c	$\nabla^2\rho_c$	$\langle u' \rangle^{(1)}$	$\langle s' \rangle^{(1)}$	$\langle t' \rangle^{(1)}$	$e_x(\vec{r}_c)$	$e_c(\vec{r}_c)$	$\langle \delta e_x \rangle^{(2)}$	$\langle \delta e_c \rangle^{(2)}$
F5	-	-	-	-	-	-	-	-	-
F6	0.010	0.043	0.029	2.15	1.55	-1.60	-0.38	-2.66	1.74
F7	0.011	0.046	0.033	2.12	1.56	-1.85	-0.43	-2.99	1.95
F8	-	-	-	-	-	-	-	-	-
F9	-	-	-	-	-	-	-	-	-
F10	0.010	0.042	0.028	2.12	1.53	-1.56	-0.37	-2.58	1.63
F11	-	-	-	-	-	-	-	-	-
F12	0.011	0.046	0.030	2.09	1.53	-1.73	-0.40	-2.84	1.76
F13	0.011	0.045	0.032	2.10	1.54	-1.80	-0.42	-2.89	1.86
F14	-	-	-	-	-	-	-	-	-
FMe5	-	-	-	-	-	-	-	-	-
FMe6	-	-	-	-	-	-	-	-	-
FMe7	-	-	-	-	-	-	-	-	-
FMe8	-	-	-	-	-	-	-	-	-
FMe9	-	-	-	-	-	-	-	-	-
FMe10	-	-	-	-	-	-	-	-	-
FMe11	-	-	-	-	-	-	-	-	-
FMe12	-	-	-	-	-	-	-	-	-
FMe13	-	-	-	-	-	-	-	-	-
FMe14	-	-	-	-	-	-	-	-	-
Cl5	0.010	0.039	0.028	2.00	1.45	-1.67	-0.39	-2.43	1.55
Cl6	0.011	0.042	0.031	1.96	1.45	-1.89	-0.44	-2.68	1.67
Cl7	0.013	0.047	0.035	1.90	1.44	-2.21	-0.50	-3.05	1.83
Cl8	0.010	0.039	0.027	1.98	1.44	-1.62	-0.38	-2.36	1.47
Cl9	0.011	0.040	0.028	1.96	1.43	-1.72	-0.40	-2.46	1.53
Cl10	0.011	0.042	0.030	1.94	1.43	-1.85	-0.43	-2.60	1.60
Cl11	0.011	0.041	0.029	2.12	1.46	-1.71	-0.40	-2.58	1.58
Cl12	0.012	0.045	0.032	1.91	1.43	-2.02	-0.46	-2.81	1.69
Cl13	0.013	0.046	0.034	1.89	1.42	-2.15	-0.49	-2.95	1.76
Cl14	0.012	0.046	0.033	1.95	1.45	-2.01	-0.46	-2.91	1.75
ClMe5	-	-	-	-	-	-	-	-	-
ClMe6	-	-	-	-	-	-	-	-	-
ClMe7	-	-	-	-	-	-	-	-	-
ClMe8	-	-	-	-	-	-	-	-	-
ClMe9	-	-	-	-	-	-	-	-	-
ClMe10	-	-	-	-	-	-	-	-	-
ClMe11	-	-	-	-	-	-	-	-	-
ClMe12	-	-	-	-	-	-	-	-	-
ClMe13	-	-	-	-	-	-	-	-	-
ClMe14	-	-	-	-	-	-	-	-	-
Br5	0.011	0.037	0.027	1.83	1.34	-1.78	-0.41	-2.25	0.00
Br6	0.012	0.040	0.040	1.78	1.33	-1.99	-0.46	-2.45	1.43
Br7	0.013	0.044	0.034	1.74	1.32	-2.33	-0.53	-2.80	1.58
Br8	0.010	0.036	0.026	1.83	1.33	-1.70	-0.40	-2.17	1.29
Br9	0.011	0.037	0.027	1.80	1.32	-1.80	-0.42	-2.25	1.27
Br10	0.012	0.039	0.029	1.77	1.31	-1.94	-0.45	-2.38	1.38
Br11	0.011	0.038	0.027	1.84	1.35	-1.78	-0.41	-2.31	1.37
Br12	0.012	0.042	0.031	1.75	1.32	-2.12	-0.48	-2.59	1.47
Br13	0.013	0.043	0.033	1.72	1.31	-2.28	-0.52	-2.72	1.52
Br14	0.012	0.043	0.031	1.79	1.34	-2.08	-0.48	-2.64	1.51
BrMe5	-	-	-	-	-	-	-	-	-
BrMe6	-	-	-	-	-	-	-	-	-
BrMe7	-	-	-	-	-	-	-	-	-
BrMe8	-	-	-	-	-	-	-	-	-
BrMe9	-	-	-	-	-	-	-	-	-
BrMe10	-	-	-	-	-	-	-	-	-
BrMe11	-	-	-	-	-	-	-	-	-
BrMe12	-	-	-	-	-	-	-	-	-
BrMe13	-	-	-	-	-	-	-	-	-
BrMe14	-	-	-	-	-	-	-	-	-

TABLE S7. Selected O…O, O…S, and O…X bond critical points properties (in atomic units) for the **O*i*** and **S*i*** compounds.

	ρ_c	$\nabla^2\rho_c$	$\langle u' \rangle^{(1)}$	$\langle s' \rangle^{(1)}$	$\langle t' \rangle^{(1)}$	$10^3 e_x(\vec{r}_c)$	$10^3 e_c(\vec{r}_c)$	$10^3 \langle \delta e_x \rangle^{(2)}$	$10^3 \langle \delta e_c \rangle^{(2)}$
O1	0.009	0.037	0.024	2.16	1.52	-1.35	-0.32	-2.26	1 .49
O8	-	-	-	-	-	-	-	-	-
O9	-	-	-	-	-	-	-	-	-
O10	-	-	-	-	-	-	-	-	-
O11	0.010	0.047	0.030	2.11	1.54	-1.70	-0.40	-2.88	1.76
O12	0.010	0.046	0.046	2.10	1.53	-1.63	-0.38	-2.82	1.74
O13	0.012	0.047	0.033	2.07	1.54	-1.92	-0.44	-3.02	1.93
O14	0.021	0.045	0.032	2.11	1.55	-1.79	-0.42	-2.87	1.87
O15	0.017	0.043	0.029	2.09	1.52	-1.65	-0.39	-2.66	1.70
O16	0.019	0.045	0.031	2.09	1.54	-1.79	-0.42	-2.85	1.84
O17	0.016	0.047	0.030	2.10	1.54	-1.71	-0.40	-2.88	1.78
O18	0.022	0.045	0.032	2.09	1.54	-1.81	-0.42	-2.85	1.85
S1	0.017	0.055	0.042	1.56	1.23	-3.25	-0.70	-3.52	1.71
S8	0.014	0.046	0.034	1.66	1.27	-2.44	-0.55	-2.86	1.49
S9	0.014	0.047	0.035	1.64	1.26	-2.52	-0.56	-2.89	1.50
S10	0.014	0.049	0.036	1.67	1.30	-2.56	-0.57	-3.03	1.63
S11	0.016	0.054	0.040	1.63	1.28	-2.97	-0.65	-3.44	1.74
S12	0.016	0.054	0.041	1.62	1.27	-3.00	-0.66	-3.45	1.74
S13	0.022	0.071	0.057	1.47	1.21	-4.61	-0.95	-4.79	2.11
S14	0.011	0.066	0.052	1.49	1.22	-4.17	-0.87	-4.36	1.98
S15	0.010	0.056	0.056	1.56	1.24	-3.27	-0.71	-3.58	1.74
S16	0.011	0.062	0.049	1.50	1.22	-3.85	-0.82	-4.05	1.87
S17	0.011	0.055	0.042	1.62	1.27	-3.07	-0.67	-3.52	1.76
S18	0.011	0.069	0.056	1.45	1.20	-4.65	-0.96	-4.69	2.07
Oph1	0.013	0.056	0.041	2.07	1.57	-2.34	-0.53	-3.73	2.33
Oph2	0.013	0.057	0.041	2.07	1.57	-2.34	-0.53	-3.74	2.34
Oph3	0.014	0.056	0.041	2.07	1.57	-2.39	-0.54	-3.82	2.37
Oph4	-	-	-	-	-	-	-	-	-
Oph5	0.013	0.056	0.040	2.07	1.57	-2.32	-0.52	-3.71	2.31
Oph6	0.014	0.058	0.042	2.01	1.58	-2.43	-0.55	-3.88	2.41
Oph7	-	-	-	-	-	-	-	-	-
Sph1	0.020	0.066	0.051	1.53	1.24	-4.00	-0.84	-4.36	2.01
Sph2	0.020	0.066	0.051	1.53	1.24	-3.99	-0.84	-4.36	2.02
Sph3	0.021	0.070	0.055	1.53	1.25	-4.27	-0.89	-4.69	2.15
Sph4	-	-	-	-	-	-	-	-	-
Sph5	0.020	0.065	0.051	1.53	1.24	-3.95	-0.83	-4.32	2.00
Sph6	0.021	0.071	0.055	1.53	1.25	-4.34	-0.90	-4.75	2.16
Sph7	-	-	-	-	-	-	-	-	-
Fph1a	0.014	0.062	0.046	2.22	1.70	-2.47	-0.55	-4.31	2.87
Fph1b	0.012	0.051	0.037	2.07	1.55	-2.13	-0.49	-3.35	2.13
Fph1c	0.015	0.065	0.049	2.22	1.71	-2.29	-0.59	-4.61	3.04
Fph1d	0.013	0.054	0.040	2.06	1.56	-2.29	-0.52	-3.60	2.26
Fph1e	0.014	0.064	0.048	2.22	1.70	-2.58	-0.57	-4.50	2.97
Fph1f	0.013	0.053	0.039	2.06	1.56	-2.23	-0.51	-3.49	2.20
Clph1a	0.015	0.062	0.046	1.99	1.54	-2.73	-0.60	-4.19	2.49
Clph1b	0.014	0.054	0.040	1.85	1.43	-2.60	-0.58	-3.54	2.03
Clph1c	0.015	0.063	0.047	1.96	1.52	-2.84	-0.62	-4.25	2.49
Clph1d	0.015	0.058	0.043	1.84	1.43	-2.81	-0.62	-3.84	2.15
Clph1e	0.016	0.064	0.047	1.97	1.53	-2.86	-0.63	-4.33	2.55
Clph1f	0.015	0.059	0.044	1.84	1.43	-2.84	-0.63	-3.88	2.18
Brph1a	0.015	0.056	0.041	1.82	1.41	-2.71	-0.60	-3.64	2.03
Brph1b	0.015	0.050	0.038	1.70	1.31	-2.69	-0.60	-3.20	1.72
Brph1c	0.015	0.053	0.040	1.79	1.38	-2.65	-0.59	-3.43	1.91
Brph1d	0.015	0.053	0.040	1.69	1.31	-2.81	-0.62	-3.37	1.77
Brph1e	0.015	0.054	0.041	1.79	1.39	-2.70	-0.60	-3.53	1.96
Brph1f	0.015	0.053	0.040	1.69	1.31	-2.84	-0.62	-3.39	1.79

TABLE S8. Selected bond critical points properties (in atomic units) for the intramolecular hydrogen bonds.

	ρ_c	$\nabla^2\rho_c$	$\langle u' \rangle^{(1)}$	$\langle s' \rangle^{(1)}$	$\langle t' \rangle^{(1)}$	$10^3 e_x(\vec{r}_c)$	$10^3 e_c(\vec{r}_c)$	$10^3 \langle \delta e_x \rangle^{(2)}$	$10^3 \langle \delta e_c \rangle^{(2)}$
Oh1	0.049	0.135	0.172	1.56	1.47	-13.14	-2.35	-12.64	6.92
Oh2	0.051	0.139	0.181	1.55	1.47	-13.98	-2.48	-13.19	7.20
Oh3	0.035	0.113	0.119	1.71	1.52	-8.31	-1.58	-9.57	5.35
Oh4	0.035	0.115	0.122	1.72	1.53	-8.49	-1.61	-9.81	5.50
Oh5	0.034	0.112	0.117	1.74	1.54	-8.06	-1.54	-9.48	5.34
Oh6	0.040	0.125	0.141	1.65	1.50	-10.26	-1.90	-11.04	6.04
Oh7	0.048	0.136	0.171	1.57	1.47	-13.00	-2.33	-12.68	6.87
Oh8	0.056	0.146	0.200	1.52	1.46	-15.67	-2.73	-14.25	7.77
Sh1	0.031	0.098	0.100	1.68	1.46	-7.10	-1.38	-7.94	4.37
Sh2	0.032	0.103	0.106	1.66	1.46	-7.65	-1.48	-8.46	4.59
Sh3	0.023	0.078	0.079	1.77	1.48	-4.89	-1.00	-5.92	3.42
Sh4	0.023	0.079	0.074	1.78	1.49	-4.94	-1.01	-6.04	3.50
Sh5	0.023	0.077	0.071	1.79	1.49	-4.75	-0.98	-5.84	3.40
Sh6	0.027	0.088	0.086	1.72	1.47	-5.93	-1.19	-6.93	3.88
Sh7	0.032	0.102	0.105	1.66	1.46	-7.53	-1.46	-8.37	4.53
Sh8	0.034	0.109	0.113	1.65	1.46	-8.24	-1.57	-9.04	4.85
OphH1	0.041	0.126	0.144	1.66	1.52	-10.36	-1.91	-11.23	6.20
OphH2	0.050	0.145	0.181	1.59	1.50	-13.61	-2.42	-13.64	7.40
OphH3	0.039	0.129	0.140	1.71	1.56	-9.75	-1.82	-11.35	6.26
OphH4a	0.041	0.132	0.147	1.67	1.53	-10.55	-1.94	-11.69	6.39
OphH4b	0.041	0.131	0.147	1.67	1.53	-10.47	-1.93	-11.64	6.36
OphH4c	0.043	0.134	0.153	1.66	1.54	-11.01	-2.02	-12.03	6.55
OphH5	0.051	0.147	0.184	1.58	1.50	-13.91	-2.46	-13.86	7.47
SphH1	0.032	0.105	0.108	1.69	1.48	-7.64	-1.47	-8.69	4.75
SphH2	0.038	0.123	0.132	1.64	1.48	-9.59	-1.79	-10.57	5.58
SphH3	0.030	0.106	0.102	1.76	1.53	-6.93	-1.35	-8.58	4.71
SphH4a	0.033	0.110	0.110	1.70	1.50	-7.69	-1.48	-9.05	4.89
SphH4b	0.032	0.109	0.109	1.71	1.50	-7.59	-1.47	-8.97	4.85
SphH4c	0.035	0.119	0.121	1.68	1.51	-8.56	-1.63	-9.94	5.31
SphH5	0.030	0.100	0.097	1.71	1.48	-6.80	-1.33	-8.01	4.35
NNh	0.046	0.113	0.148	1.45	1.35	-12.23	-2.21	-10.30	5.46
PD	0.021	0.080	0.071	1.97	1.62	-4.32	-0.90	-6.14	3.81
BD	0.031	0.109	0.109	1.84	1.60	-7.06	-1.38	-9.09	5.31