Supplementary material

DFT approach to the charge transport related properties in columnar stacked π-conjugated N-heterocycles cores including electron donor and acceptor units

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SOME COMMENTS ABOUT THE QTAIM ANALYSIS

The eigenvalues λ_i of the Hessian matrix of electron density ρ_b rule the criteria for classifying the so-called critical points, CP, according to two indexes, i.e. (r, s). Here, r and s stand for the number of non-null λ_i and the difference between the number of positive and negative λ_i, respectively. Thus, CPs (3,-1) mean bond critical points (BCP), CPs (3, 1) mean ring critical point (RCP) and CPs (3, 3) mean cage critical point (CCP).

The sign of the Laplacian of electron density, $\nabla^2\rho_b$, at these CPs points the charge density is either locally concentrated [$\nabla^2\rho_b < 0$] or locally depleted [$\nabla^2\rho_b > 0$]. In the former case, the electrons are shared by both nuclei and it is typical for covalent interactions. The latter case is associated with closed-shell type interactions, such as H-bonds, ionic bonding, and even van der Waals interactions.

An energy interpretation of these kind of interactions can be performed through the virial theorem which relates $\nabla^2\rho_b$ to the values of the potential, $V_b < 0$, and kinetic, $G_b > 0$, energy densities at the CP, for a system in electrostatic equilibrium. Thus, the stability of the shared interaction in regions where $\nabla^2\rho_b < 0$ is due to the lowering of potential energy term, while for closed-shell interactions, $\nabla^2\rho_b > 0$, the kinetic energy term is the dominant one.

In addition, Cremer and Kraka have proposed the use of the total energy density, H_b, evaluated at the CP, defined as $H_b = V_b + G_b$.[1] H_b takes negative values for shared-type atomic interactions and reflects the covalent character of the bonding, while positive values for H_b are associated to closed-shell interactions.

Furthermore, in order to characterize the strength of closed-shell interactions we have calculated the indexes $|V_b|/G_b$ and bond-degree (BD) H_b/ρ_b.[2] The BD index can be interpreted as the softening degree (SD) for interactions where $H_b > 0$ in such a way that the weaker the interaction the greater the SD index. As stated by Matta and Boyd $|V_b|/G_b < 1$ for pure closed-shell type interactions as it is the case of the H-bonds described above.[3]

The dependence of $|V_b|/G_b$ and SD with the interatomic distance is plotted in Figures 3S and 4S, respectively. Thus, the ratio $|V_b|/G_b$ increases from 0 to 1, leading to a decrease of SD as the internuclear distance shortens, and then, closed-shell interactions become stronger.

As seen in Table 1S**,** the BCPs associated to intramolecular, H-bond interactions observed for each (2,3) and (2,4) couples were also found in the corresponding single molecule. Thus, $S_{thio}\cdots H_{carb}$ contacts are found for *1b*, *1c* and *2c*. However, despite H_{carb} only intervenes in the $C_{thio}\cdots H_{carb}$ contacts in single *1b* and *1c*, new $H_{thio}\cdots H_{carb}$ contacts appeared in the couple *1c*. Finally, as discussed for the single disc, $N_{triazol}$ atoms are H-bonded with metoxyphenyl (*2a*), and thiophene in (*2b***,** *2c***)**.

For couples (2, 3) of *1a* and *1b*, there are two ($C_{triaz}\cdots C_{triaz}$) BCPs and four ($C_{triaz}\cdots N_{triaz}$) BCPs, while for *1c* only one ($C_{triaz}\cdots N_{triaz}$) BCP is found connecting neighboring triazine rings. Also, two (six) BCPs ($S_{thio}\cdots C_{thio}$) between consecutive discs for *1b*(*1c*) are found. Note that for tristriazolotriazine derivatives, the number of BCPs ($C_{triaz}\cdots N_{triaz}$) for (2, 3) couples associated to neighboring discs increases from three (*2a*), nine (*2b*) to eleven (*2c*).

For triazine derivatives, however, the total number of BCPs for (2, 3) couples increases from two in *1a* ($C_{triaz}\cdots C_{triaz}$), six in *1b* (two $S_{thio}\cdots C_{thio}$, four $C_{triaz}\cdots N_{triaz}$) to seven in *1c* (six $S_{thio}\cdots C_{thio}$ and one $C_{triaz}\cdots N_{triaz}$).

For *1b*, *1c* and *2c*, the distance between N-carbazolyl rings linked to (2,4) couples is around 3.8 Å and they stack in an almost parallel arrangement giving rise to a richer, intermolecular network and then to an ordered, helical structure.

(1) D. Cremer, E. Kraka, *Angew.Chem.*, 1984, **23**, 627-628

(2) E. Espinosa, I. Alkorta, J. Elguero, E. Molins, *J. Chem. Phys.,* 2002, **117**, 5529-5542

(3) C. Matta, R.J. Boyd, The Quantum Theory of Atoms in Molecules, Wiley-VCH, Weinheim, 2007.

Figure 1S. Rotational barrier for the dimer of 1a (left) and 2a (right) at B3LYP/6-31G* level.

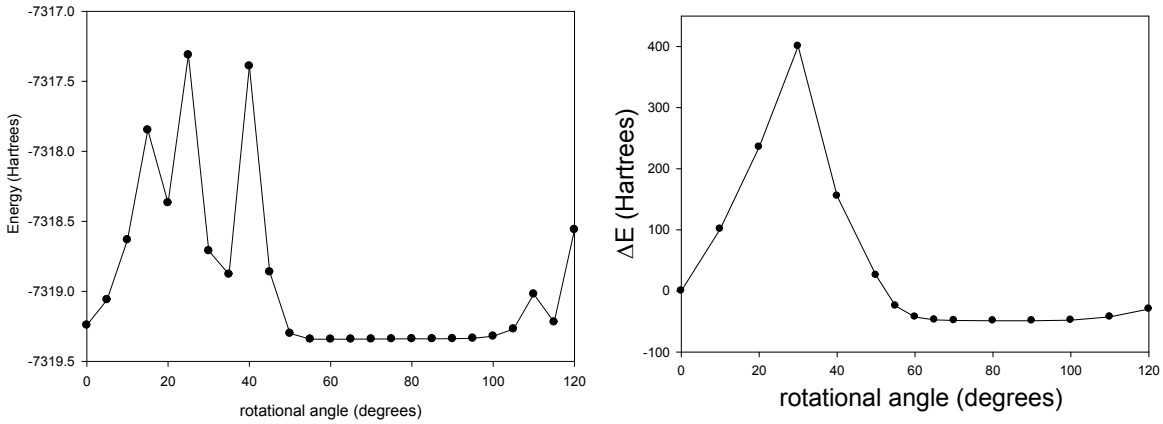

Figure 2S. Representation of the intramolecular bond paths (---) in single molecules of the selected compounds (o Hydrogen; ● Carbon; ● Oxygen; ● Sulfur; ● Nitrogen).

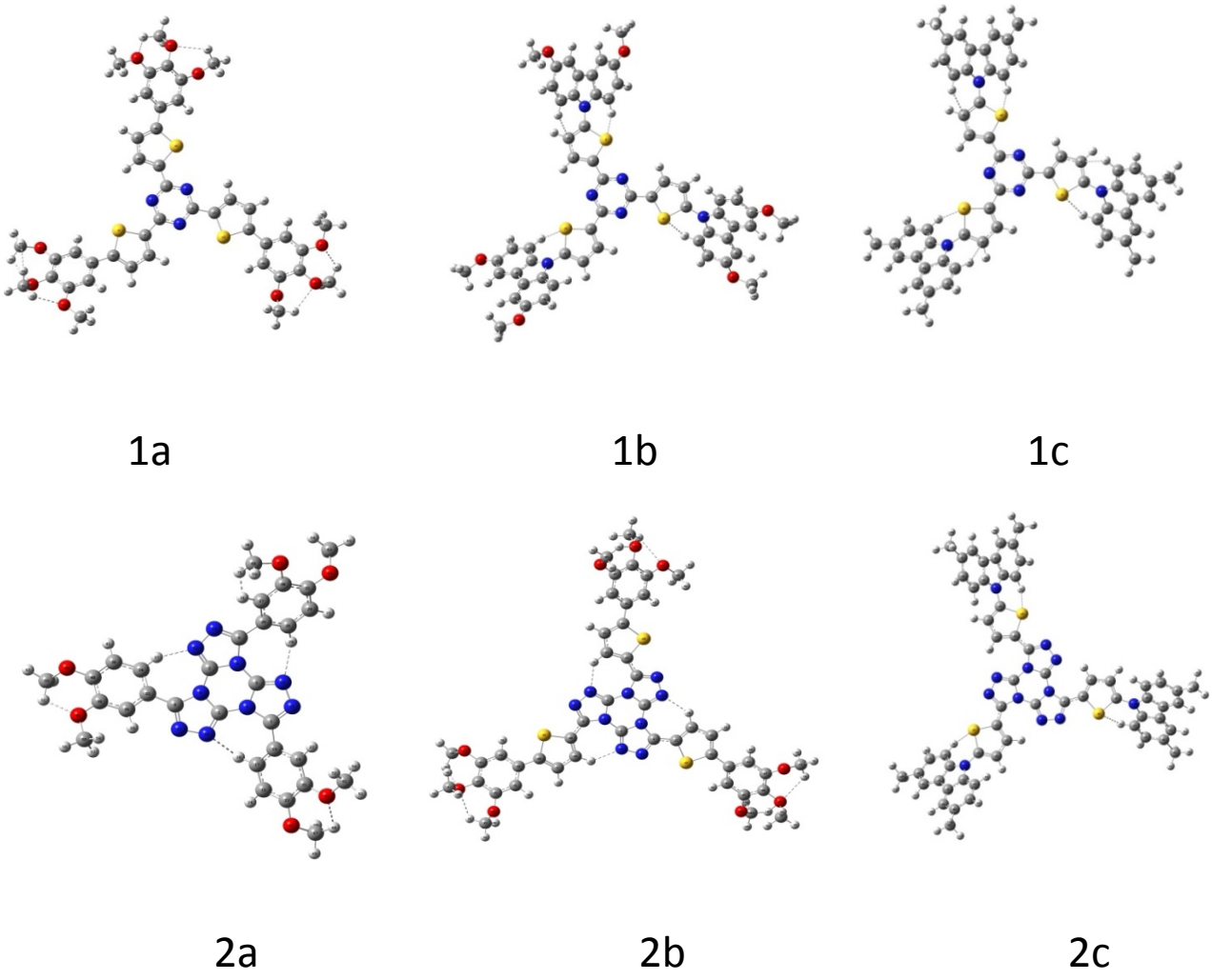

Figure 3S. Dependence of $|V_b|/G_b$ on the interatomic distance.

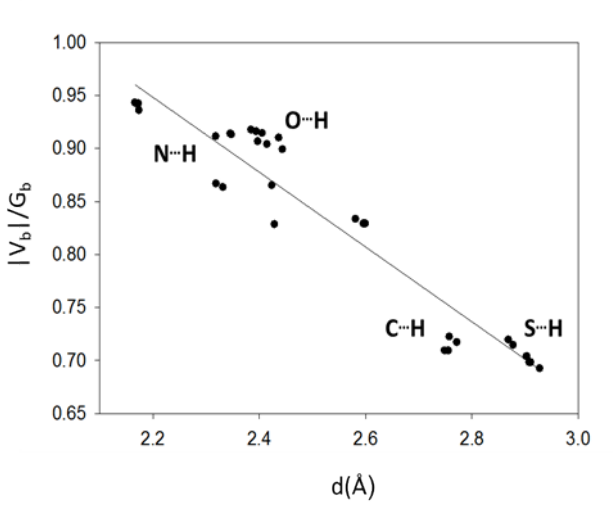

Figure 4S: Dependence of the bond-degree (BD) H_b/ρ_b on the interatomic distance.

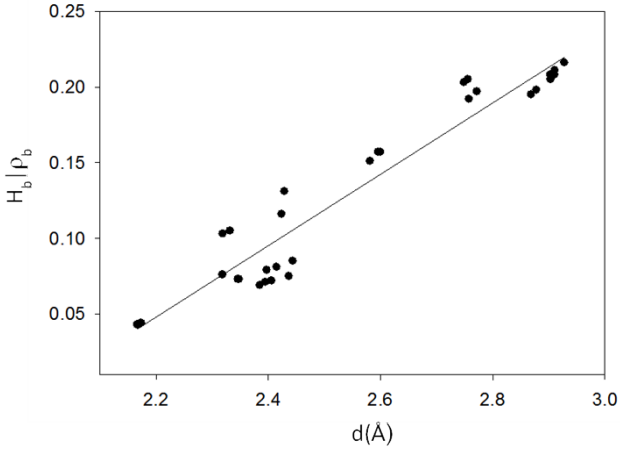

Figure 5S. Representation of the inter and intra molecular bond paths (---) for the (2,4) couples of the six clusters studied (o Hydrogen; • Carbon; • Oxygen; • Sulfur; • Nitrogen).

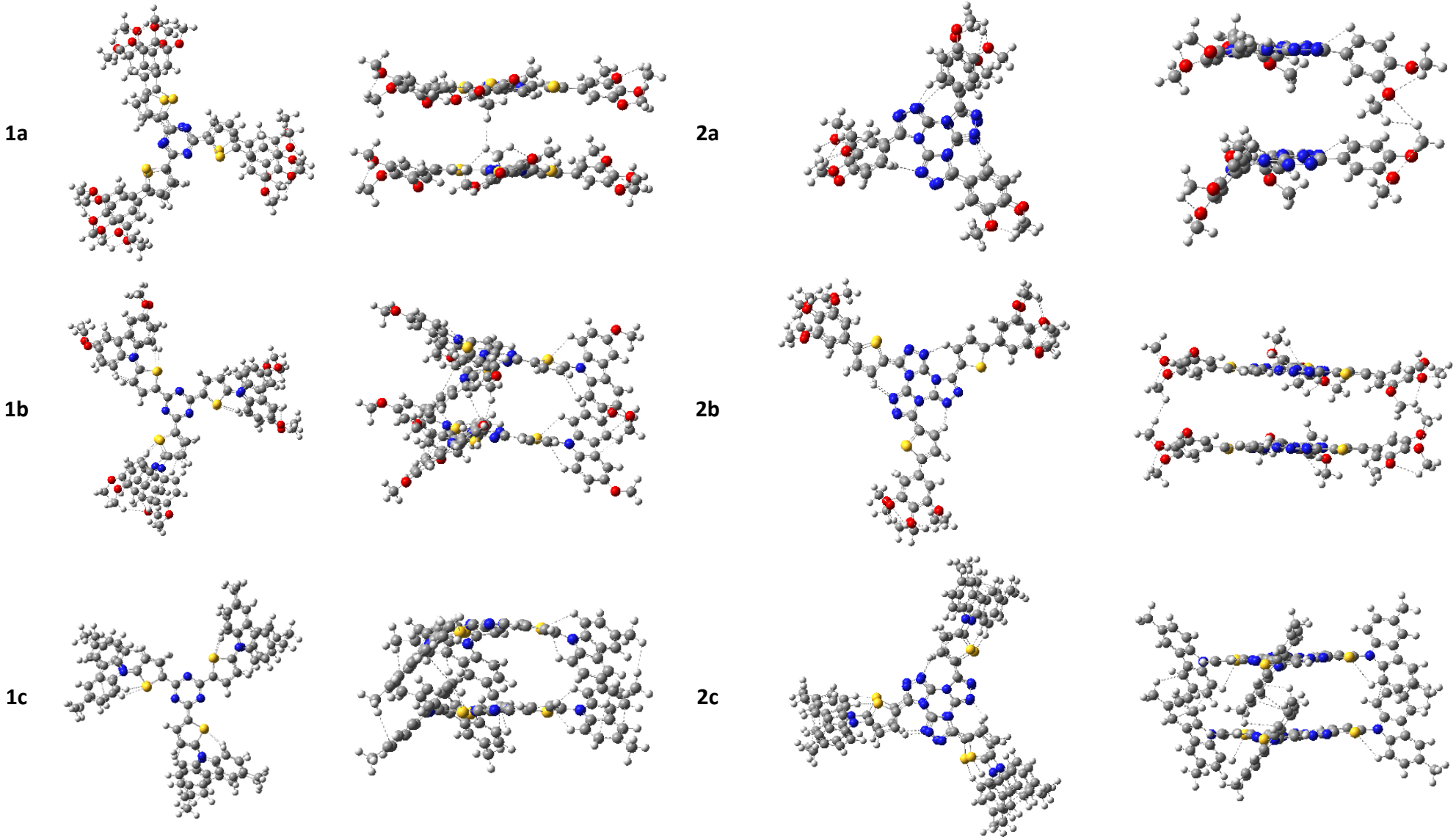

Table 1S. Topological properties for single disc and (2,3) and (2,4) couples of each compound studied at the B3LYP/6-31G* level.

Single disc 1a.

Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
O52…H92	2.3975	0.0127	0.0466	0.0107	-0.0097	0.0010
O84…H49	2.5815	0.0086	0.0362	0.0078	-0.0065	0.0013
O83…H62	2.3186	0.0145	0.0538	0.0124	-0.0113	0.0011
O82…H68	2.4241	0.0146	0.0573	0.0126	-0.0109	0.0017
O87…H76	2.5962	0.0083	0.0358	0.0076	-0.0063	0.0013
O86…H80	2.3947	0.0127	0.0469	0.0107	-0.0098	0.0009

Single disc 1b.

Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
S9…H24	2.903	0.0077	0.0281	0.0054	-0.0038	0.0016
S42…H75	2.911	0.0076	0.0276	0.0053	-0.0037	0.0016
S35…H54	2.928	0.0074	0.0270	0.0052	-0.0036	0.0016
C10…H21	2.772	0.0076	0.0276	0.0053	-0.0038	0.0015

Single disc 1c.

Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
S9…H24	2.877	0.0081	0.0292	0.0057	-0.0057	0.0000
S42…H75	2.869	0.0082	0.0296	0.0057	-0.0041	0.0016
S35…H54	2.878	0.0081	0.0292	0.0056	-0.0040	0.0016
C10…H21	2.756	0.0078	0.0283	0.0055	-0.0039	0.0016
C43…H72	2.749	0.0079	0.0285	0.0055	-0.0039	0.0016
C36…H57	2.758	0.0078	0.0282	0.0054	-0.0039	0.0015

Single disc 2a.

Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
N14…H29	2.429	0.0130	0.0463	0.0099	-0.0082	0.0017
N12…H37	2.332	0.0153	0.0531	0.0117	-0.0101	0.0016
N10…H20	2.319	0.0156	0.0541	0.0120	-0.0104	0.0016
O43…H48	2.348	0.0137	0.0504	0.0115	-0.0105	0.0010
O46…H61	2.346	0.0137	0.0506	0.0116	-0.0106	0.0010
H31…H71	1.418	0.0420	0.1417	0.0381	-0.0408	-0.0027

Single disc 2b.

Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
O66…H86	2.600	0.0083	0.0358	0.0076	-0.0063	0.0013
O65…H91	2.385	0.0130	0.0476	0.0109	-0.0100	0.0009
O61…H70	2.437	0.0120	0.0441	0.0100	-0.0091	0.0009
O61…H95	2.415	0.0123	0.0454	0.0104	-0.0094	0.0010
O68…H105	2.444	0.0118	0.0437	0.0099	-0.0089	0.0010
O68…H74	2.406	0.0125	0.0460	0.0105	-0.0096	0.0009
N14…H20	2.170	0.0207	0.0662	0.0156	-0.0147	0.0009
N10…H26	2.173	0.0206	0.0660	0.0156	-0.0147	0.0009
N12…H32	2.174	0.0205	0.0659	0.0156	-0.0146	0.0009

Single disc 2c.

Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
S30…H44	2.9103	0.0077	0.0278	0.0053	-0.0037	0.0016
S24…H80	2.9083	0.0077	0.0279	0.0053	-0.0037	0.0016
S18…H62	2.9037	0.0078	0.0280	0.0054	-0.0038	0.0016
N14…H20	2.1673	0.0208	0.0665	0.0157	-0.0148	0.0009
N10…H26	2.1665	0.0208	0.0666	0.0158	-0.0149	0.0009
N12…H32	2.1674	0.0208	0.0665	0.0157	-0.0148	0.0009

(2,4) Couple of 1a.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Methoxy	H75…H161	2.2221	0.0072	0.0255	0.0049	-0.0035	0.0015
Intramolecular interactions	Methoxy	O85…H50	2.2831	0.0155	0.0560	0.0131	-0.0122	0.0009
		O53…H93	2.1594	0.0199	0.0695	0.0168	-0.0162	0.0006
		O88…H77	2.2625	0.0161	0.0578	0.0136	-0.0127	0.0009
		O87…H81	2.1508	0.0199	0.0705	0.0170	-0.0163	0.0007
		O84…H63	2.2457	0.0167	0.0601	0.0142	-0.0133	0.0009
		O83…H69	2.3824	0.0162	0.0642	0.0142	-0.0123	0.0019
		O149…H18	2.1713	0.0194	0.0678	0.0164	-0.0158	0.0006
		O181…H146	2.2827	0.0153	0.0557	0.0130	-0.0121	0.0009
		O183…H177	2.1755	0.0195	0.0673	0.0163	-0.0158	0.0005
		O184…H173	2.3507	0.0137	0.0502	0.0116	-0.0106	0.0010
		O180…H159	2.2870	0.0154	0.0560	0.0131	-0.0121	0.0010
		O179…H165	2.4039	0.0159	0.0633	0.0140	-0.0121	0.0019
		H65…H68	2.3512	0.0061	0.0254	0.0049	-0.0034	0.0015
		H161…H164	2.2973	0.0068	0.0272	0.0052	-0.0037	0.0015

(2,4) Couple of 1b.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Methoxy	O90…H228	2.4393	0.0102	0.0348	0.0081	-0.0074	0.0007
		O90…H175	2.7566	0.0063	0.0246	0.0050	-0.0039	0.0011
		O203…H105	2.4877	0.0097	0.0326	0.0075	-0.0068	0.0007
	Carbazolyl (C) Methoxy	C22…H224	2.7628	0.0084	0.0306	0.0060	-0.0043	0.0017
		C68…H208	2.5575	0.0103	0.0349	0.0072	-0.0056	0.0016
		C17…O200	3.1203	0.0080	0.0274	0.0060	-0.0052	0.0008
		C76…O203	3.1277	0.0080	0.0274	0.0061	-0.0053	0.0008
		C140…C80	3.2167	0.0079	0.0247	0.0050	-0.0037	0.0013
Intramolecular interactions	Thiophenyl (S, C) Carbazolyl (H)	S35…H54	2.7982	0.0092	0.0340	0.0067	-0.0049	0.0018
		S42…H75	2.8166	0.0087	0.0317	0.0062	-0.0045	0.0017
		S9…H24	2.8328	0.0086	0.0319	0.0062	-0.0044	0.0018
		S123…H138	2.7351	0.0104	0.0382	0.0076	-0.0057	0.0019
		S156…H189	2.7176	0.0105	0.0381	0.0077	-0.0058	0.0019
		S149…H168	2.7238	0.0103	0.0375	0.0075	-0.0057	0.0018
		C36…H57	2.6367	0.0094	0.0346	0.0067	-0.0048	0.0019
		C43…H72	2.6039	0.0101	0.0380	0.0074	-0.0053	0.0021
		C10…H21	2.5992	0.0101	0.0382	0.0074	-0.0053	0.0021
		C124…H135	2.6649	0.0090	0.0343	0.0066	-0.0046	0.0020
		C157…H186	2.5867	0.0108	0.0433	0.0083	-0.0058	0.0025
		C150…H171	2.6681	0.0090	0.0335	0.0065	-0.0046	0.0019

(2,4) Couple of 1c.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Methyl	H99…H214	2.2276	0.0075	0.0271	0.0052	-0.0037	0.0015
		C104…H194	2.6264	0.0080	0.0312	0.0061	-0.0045	0.0016
		C84…H206	2.6352	0.0077	0.0301	0.0059	-0.0044	0.0015
	Carbazolyl (C) Methyl (H)	C178…H95	2.6132	0.0098	0.0315	0.0066	-0.0053	0.0013
		C164…H102	2.6481	0.0092	0.0298	0.0062	-0.0049	0.0013
		C180…H93	2.8281	0.0074	0.0244	0.0048	-0.0036	0.0012
		C75…H194	2.7937	0.0068	0.0243	0.0048	-0.0035	0.0013
		C128…H90	2.6713	0.0088	0.0286	0.0059	-0.0047	0.0012
		C50…C131	3.1820	0.0084	0.0258	0.0053	-0.0041	0.0012
		C130…C88	3.3692	0.0069	0.0239	0.0048	-0.0036	0.0012
Intramolecular interactions	Thiophenyl (S, C) Carbazolyl (H)	S9…H24	2.7272	0.0102	0.0381	0.0076	-0.0057	0.0019
		S35…H54	2.7283	0.0101	0.0368	0.0074	-0.0056	0.0018
		S42…H74	2.6865	0.0107	0.0395	0.0080	-0.0062	0.0018
		S143…H162	2.7935	0.0096	0.0356	0.0070	-0.0051	0.0019
		S150…H182	2.7035	0.0107	0.0390	0.0079	-0.0060	0.0019
		S117…H132	2.9349	0.0080	0.0304	0.0059	-0.0041	0.0017
		C144…H165	2.6247	0.0096	0.0358	0.0069	-0.0049	0.0020
		C151…H179	2.5761	0.0106	0.0408	0.0080	-0.0057	0.0023
		C36…H57	2.5730	0.0109	0.0429	0.0083	-0.0059	0.0024
	Carbazolyl	H13…H21	2.0731	0.0122	0.0498	0.0097	-0.0070	0.0027
	Thioph…Carbaz	H46…H71	2.0867	0.0124	0.0515	0.0100	-0.0071	0.0029

(2,4) Couple of 2a.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Methoxy	O139…H50	2.5774	0.0073	0.0269	0.0059	-0.0050	0.0009
		H50…H142	2.2634	0.0076	0.0303	0.0058	-0.0040	0.0018
Intramolecular interactions	Triazolyl (N) Phenyl (H)	N10…H20	2.2309	0.0185	0.0647	0.0146	-0.0130	0.0016
		N12…H37	2.4518	0.0129	0.0485	0.0100	-0.0080	0.0020
		N14…H29	2.6827	0.0101	0.0348	0.0072	-0.0058	0.0014
		N86…H101	2.7555	0.0086	0.0291	0.0060	-0.0047	0.0013
		N82…H92	2.1389	0.0220	0.0741	0.0174	-0.0162	0.0011
		N84…H109	2.0592	0.0256	0.0826	0.0201	-0.0195	0.0006
	Methoxy	O43…H48	2.4554	0.0108	0.0415	0.0093	-0.0082	0.0011
		O67…H64	2.3551	0.0132	0.0486	0.0111	-0.0101	0.0010
		O139…H136	2.3687	0.0129	0.0475	0.0109	-0.0099	0.0010
		O118…H133	2.2606	0.0161	0.0588	0.0137	-0.0126	0.0011
		O115…H120	2.2801	0.0154	0.0561	0.0130	-0.0121	0.0009

(2,4) Couple of 2b.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Methyl	H104…H106	2.2954	0.0061	0.0222	0.0042	-0.0028	0.0014
		H76…H194	2.4542	0.0052	0.0201	0.0037	-0.0025	0.0012
Intramolecular interactions	Triazol (N) Thiophenyl (H)	N14…H27	2.1507	0.0214	0.0688	0.0163	-0.0154	0.0009
		N4…H24	2.1493	0.0215	0.0687	0.0163	-0.0155	0.0008
		N11…H36	2.1280	0.0224	0.0721	0.0172	-0.0164	0.0008
		N143…H136	2.1051	0.0235	0.0754	0.0181	-0.0174	0.0007
		N149…H158	2.1591	0.0211	0.0675	0.0160	-0.0151	0.0009
		N141…H161	2.1772	0.0203	0.0650	0.0153	-0.0144	0.0009
	Methoxy	O87…H100	2.2982	0.0153	0.0546	0.0128	-0.0119	0.0009
		O87…H99	2.3437	0.0145	0.0510	0.0120	-0.0112	0.0008
		O71…H105	2.4363	0.0119	0.0436	0.0099	-0.0090	0.0009
		O108…H128	2.4446	0.0117	0.0434	0.0099	-0.0089	0.0010
		O117…H110	2.3661	0.0138	0.0492	0.0115	-0.0107	0.0008
		O117…H133	2.2886	0.0158	0.0559	0.0132	-0.0124	0.0008
		O184…H208	2.4660	0.0108	0.0416	0.0093	-0.0082	0.0010
		O188…H201	2.3367	0.0142	0.0512	0.0119	-0.0110	0.0009
		O59…H94	2.4169	0.0124	0.0449	0.0103	-0.0094	0.0009
		O67…H86	2.3477	0.0143	0.0504	0.0119	-0.0111	0.0008
		O67…H82	2.3312	0.0143	0.0517	0.0120	-0.0111	0.0009
		O185…H195	2.2783	0.0164	0.0581	0.0137	-0.0128	0.0009
		O185…H194	2.3497	0.0143	0.0505	0.0119	-0.0111	0.0008
		O64…H76	2.3449	0.1399	0.0503	0.0117	-0.0108	0.0009
		O56…H90	2.4778	0.0106	0.0409	0.0091	-0.0080	0.0011
		O180…H207	2.4409	0.0118	0.0434	0.0099	-0.0089	0.0010

(2,4) Couple of 2c.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Carbazolyl (C) Methyl (H)	C162…H106	2.7425	0.0078	0.0272	0.0054	-0.0040	0.0014
		C66…H210	2.7759	0.0073	0.0257	0.0051	-0.0037	0.0014
		C48…H226	2.7879	0.0071	0.0250	0.0049	-0.0036	0.0013
		C198…H98	2.7425	0.0077	0.0269	0.0053	-0.0039	0.0014
		C84…H218	2.7355	0.0077	0.0266	0.0053	-0.0039	0.0014
		C180…H114	2.7689	0.0072	0.0255	0.0050	-0.0037	0.0013
	Carbazolyl	C59…C156	3.1139	0.0096	0.0283	0.0059	-0.0048	0.0011
		C70…C166	3.2685	0.0082	0.0238	0.0049	-0.0038	0.0011
		C52…C202	3.2802	0.0080	0.0230	0.0047	-0.0037	0.0010
		C41…C192	3.0883	0.0100	0.0296	0.0062	-0.0050	0.0012
		C88…C184	3.2990	0.0078	0.0226	0.0046	-0.0036	0.0010
		C77…C174	3.1204	0.0095	0.0278	0.0058	-0.0047	0.0011
Intramolecular interactions	Triazol (N) Thiophenyl (H)	N127…H143	2.0987	0.0237	0.0755	0.0182	-0.0175	0.0007
		N129…H149	2.0763	0.0247	0.0790	0.0191	-0.0185	0.0006
		N131…H137	2.0760	0.0248	0.0791	0.0192	-0.0186	0.0006
		N14…H20	2.0928	0.0240	0.0767	0.0185	-0.0178	0.0007
		N12…H32	2.0591	0.0256	0.0821	0.0200	-0.0194	0.0006
		N10…H26	2.0901	0.0241	0.0770	0.0186	-0.0179	0.0007
	Thiophenyl (S) Carbazolyl (H)	S24…H80	2.8047	0.0091	0.0325	0.0064	-0.0047	0.0017
		S30…H44	2.8021	0.0091	0.0325	0.0064	-0.0047	0.0017
		S18…H62	2.7999	0.0091	0.0327	0.0065	-0.0047	0.0018
		S147…H161	2.9376	0.0075	0.0274	0.0052	-0.0036	0.0016
		S141…H197	2.9241	0.0076	0.0279	0.0053	-0.0037	0.0016
		S135…H179	2.9207	0.0077	0.0280	0.0054	-0.0037	0.0017

(2,3) Couple of 1a.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Triazine	C2…C98	3.0609	0.0079	0.0301	0.0059	-0.0043	0.0016
		C1…C99	3.0787	0.0078	0.0293	0.0058	-0.0042	0.0016
	Methoxy	O85…H168	2.4291	0.0108	0.0391	0.0088	-0.0079	0.0009
		C165…H78	2.7362	0.0066	0.0276	0.0052	-0.0035	0.0017
Intramolecular interactions	Methoxy	O84…H49	2.2831	0.0155	0.0559	0.0131	-0.0122	0.0009
		O83…H62	2.2457	0.0167	0.0601	0.0142	-0.0133	0.0009
		O82…H68	2.3824	0.0162	0.0641	0.0142	-0.0123	0.0019
		O52…H92	2.1594	0.0199	0.0694	0.0168	-0.0162	0.0006
		O86…H80	2.1508	0.0199	0.0704	0.0170	-0.0163	0.0007
		O87…H76	2.2625	0.0160	0.0579	0.0136	-0.0127	0.0009
		O148…H188	2.1138	0.0216	0.0754	0.0184	-0.0179	0.0005
		O179…H158	2.2831	0.0156	0.0564	0.0132	-0.0123	0.0009
		O180…H145	2.3049	0.0148	0.0536	0.0125	-0.0116	0.0009
		O182…H176	2.1237	0.0213	0.0736	0.0180	-0.0176	0.0004
		O183…H172	2.2927	0.0150	0.0548	0.0128	-0.0118	0.0010
		H64…H67	2.3512	0.0061	0.0254	0.0049	-0.0034	0.0015
		H160…H163	2.3103	0.0066	0.0262	0.0051	-0.0036	0.0015

(2,3) Couple of 1b.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Thiophenyl Carbazolyl	H24…H125	2.7054	0.0078	0.0310	0.0059	-0.0041	0.0018
		H24…H127	2.3506	0.0064	0.0266	0.0049	-0.0032	0.0017
		H54…H153	2.1158	0.0088	0.0338	0.0066	-0.0048	0.0018
		H81…H160	2.8395	0.0069	0.0272	0.0052	-0.0035	0.0017
	Thiophenyl (C) Carbazolyl (H)	C157…H75	2.5618	0.0095	0.0369	0.0073	-0.0054	0.0019
		C49…H171	2.6205	0.0091	0.0353	0.0069	-0.0049	0.0020
	Thiophenyl	S149…C8	3.1668	0.0117	0.0389	0.0079	-0.0062	0.0017
		S123…C41	3.2448	0.0100	0.0321	0.0065	-0.0050	0.0015
		S9…H125	2.9626	0.0077	0.0266	0.0050	-0.0034	0.0016
	Triazine	N4…C116	3.1157	0.0078	0.0259	0.0055	-0.0045	0.0010
		N119…C1	3.1075	0.0080	0.0265	0.0057	-0.0047	0.0010
		N6…C115	3.1117	0.0080	0.0269	0.0057	-0.0047	0.0010
		N120…C2	3.1058	0.0082	0.0270	0.0057	-0.0046	0.0011
Intramolecular interactions	Thiophenyl (S, C) Carbazolyl (H)	S156…H189	2.8564	0.0081	0.0294	0.0057	-0.0040	0.0017
		S42…H75	2.8166	0.0087	0.0320	0.0063	-0.0045	0.0017
		S123…H138	2.7873	0.0096	0.0356	0.0070	-0.0051	0.0019
		S35…H54	2.7982	0.0093	0.0344	0.0068	-0.0049	0.0018
		S149…H168	2.8115	0.0091	0.0339	0.0066	-0.0048	0.0018
		S9…H24	2.8328	0.0087	0.0322	0.0063	-0.0045	0.0018
		C157…H186	2.5926	0.0103	0.0390	0.0076	-0.0055	0.0021
		C36…H57	2.6367	0.0094	0.0346	0.0067	-0.0048	0.0019
		C124…H135	2.6782	0.0087	0.0318	0.0062	-0.0044	0.0018
		C43…H72	2.6039	0.0101	0.0379	0.0074	-0.0053	0.0021
		C150…H171	2.6680	0.0089	0.0322	0.0063	-0.0045	0.0018

(2,3) Couple of 1c.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Thiophenyl Carbazolyl	H46…H182	2.1480	0.0097	0.0402	0.0077	-0.0054	0.0023
		H39…H162	2.2938	0.0073	0.0298	0.0055	-0.0036	0.0019
	Carbazolyl	C161…H57	2.7225	0.0085	0.0287	0.0056	-0.0041	0.0015
	Thiophenyl	S9…C149	3.1742	0.0116	0.0375	0.0077	-0.0061	0.0016
		S35…C116	3.2780	0.0098	0.0332	0.0065	-0.0047	0.0018
		S42…C142	3.0550	0.0144	0.0454	0.0097	-0.0081	0.0016
		S117…C8	3.2874	0.0093	0.0291	0.0059	-0.0046	0.0013
		S143…C34	3.3282	0.0087	0.0267	0.0054	-0.0041	0.0013
		S150…C41	3.3312	0.0086	0.0278	0.0055	-0.0041	0.0014
	Triazine	N5…C109	3.1506	0.0075	0.0247	0.0052	-0.0043	0.0009
Intramolecular interactions	Thiophenyl (S, C) Carbazolyl (H)	S150…H182	2.8589	0.0088	0.0332	0.0064	-0.0046	0.0018
		S42…H74	2.6865	0.0107	0.0394	0.0080	-0.0062	0.0018
		S143…H162	2.8624	0.0085	0.0326	0.0063	-0.0045	0.0018
		S35…H54	2.7283	0.0101	0.0367	0.0074	-0.0056	0.0018
		S117…H132	2.8056	0.0093	0.0353	0.0069	-0.0050	0.0019
		S9…H24	2.7272	0.0102	0.0381	0.0076	-0.0057	0.0019
		C151…H179	2.6520	0.0091	0.0322	0.0063	-0.0046	0.0017
		C36…H57	2.5730	0.0108	0.0431	0.0084	-0.0060	0.0024
		C118…H129	2.5776	0.0110	0.0441	0.0085	-0.0060	0.0025
		C144…H165	2.5334	0.0115	0.0437	0.0086	-0.0063	0.0023
	Thiophenyl Carbazolyl	H13…H21	2.0731	0.0122	0.0502	0.0098	-0.0071	0.0027
		H46…H71	2.0867	0.0123	0.0519	0.0101	-0.0072	0.0029

(2,3) Couple of 2a.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Triazolyl (N) Pheyl (H)	N14…H103	2.5185	0.0112	0.0421	0.0087	-0.0068	0.0019
		N87…H20	2.5514	0.0109	0.0394	0.0080	-0.0062	0.0018
	Phenyl	H29…H103	2.1263	0.0080	0.0330	0.0064	-0.0046	0.0018
		H20…H94	2.2661	0.0066	0.0278	0.0052	-0.0034	0.0018
		H37…H111	2.1649	0.0076	0.0315	0.0060	-0.0042	0.0018
	Methoxy…Phenyl	H24…H124	2.1250	0.0093	0.0367	0.0072	-0.0053	0.0019
	Methoxy	H41…H130	2.1024	0.0098	0.0393	0.0077	-0.0057	0.0020
	Triazine	N5…C75	3.1895	0.0072	0.0238	0.0052	-0.0044	0.0008
		N77…C1	3.1943	0.0074	0.0240	0.0053	-0.0046	0.0007
	Triazol	N10…C79	3.1790	0.0073	0.0240	0.0051	-0.0042	0.0009
Intramolecular interactions	Triazolyl (N) Phenyl (H)	N14…H29	2.6689	0.0100	0.0351	0.0073	-0.0057	0.0016
		N10…H20	2.1607	0.0211	0.0700	0.0164	-0.0154	0.0010
		N12…H37	2.3718	0.0142	0.0502	0.0109	-0.0092	0.0017
		N84…H109	2.0592	0.0255	0.0828	0.0201	-0.0195	0.0006
		N85…H29	2.1689	0.0188	0.0618	0.0145	-0.0136	0.0009
		N83…H37	2.5262	0.0107	0.0376	0.0078	-0.0063	0.0015
		N82…H92	2.1389	0.0219	0.0742	0.0174	-0.0162	0.0012
		N86…H101	2.7555	0.0086	0.0291	0.0060	-0.0047	0.0013
	Methoxy	O43…H48	2.2975	0.0150	0.0543	0.0126	-0.0116	0.0010
		O46…H61	2.2979	0.0150	0.0544	0.0126	-0.0116	0.0010
		O67…H64	2.2990	0.0148	0.0536	0.0125	-0.0115	0.0010
		O115…H120	2.2801	0.0154	0.0560	0.0130	-0.0121	0.0009
		O118…H133	2.2606	0.0161	0.0588	0.0137	-0.0126	0.0011
		O139…H136	2.2369	0.0129	0.0473	0.0109	-0.0099	0.0010

(2,3) Couple of 2b.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Triazine	N2…C112	3.1296	0.0081	0.0278	0.0061	-0.0051	0.0010
		N3…C121	3.1635	0.0080	0.0268	0.0059	-0.0051	0.0008
		N10…C111	3.1434	0.0082	0.0270	0.0059	-0.0050	0.0009
		N109…C5	3.1394	0.0083	0.0280	0.0062	-0.0053	0.0009
		N115…C7	3.1933	0.0072	0.0252	0.0054	-0.0046	0.0008
		N116…C1	3.1543	0.0080	0.0264	0.0058	-0.0049	0.0009
	Triazol…Thiop	N124… C17	3.0956	0.0086	0.0261	0.0057	-0.0048	0.0009
	Triazolyl	N11… C107	3.1279	0.0077	0.0258	0.0055	-0.0045	0.0010
		N127…C8	3.1459	0.0074	0.0249	0.0053	-0.0043	0.0010
Intramolecular interactions	Methoxy	O71…H105	2.4363	0.0119	0.0436	0.0100	-0.0090	0.0009
		O87…H100	2.2982	0.0153	0.0546	0.0128	-0.0119	0.0009
		O64…H76	2.3449	0.0140	0.0502	0.0117	-0.0108	0.0009
		O56…H90	2.4778	0.0106	0.0409	0.0091	-0.0080	0.0011
		O59…H94	2.4169	0.0124	0.0449	0.0103	-0.0094	0.0009
		O67…H82	2.3312	0.0143	0.0517	0.0120	-0.0111	0.0009
		O185…H197	2.3141	0.0153	0.0535	0.0127	-0.0120	0.0007
		O185…H193	2.3015	0.0153	0.0545	0.0128	-0.0119	0.0009
		O181…H206	2.4495	0.0116	0.0427	0.0097	-0.0087	0.0010
		O184…H208	2.4564	0.0110	0.0420	0.0094	-0.0083	0.0011
		O188…H201	2.3704	0.0132	0.0481	0.0111	-0.0101	0.0010
		O148…H178	2.4182	0.0124	0.0450	0.0103	-0.0094	0.0009
		O154…H163	2.3683	0.0137	0.0488	0.0114	-0.0106	0.0008
		O154…H165	2.3061	0.0151	0.0540	0.0126	-0.0117	0.0009
		N11…H36	2.1280	0.0223	0.0722	0.0172	-0.0163	0.0009
		N4…H24	2.1493	0.0215	0.0690	0.0164	-0.0155	0.0009
	Triazolyl (N) Thiophenyl (H)	N117…H119	2.1619	0.0208	0.0669	0.0158	-0.0149	0.0009
		N127…H145	2.1249	0.0224	0.0726	0.0173	-0.0164	0.0009
		N108…H142	2.1384	0.0219	0.0705	0.0168	-0.0159	0.0009
		N14…H27	2.1507	0.0213	0.0689	0.0163	-0.0154	0.0009

(2,3) Couple of 2c.

	Involved Group	Bond (X···Y)	R_{AB} (Å)	ρ_b (au)	$\nabla^2\rho_b$ (au)	G_b (au)	V_b (au)	H_b (au)
Intermolecular interactions	Triazine	N122…C1	3.0967	0.0087	0.0288	0.0063	-0.0055	0.0008
		N123…C2	3.0911	0.0088	0.0290	0.0064	-0.0055	0.0009
		N121…C3	3.1044	0.0085	0.0284	0.0062	-0.0054	0.0008
		N5…C120	3.0888	0.0088	0.0291	0.0064	-0.0055	0.0009
		N4…C119	3.0885	0.0088	0.0291	0.0064	-0.0056	0.0008
		N6…C118	3.0889	0.0087	0.0291	0.0064	-0.0055	0.0009
	Triazolyl	N12…C125	3.1300	0.0079	0.0261	0.0055	-0.0046	0.0009
		N129…C9	3.1599	0.0074	0.0247	0.0052	-0.0043	0.0009
		N127…C8	3.1805	0.0072	0.0240	0.0051	-0.0041	0.0010
		N14…C126	3.1426	0.0077	0.0254	0.0054	-0.0044	0.0010
		N10…C124	3.1240	0.0079	0.0261	0.0056	-0.0046	0.0010
Intramolecular interactions	Triazol (N) Thiophenyl (H)	N12…H32	2.1045	0.0233	0.0753	0.0181	-0.0173	0.0008
		N14…H20	2.0927	0.0239	0.0772	0.0186	-0.0179	0.0007
		N10…H26	2.1138	0.0229	0.0742	0.0177	-0.0169	0.0008
		N129…H149	2.0763	0.0247	0.0792	0.0192	-0.0185	0.0007
		N127…H143	2.0987	0.0236	0.0757	0.0182	-0.0175	0.0007
		N131…H137	2.0760	0.0247	0.0793	0.0192	-0.0186	0.0006
	Thiophenyl (S) Carbazolyl (H)	S18…H62	2.9214	0.0076	0.0272	0.0052	-0.0036	0.0016
		S30…H44	2.9309	0.0075	0.0268	0.0051	-0.0036	0.0015
		S24…H80	2.9272	0.0075	0.0270	0.0052	-0.0036	0.0016
		S147…H161	2.9376	0.0075	0.0273	0.0052	-0.0036	0.0016
		S141…H197	2.9241	0.0076	0.0279	0.0053	-0.0037	0.0016
		S135…H179	2.9207	0.0077	0.0280	0.0054	-0.0037	0.0017