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## Intramolecular Six-Membered and Three-Center C–H···O Hydrogen Bonding in 1,4-Diphenyl-1,2,3-Triazoles

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**ABSTRACT:** This paper reports the first example of the intramolecular three-center C–H···O hydrogen bonding. Nine 1,4-di(2-methoxy and/or *i*-butoxy)phenyl-1,2,3-triazole derivatives, that is, **1–9**, are prepared. The X-ray diffraction studies reveal that **1**, **2**, and **4**, which bear a methoxyl or *i*-butoxyl group on the N-1- or C-4-substituted benzene ring, form a six-membered C–H···O hydrogen bond between the C<sup>5</sup>–H of their triazole unit and the alkoxy O, while **5–8**, which bear two methoxyl and/or *i*-butoxyl groups on the similar benzene rings, form two three-center C–H···O hydrogen bonds. It is also found that in most cases the hydrogen bond on the C-4 side is shorter than that on the N-1 side and both of them can be stabilized by the aromatic stacking and other intermolecular interactions. The (NOESY) <sup>1</sup>H NMR experiments in CDCl<sub>3</sub> and CDCl<sub>3</sub>–DMSO-*d*<sub>6</sub> mixture (4:1) support that both the six-membered and the three-center C–H···O hydrogen bonds also exist in solution.

## Introduction

Hydrogen bonding plays an important role in the conformation, interaction, and recognition of both organic and biological structures.<sup>1,2</sup> Therefore, the evaluation of new hydrogen bonding patterns has attracted considerable interest in several decades. Strong or conventional O–H···O, O–H···N, N–H···O, and N–H···N hydrogen bonds (5–15 kcal/mol) have been well established in as early as the 1940s.<sup>3–5</sup> In the context of weak hydrogen bonding, the landmark study by Taylor and Kennard has stimulated increasing interest in the C–H···O hydrogen bond.<sup>6</sup> Systematic studies by Desiraju and others reveal that this weak interaction is equally important as the conventional analogues in both small-molecule and biological crystallography and molecular recognition.<sup>7–10</sup>

It is well-known that two strong N–H···O or N–H···N hydrogen bonds in aromatic amides could combine together to form stable intramolecular three-center hydrogen bonds, in which one amide H is shared by two acceptor O or N atoms or one acceptor O or N is shared by two amide H atoms.<sup>5</sup> On the basis of this hydrogen bonding pattern, quite a number of folded or extended secondary structures have been constructed from oligomeric aromatic amides.<sup>11,12</sup> Previously, we found that the F atom could also serve as the acceptor to create a similar three-center pattern.<sup>13</sup> Recently, it was reported that 1,4-diarylated 1,2,3-triazole linear and macrocyclic derivatives formed intermolecular C<sup>5</sup>–H···Cl<sup>–</sup> hydrogen bonding<sup>14–16</sup> due to the strong electron-deficient nature of the heterocycle.<sup>17</sup> With the increasing applications of the click chemistry in studies in biological, materials, and supramolecular sciences,<sup>18–20</sup> we became interested in detecting if the C<sup>5</sup>–H atom of 1,2,3-triazole serves as a donor for intramolecular hydrogen bonding because such a hydrogen bonding pattern is potentially useful in tuning the conformation or shape of molecular backbones constructed through the click chemistry. In this paper, we report that both two- and

three-center hydrogen bonds can be formed from alkoxy-substituted derivatives.

## Results and Discussion

A number of 1,2,3-triazole derivatives were prepared. For eight of them, that is, compounds **1–8**, single crystals suitable for the X-ray analysis were grown by slow evaporation of their solution in a suitable solvent at 10 °C. Compound **3**, which cannot form any intramolecular hydrogen bonding, was prepared as a control compound. All the compounds were prepared by the 1,3-dipolar addition of the corresponding azides to phenylacetylenes. The detailed synthesis and characterization are provided in the Supporting Information. The crystal data and structure refinements are summarized in Table 1.

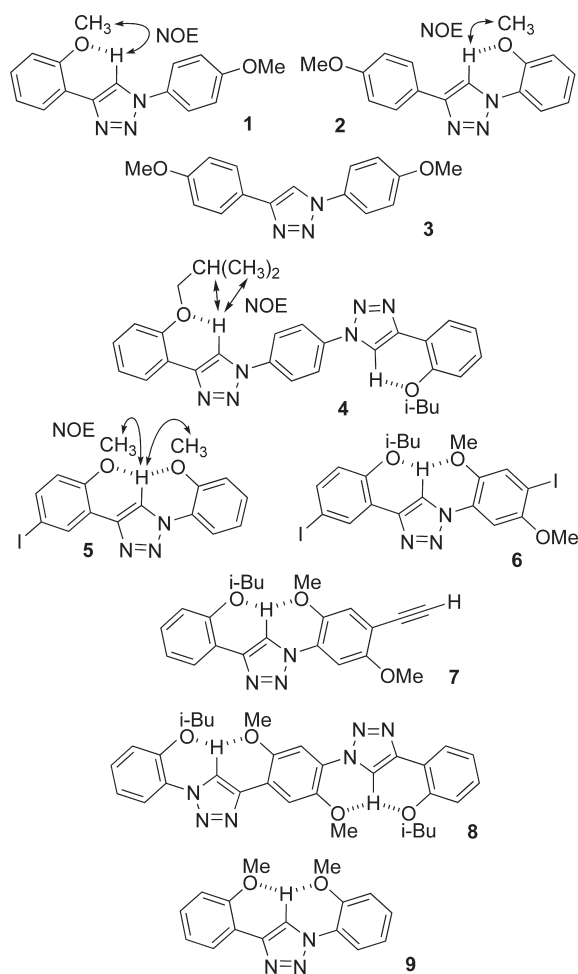
The crystal structures and geometric data of **1–3** are presented in Figures 1–3, respectively. Compound **1** formed a strong six-membered C<sup>5</sup>–H···O hydrogen bond. The H···O distance (*d*) is 2.31 Å, which is significantly shorter than the sum of their van der Waals radii (*d*<sub>0</sub>, 2.72 Å; *d*/*d*<sub>0</sub> = 0.85).<sup>21</sup> The torsion angle of the hydrogen-bonded benzene ring from the triazole unit (2.9°) was remarkably smaller than that of its another benzene ring at N-1 (30.5°) and that (26.3°) of the same benzene ring of its isomer **3** (Figure 3). All these results supported the formation of the intramolecular C<sup>5</sup>–H···O hydrogen bond. The (C<sup>5</sup>)H···O distance (*d*) of **2** (2.54 Å) was longer than that of **1**, but still notably shorter than the sum of the van der Waals radii (*d*/*d*<sub>0</sub> = 0.93) (Figure 2), suggesting the formation of another six-membered C<sup>5</sup>–H···O hydrogen bond. This difference may be ascribed to the fact that the methoxyl oxygen of **2** is weaker as a hydrogen bonding acceptor than that of **1** due to the electron-withdrawing feature of N-1 of the triazole unit. Another factor that might cause this difference is the asymmetric feature of the triazole, as reflected by the different lengths (1.35 and 1.31 Å) of the N<sup>1</sup>–N<sup>2</sup> and N<sup>2</sup>–N<sup>3</sup> bonds. The torsion angle (40.1°) of the benzene ring of **2** at N-1 is larger than that of **1** (30.5°) and **3** (28.7°). This result should not be regarded as evidence that the formation of the C–H···O

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Table 1. The X-ray Data Collection and Structure Analysis Details for Compounds 1–8

compound	1	2	3	4	5	6	7	8
empirical formula	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>	C <sub>30</sub> H <sub>32</sub> N <sub>6</sub> O <sub>2</sub>	C <sub>16</sub> H <sub>14</sub> IN <sub>3</sub> O <sub>2</sub>	C <sub>20</sub> H <sub>21</sub> I <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>	C <sub>32</sub> H <sub>36</sub> N <sub>6</sub> O <sub>4</sub>
formula weight	281.31	281.31	281.31	508.62	407.20	605.20	377.43	568.67
crystal system	monoclinic	monoclinic	monoclinic	triclinic	triclinic	triclinic	triclinic	monoclinic
space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>Cc</i>	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> (Å)	9.632	13.087	31.737	6.006	4.119	9.022	10.5118(11)	4.987
<i>b</i> (Å)	9.8856	7.443	5.651	7.828	7.300	9.367	11.2359(12)	15.866
<i>c</i> (Å)	15.743	14.981	7.619	14.629	13.126	13.897	17.9193(19)	18.134
α (deg)	90	90	90	101.280	95.669	105.905	102.714(2)	90
β (deg)	106.780	108.472	96.54	94.111	90.190	90.768	94.130(2)	96.121
γ (deg)	90	90	90	97.453	92.231	104.24	99.117(2)	90
<i>V</i> (Å <sup>3</sup> )	1434.3	1384.14	1357.5	667.8	392.47	1090.65	2025.9(4)	1426.6
<i>Z</i>	4	4	4	1	1	2	4	2
<i>D</i> <sub>calcd</sub> (g/cm <sup>3</sup> )	1.303	1.350	1.376	1.265	1.723	1.843	1.237	1.324
abs coeff (mm <sup>−1</sup> )	0.088	0.092	0.093	0.082	2.050	2.908	0.084	0.089
temperature (K)	293	293	296	293	293	293	293	293
GOF	1.066	0.979	1.080	0.994	1.049	1.047	0.840	0.962

hydrogen bond in **2** is not favored energetically because their structures and stacking patterns were different, and there also



existed the influence of additional intermolecular weak interactions on the whole molecular conformation in the crystal. For compound **1**, the benzene rings of the neighboring molecules stacked to give rise to a dimeric structure (Figure 1), while for compound **3**, the triazole units stacked. In addition, it also formed weaker intermolecular bifurcated C<sup>5</sup>–H···N<sup>2</sup> and C<sup>5</sup>–H···N<sup>3</sup> interactions.<sup>22</sup> All these interactions, which were not observed for **2**, should promote the coplanarity of the aromatic units of **1** and **3** and favor the formation of the intramolecular C<sup>5</sup>–H···O hydrogen bond in **1**.

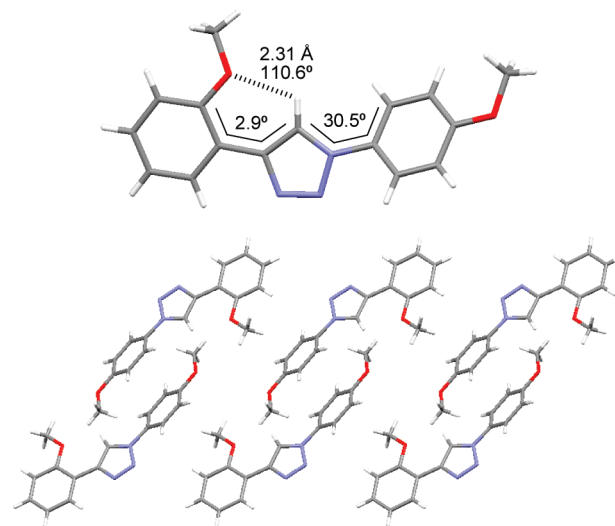


Figure 1. The crystal structure and packing pattern, highlighting the dimeric stacking interaction of the N-1 benzene ring, of compound **1**.

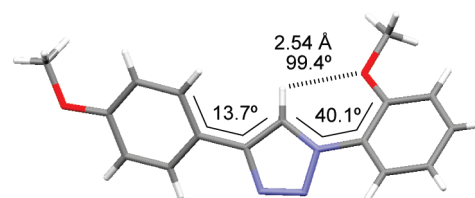
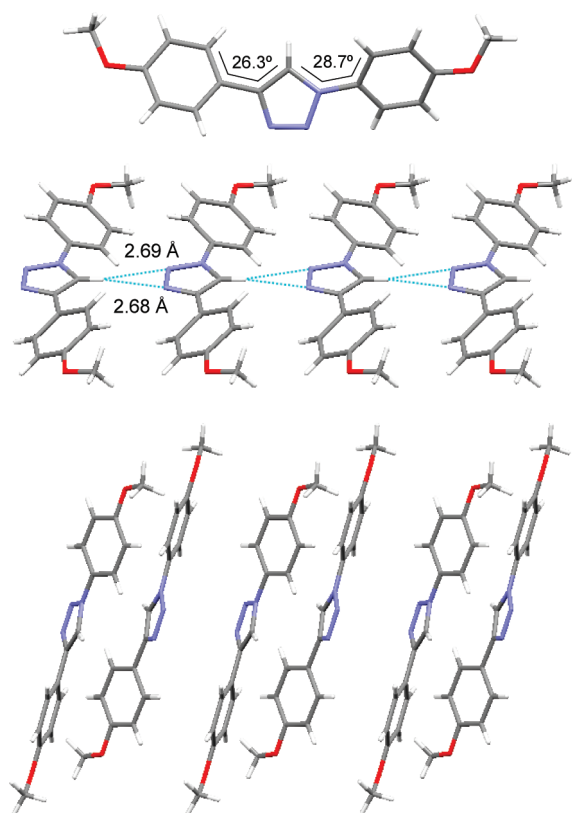


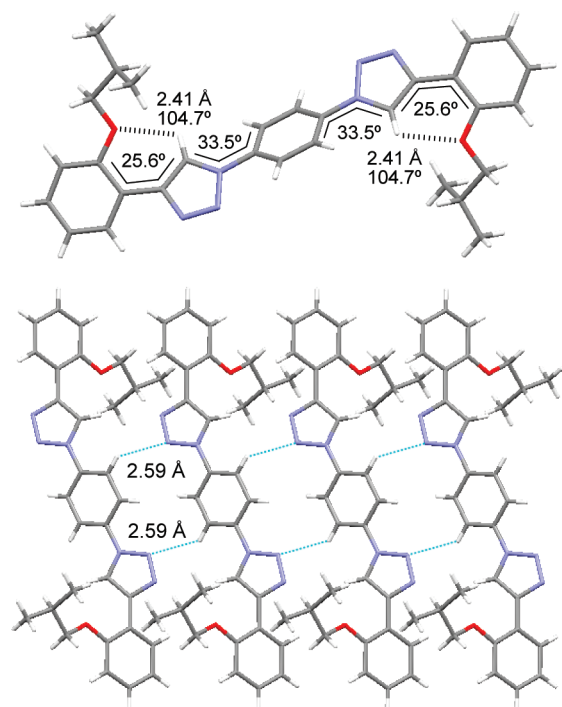
Figure 2. The crystal structure of compound **2**, highlighting a weak intramolecular six-membered C<sup>5</sup>–H···O hydrogen bond.

To get more insight into the factors that affect the stability of the intramolecular C–H···O hydrogen bonding, compound **4** was also prepared. Its crystal structure is shown in Figure 4. Both *i*-butoxyl oxygen atoms formed the expected C–H···O hydrogen bonding (*d* = 2.41 Å), although it is longer than that observed in compound **1**. Possibly owing to the larger *i*-butyl group, no aromatic stacking was observed in the packing structure of **4**. Instead, the central benzene ring formed two intermolecular C–H···N<sup>2</sup> hydrogen bonds. This result implies that this intramolecular C–H···O hydrogen bond may tolerate the introduction of a larger alkoxy group.

Compounds **5** and **6** were then prepared to detect the formation of the three-center C–H···O hydrogen bonding pattern. The crystal structure of their iodine-free analogue **9** is

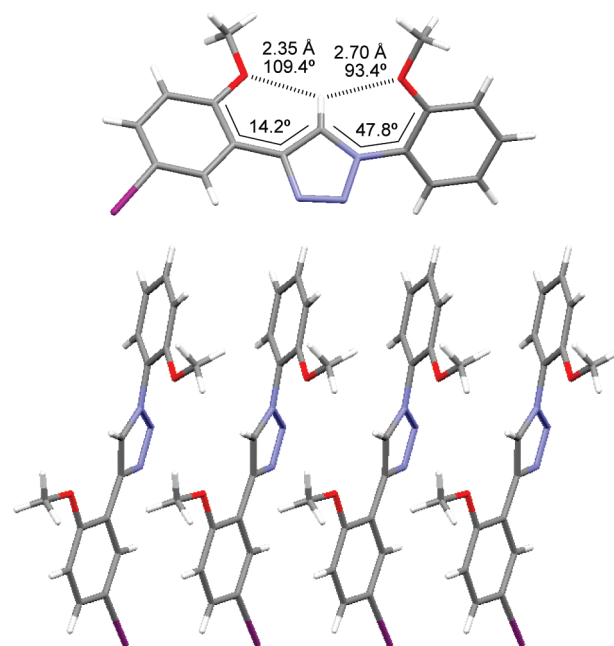


**Figure 3.** The crystal structure and packing patterns, highlighting the intermolecular bifurcated  $C^5-H \cdots N$  and stacking interactions, of compound **3**.



**Figure 4.** The crystal structure and packing pattern of compound **4**, highlighting the intramolecular six-membered  $C^5-H \cdots O$  and intermolecular  $C-H \cdots N^2$  hydrogen bonds.

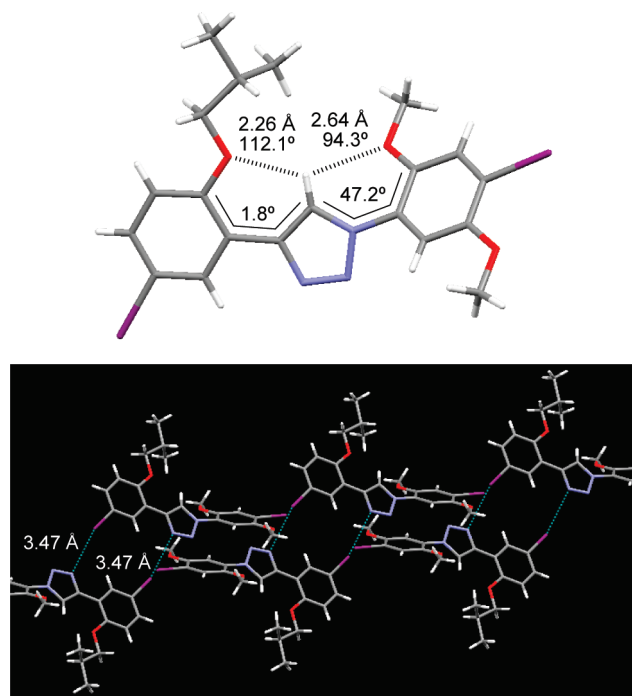
not available at the present stage. The crystal structure of **5** is provided in Figure 5. The intramolecular  $C-H \cdots O$  hydrogen bond ( $d = 2.35 \text{ \AA}$ ) on the C-4 side was still quite strong,



**Figure 5.** The crystal structure and packing pattern of compound **5**, highlighting two three-center  $C^5-H \cdots O$  hydrogen bonds and the stacking of the backbone.

while the  $(C^5)H \cdots O$  distance ( $2.70 \text{ \AA}$ ) on the N-1 side was just slightly shorter than the sum of the van der Waals radii. This result was consistent with the different torsion angles of the two appended benzene rings from the triazole unit ( $14.2$  and  $47.8^\circ$ ). The backbones stacked strongly, which should stabilize the three-center hydrogen bonds. However, the two hydrogen bonds might weaken each other, as observed for the conventional three-center  $N-H \cdots O$  or  $N-H \cdots N$  hydrogen bonding patterns.<sup>5</sup> The crystal structure of compound **6** reflects the complexity of the molecular conformation (Figure 6), which was controlled both intra- and intermolecular interactions. Despite the existence of a large *i*-butyl group, this compound still exhibited the strongest  $C-H \cdots O$  hydrogen bond on the C-4 side ( $d = 2.26 \text{ \AA}$ ,  $d/d_0 = 0.83$ ). The packing pattern revealed that this hydrogen bond was stabilized by two intermolecular  $N^3 \cdots I$  halogen bonds ( $d = 3.47 \text{ \AA}$ ),<sup>23,24</sup> which promoted the coplanarity of the benzene and triazole rings, as evidenced by the smallest torsion angle of the two aromatic rings ( $1.8^\circ$ ). Only the iodine atom on the  $C^4$ -substituted benzene ring formed such halogen bonds, reflecting its geometrical matching with the N-3 atom. The  $C-H \cdots O$  hydrogen bond ( $d = 2.64 \text{ \AA}$ ) on the N-1 side was longer than that on the C-4 side, but slightly shorter than that observed for compound **5**. The  $N^1$ -substituted benzene ring stacked intermolecularly, which might weaken the intramolecular hydrogen bonding by causing the large torsion from the triazole unit.

The crystal structure of **7** gave rise to two conformers (Figure 7), both of which exhibited the expected three-center  $C-H \cdots O$  hydrogen bonding pattern. Remarkably, for both conformers, the  $(C^5)H \cdots O$  distance ( $d = 2.30$  and  $2.34 \text{ \AA}$ ) on the N-1 side was shorter than that ( $d = 2.36$  and  $2.37 \text{ \AA}$ ) on the C-4 side. Consistently, the torsion angle of the benzene ring at N-1 in both conformers was also considerably smaller than that observed for **2**, **5**, and **6**. Clearly, the packing pattern and other intermolecular interactions helped to stabilize the intramolecular  $C-H \cdots O$  hydrogen bond on the N-1 side. The first interaction was the aromatic stacking of the backbones,

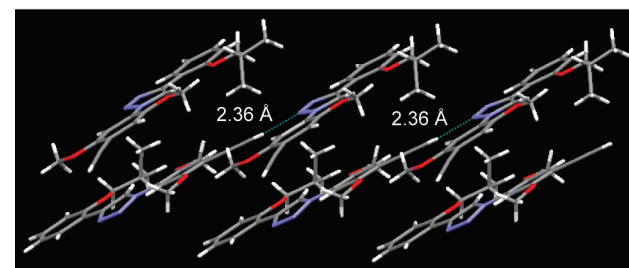
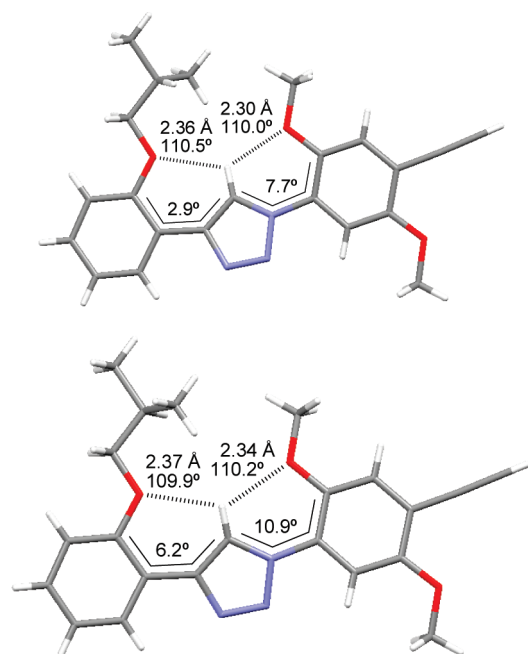


**Figure 6.** The crystal structure and packing pattern of compound **6**, highlighting two intramolecular three-center  $C^5-H\cdots O$  hydrogen bonds and two intermolecular  $N^3\cdots I$  halogen bonds.

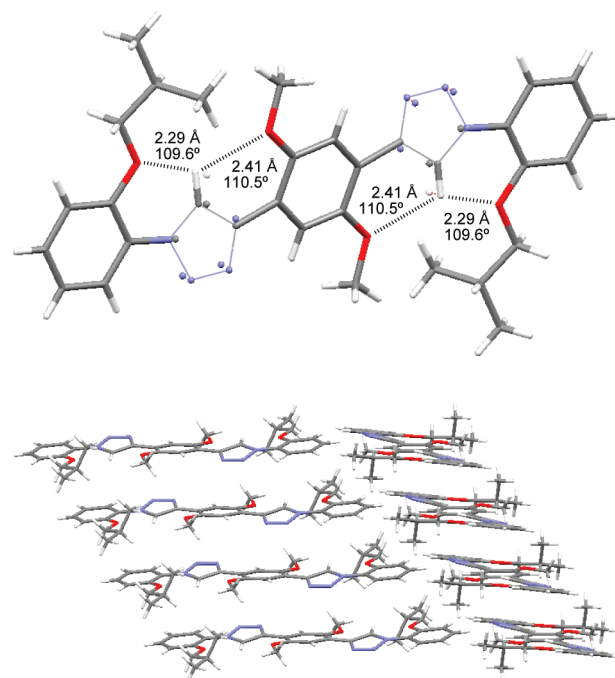
which should reduce the torsion of the benzene rings from the triazole ring. Another interaction is a relatively strong intermolecular  $C-H\cdots N$  hydrogen bond ( $d = 2.36$  Å,  $d/d_0 = 0.86$ ) formed between the acetylene hydrogen of the second conformer and N-2 of the first conformer, which should also reduce the torsion of the appended benzene rings from the triazole unit. This result shows that the relatively weak intramolecular  $C-H\cdots O$  hydrogen bond on the N-1 side may be greatly strengthened by introducing other intermolecular interactions.

To investigate the scope of this new three-center  $C-H\cdots O$  hydrogen bonding pattern, compound **8**, which contains two sets of 1,4-diphenyltriazole units, was prepared. The X-ray diffraction analysis showed that the two triazole units were disordered, which may be attributed to the alternate arrangement of the molecules in the packing structure, which was possible because the conformation of the molecule was quite symmetric (Figure 8).<sup>25</sup> Nevertheless, both ( $C^5$ )H atoms formed stable three-center  $C-H\cdots O$  hydrogen bonds with identical bonding distances and angles (Figure 8). The aromatic backbones stacked in two different directions, which should considerably stabilized the intramolecular hydrogen bonding. The whole backbone is straight and planar, reminiscent of the straight secondary structures formed by aromatic amide oligomers that are induced by three-center  $N-H\cdots O$  or  $N-H\cdots N$  hydrogen bonds.<sup>26</sup>

The  $^1H$  NMR spectra of compounds **9** and **1–3** in  $CDCl_3$  (10 mM) exhibited the signals of the ( $C^5$ )H atoms at 8.52, 8.39, 8.24, and 8.03 ppm, respectively. Compared to that of **3**, the signals of **9**, **1**, and **2** all shifted downfield pronouncedly, indicating the formation of the intramolecular six-membered  $C-H\cdots O$  hydrogen bonding, while the largest chemical shift of **9** well supported the formation of the three-center hydrogen bonding pattern. Compared to that in  $CDCl_3$ , the signal of the hydrogen atom on C-5 of **9** and **1–3** (5 mM) in the  $^1H$  NMR spectra in  $CDCl_3$  and DMSO- $d_6$  mixture (4:1 v/v) shifted

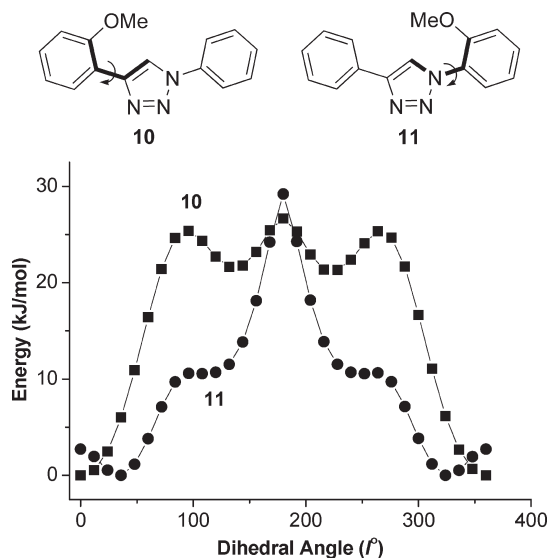


**Figure 7.** The crystal structures, with two conformational isomers, and packing pattern of compound **7**, highlighting the intramolecular three-center  $C^5-H\cdots O$  hydrogen bonds and intermolecular  $C\equiv C-H\cdots N^2$  hydrogen bond.



**Figure 8.** The crystal structure and packing pattern of compound **8**.





**Figure 9.** The torsion energies of **10** and **11** calculated at the 6-31G\*\* level using B3LYP method (the minimum calculated potential energy was set to zero).

downfield by 0.03, 0.08, 0.10, and 0.31 ppm, respectively. The smaller values observed for **9**, **1**, and **2** further supported that the hydrogen atom was engaged in the intramolecular hydrogen bonding and therefore less sensitive to the increase of the polarity of the solvent. 2D NOESY spectra of **1**, **2**, **4**, and **5** in CDCl<sub>3</sub> (10 mM) also exhibited NOE contacts between the (C<sup>5</sup>)H atom and the CH<sub>3</sub> and CH (for *i*-butyl) hydrogen atoms but not the H-6 atom on the appended benzene rings, which also evidenced the formation of the hydrogen bonding.

To get insight into the factors that control the low energy conformations for the formation of the new C—H···O hydrogen bonds, the quantum calculations were further performed for model compounds **10** and **11**. Their energy profiles at different rotations of the related C—C and C—N bonds (see the structures) were obtained.<sup>27</sup> As shown in Figure 9, for both molecules, all the conformations at about 90° (270°) and 180° had a high energy peak or shoulder, indicating that the conjugation of the two related aromatic units and the electrostatic repulsion between their O and N<sup>3</sup> (for **10**) or N<sup>2</sup> (for **11**) atoms should also contribute to the formation of the above hydrogen bonds. It is expected that the former increased the coplanarity of the two adjacent sp<sup>2</sup> systems, while the latter helped to push the O atom to the C<sup>5</sup> side of triazole.

### Conclusion

We have demonstrated that 1,4-diphenyl-1,2,3-triazole derivatives can form relatively stable intramolecular six-membered and three-center C<sup>5</sup>—H···O hydrogen bonds. Previously, aromatic amides-based three-center hydrogen bonding patterns has been well established. The present work extends this concept by using 1,2,3-triazole as a hydrogen bonding donor. One potential application of this new hydrogen bonding pattern is to design new folded or extended structures by constructing similar diphenyl-1,2,3-triazole oligomers. In this way, multiple triazole units may be orientated convergently to bind linear guests through intermolecular hydrogen bonding. Replacement of the simple alkyl groups with suitable peptide chains may also create linear backbones in which the peptide chains bind to form sheet-like structures.

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**Supporting Information Available:** Detailed synthesis and characterizations, the calculation method, and (NOESY) <sup>1</sup>H NMR spectra and CIF files of compounds **1–8**. This information is available free of charge via the Internet at <http://pubs.acs.org/>.

### References

- (1) (a) Jeffrey, G. A.; Saenger, W. *Hydrogen Bonding in Biological Structures*; Springer-Verlag: Berlin, 1991. (b) Jeffrey, G. A. *An Introduction to Hydrogen Bonding*; Oxford University Press: New York, 1997.
- (2) (a) Nangia, A. *CrystEngComm* **2002**, *4*, 93–101. G. R. (b) Biradha, K. *CrystEngComm* **2003**, *5*, 374–384. (c) Desiraju, G. R. *Angew. Chem., Int. Ed.* **2007**, *46*, 8342–8356.
- (3) Pauling, L.; Delbruck, M. *Science* **1940**, *92*, 77–79.
- (4) (a) Gellman, S. H. *Acc. Chem. Res.* **1998**, *31*, 173–180. (b) Seebach, D.; Matthews, J. L. *Chem. Commun.* **1997**, 2015–2022. (c) Licini, G.; Prins, L. J.; Scrimin, P. *Eur. J. Org. Chem.* **2005**, 969–977.
- (5) (d) Goodman, C. M.; Choi, S.; Shandler, S.; DeGrado, W. F. *Nature Chem. Biol.* **2007**, *3*, 252–262. (e) Li, X.; Wu, Y.-D.; Yang, D. *Acc. Chem. Res.* **2008**, *41*, 1428–1438. (f) Wu, Y.-D.; Han, W.; Wang, D.-P.; Gao, Y.; Zhao, Y.-L. *Acc. Chem. Res.* **2008**, *41*, 1418–1427. (g) Saraghi, I.; Hamilton, A. D. *Chem. Soc. Rev.* **2009**, *38*, 1726–1743.
- (6) Gong, B. *Chem.—Eur. J.* **2001**, *7*, 4336–4342. (b) Huc, I. *Eur. J. Org. Chem.* **2004**, 17–29. (c) Li, Z.-T.; Hou, J.-L.; Li, C.; Yi, H.-P. *Chem.—Asian J.* **2006**, *1*, 766–778.
- (7) Taylor, R.; Kennard, O. J. *Am. Chem. Soc.* **1982**, *104*, 5063–5070.
- (8) Desiraju, G. R.; Steiner, T. *The Weak Hydrogen Bond in Structural Chemistry and Biology*; Oxford University Press: Oxford, 1999.
- (9) (a) Desiraju, G. R. *Acc. Chem. Res.* **1991**, *24*, 270–276. (b) Desiraju, G. R. *Acc. Chem. Res.* **1996**, *29*, 441–449. (c) Desiraju, G. R. *Acc. Chem. Res.* **2002**, *35*, 565–573. (d) Desiraju, G. R. *Chem. Comm.* **2005**, 2995–3001.
- (10) (a) Steiner, T. *Crystallogr. Rev.* **1996**, *6*, 1–51. (b) Wahl, M. C.; Sundaralingam, M. *Trends Biochem. Sci.* **1997**, *22*, 97–102.
- (11) Hunter, C. A. *Angew. Chem., Int. Ed.* **2004**, *43*, 5310–5324.
- (12) (a) Gong, B. *Acc. Chem. Res.* **2008**, *41*, 1376–1386. (b) Li, Z.-T.; Hou, J.-L.; Li, C. *Acc. Chem. Res.* **2008**, *41*, 1343–1353.
- (13) Bao, C.; Kauffmann, B.; Gan, Q.; Srinivas, K.; Jiang, H.; Huc, I. *Angew. Chem., Int. Ed.* **2008**, *47*, 4153–4156.
- (14) (a) Li, C.; Ren, S.-F.; Hou, J.-L.; Yi, H.-P.; Zhu, S.-Z.; Jiang, X.-K.; Li, Z.-T. *Angew. Chem., Int. Ed.* **2005**, *44*, 5725–5729. (b) Li, C.; Zhu, Y.-Y.; Yi, H.-P.; Li, C.-Z.; Jiang, X.-K.; Li, Z.-T. *Chem.—Eur. J.* **2007**, *13*, 9990–9998. (c) Zhu, Y.-Y.; Wu, J.; Li, C.; Zhu, J.; Hou, J.-L.; Li, C.-Z.; Jiang, X.-K.; Li, Z.-T. *Cryst. Growth Des.* **2007**, *7*, 1490–1496.
- (15) (a) Li, Y.; Flood, A. H. *Angew. Chem., Int. Ed.* **2008**, *47*, 2649–2652. (b) Li, Y.; Pink, M.; Karty, J. A.; Flood, A. H. *J. Am. Chem. Soc.* **2008**, *130*, 17293–17295. (c) Li, Y.; Flood, A. H. *J. Am. Chem. Soc.* **2008**, *130*, 12111–12122. (d) Li, Y.; Griend, D. A. V.; Flood, A. H. *Supramol. Chem.* **2009**, *21*, 111–117.
- (16) Juwarker, H.; Lenhardt, J. M.; Pham, D. M.; Craig, S. L. *Angew. Chem., Int. Ed.* **2008**, *47*, 3740–3743.
- (17) Hecht, S.; Meudtner, R. M. *Angew. Chem., Int. Ed.* **2008**, *47*, 4926–4930.
- (18) (a) Palmer, M. H.; Findlay, R. H.; Gaskell, A. J. *J. Chem. Soc., Perkin Trans. 2* **1974**, 420–428. (b) Horne, W. S.; Yadav, M. K.; Stout, C. D.; Ghadiri, M. R. *J. Am. Chem. Soc.* **2004**, *126*, 15366–15367.
- (19) (a) Angell, Y. L.; Burgess, K. *Chem. Soc. Rev.* **2007**, *36*, 1674–1689. (b) Weisbrod, S. H.; Marx, A. *Chem. Commun.* **2008**, 5675–5685. (c) Park, S.; Lee, M.-R.; Shin, I. *Chem. Soc. Rev.* **2008**, *37*, 1579–1591.
- (20) (a) Nandivada, H.; Jiang, X.; Lahann, J. *Adv. Mater.* **2007**, *19*, 2197–2208. (b) Lutz, J.-F. *Angew. Chem., Int. Ed.* **2007**, *46*, 1018–1025.
- (21) (a) Fournier, D.; Hoogenboom, R.; Schubert, U. S. *Chem. Soc. Rev.* **2007**, *36*, 1369–1380. (b) Lutz, J.-F. *Angew. Chem., Int. Ed.* **2008**, *47*, 2182–2184. (c) Franc, G.; Kakkar, A. *Chem. Commun.* **2008**,

- 5267–5276. (d) Meudtner, R. M.; Ostermeier, M.; Goddard, R.; Limberg, C.; Hecht, S. *Chem.–Eur. J.* **2007**, *13*, 9834–9840.
- (21) Bondi, A. *J. Phys. Chem.* **1964**, *68*, 441–451.
- (22) Low, J. N.; Cobo, J.; Noguera, M.; Sanchez, A.; Cuervo, P. A.; Abonia, R. *Acta Crystallogr.* **2002**, *E58*, o769–o771.
- (23) Metrangolo, P.; Meyer, F.; Pilati, T.; Resnati, G.; Terraneo, G. *Angew. Chem., Int. Ed.* **2008**, *47*, 6114–6127.
- (24) (a) Aakeroy, C. B.; Fasulo, M.; Schultheiss, N.; Desper, J.; Moore, C. *J. Am. Chem. Soc.* **2007**, *129*, 13772–13773. (b) Du, P.; Jiang, X.-K.; Li, Z.-T. *Tetrahedron Lett.* **2009**, *50*, 316–319.
- (25) (a) Flippen-Anderson, J. L.; Deschamps, J. R.; Gilardi, R. D.; George, C. *Cryst. Eng.* **2001**, *4*, 131–139. (b) Zhu, J.; Lin, J.-B.; Xu, Y.-X.; Shao, X.-B.; Jiang, X.-K.; Li, Z.-T. *J. Am. Chem. Soc.* **2006**, *128*, 12307–12313.
- (26) (a) Ernst, J. T.; Becerril, J.; Park, H. S.; Yin, H.; Hamilton, A. D. *Angew. Chem., Int. Ed.* **2003**, *42*, 535–539. (b) Wu, Z.-Q.; Jiang, X.-K.; Zhu, S.-Z.; Li, Z.-T. *Org. Lett.* **2004**, *6*, 229–232.
- (27) Delsuc, N.; Kawanami, T.; Julien Lefevre, J.; Shundo, A.; Ihara, H.; Takafuji, M.; Huc, I. *ChemPhysChem* **2008**, *9*, 1882–1890.