N-Alkylthienopyrroledione versus Benzothiadiazole Pulling Units in Push-Pull Copolymers Used for Photovoltaic Applications: Density Functional Theory Study

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Electronic Supplementary Information (ESI)

Experimental values of the HOMO energy levels (E_{HOMO}) and the band gaps (E_g) of 1-6

The HOMO energy levels (E_{HOMO}; in eV) from the DFT calculations on the dimer models of **1**-**6** in $CHCl_3$ are shown in Table 1 and Fig. 3a (red marks; -4.99, -4.95, -5.09, -5.21, -5.17, and -5.29) along with a collection of the experimental values from the cyclic voltammetry (CV) [black bars; -4.9, -5.3, -5.12, and -5.33 (**1**);[1-5] -4.65, -4.81, -4.86, -4.89, and -4.94 (**2**);[6-8] -5.05, -5.3, and -5.36 (**3**);[5,9,10] -5.08, -5.12, -5.2, -5.24, -5.26, -5.29, and -5.43 (**4**);[11-15] -5.09, -5.11, and -5.16 (**5**);[11,16,17] -5.33, -5.37, -5.44, -5.52, -5.57 and -5.65 (**6**);[11,18-21] The last two values for **6**,[18,19] which are converted from the oxidation onset potential (E_{ox}) using a different formula (E_{HOMO} = -E_{ox} - 5.12) from the one used for all the others (E_{HOMO} = -E_{ox} - 4.8), are excluded from the comparison.[22,23]

The experimental band gaps E_g (eV) estimated from the positions (nm) of the high- and low-energy shoulders of the lowest-energy UV/vis absorption peak (*intrinsic* band gap of a polymer chain versus *thin-film* band gap of a π-stacked phase) are summarized in Fig. 3b (black versus green bars) and in Table 1: 1.70-1.80 (690-730) vs. 1.60-1.65 (750-790) for **1**;[1,2,4,5,24-27] 1.62-1.81 (684-765) vs. 1.60-1.76 (706-777) for **2**;[6-8] 1.77-1.85 (670-700) vs. 1.57-1.80 (690-790) for **3**;[5,9,10,28-30] 1.76-2.05 (604-705) vs. 1.77-1.85 (670-701) for **4**;[11-15] 1.92-2.11 (588-645) vs. 1.81-2.07 (598-686) for **5**;[11,16,17] 1.84-2.04 (608-673) vs. 1.85-1.86 (665-671) for **6**.[11,18-21,31]

1 J. Y. Kim, K. Lee, N. E. Coates, D. Moses, T.-Q. Nguyen, M. Dante and A. J. Heeger, *Science*, 2007, **317**, 222.
2 D. Muhlbacher, M. Scharber, M. Morana, Z. Zhu, D. Waller, R. Gaudiana and C. Brabec, *Adv. Mater.*, 2006, **18**, 2884.
3 M. Koppe, H.-J. Egelhaaf, G. Dennler, M. C. Scharber, C. J. Brabec, P. Schilinsky and C. N. Hoth, *Adv. Funct. Mater.*, 2010, **20**, 338.
4 Z. Zhu, D. Waller, R. Gaudiana, M. Morana, D. Muhlbacher, M. Scharber and C. Brabec, *Macromolecules*, 2007, **40**, 1981.
5 R. C. Coffin, J. Peet, J. T. Rogers and G. C. Bazan, *Nature Chem.*, 2009, **1**, 657.
6 S. Zhang, Y. Guo, H. Fan, Y. Liu, H.-Y. Chen, G. Yang, X. Zhan, Y. Liu, Y. Li and Y. Yang, *J. Polym. Sci., Part A: Polym. Chem.*, 2009, **47**, 5498.
7 W. Yue, Y. Zhao, S. Shao, H. Tian, Z. Xie, Y. Geng and F. Wang, *J. Mater. Chem.*, 2009, **19**, 2199.
8 S. C. Price, A. C. Stuart and W. You, *Macromolecules*, 2009, **43**, 797.
9 J. Hou, H.-Y. Chen, S. Zhang, G. Li and Y. Yang, *J. Am. Chem. Soc.*, 2008, **130**, 16144.
10 M. C. Scharber, M. Koppe, J. Gao, F. Cordella, M. A. Loi, P. Denk, M. Morana, H.-J. Egelhaaf, K. Forberich, G. Dennler, R. Gaudiana, D. Waller, Z. Zhu, X. Shi and C. J. Brabec, *Adv. Mater.*, 2010, **22**, 367.
11 Y. Zhang, J. Zou, H.-L. Yip, Y. Sun, J. A. Davies, K.-S. Chen, O. Acton and A. K.-Y. Jen, *J. Mater. Chem.*, 2011, **21**, 3895.
12 Z. Li, S.-W. Tsang, X. Du, L. Scoles, G. Robertson, Y. Zhang, F. Toll, Y. Tao, J. Lu and J. Ding, *Adv. Funct. Mater.*, 2011, **21**, 3331.
13 X. Guo, H. Xin, F. S. Kim, A. D. T. Liyanage, S. A. Jenekhe and M. D. Watson, *Macromolecules*, 2011, **44**, 269.
14 C. M. MacNeill, E. D. Peterson, R. E. Noftle, D. L. Carroll and R. C. Coffin, *Synth. Met.*, 2011, **161**, 1137.
15 Z. Lin, J. Bjorgaard, A. G. Yavuz, A. Iyer and M. E. Kose, *RSC Adv.*, 2012, **2**, 642.
16 E. Zhou, J. Cong, K. Tajima, C. Yang and K. Hashimoto, *Macromol. Chem. Phys.*, 2011, **212**, 305.
17 X. Hu, M. Shi, L. Zuo, Y. Nan, Y. Liu, L. Fu and H. Chen, *Polymer*, 2011, **52**, 2559.
18 T.-Y. Chu, J. Lu, S. Beaupre, Y. Zhang, J.-R. Pouliot, S. Wakim, J. Zhou, M. Leclerc, Z. Li, J. Ding and Y. Tao, *J. Am. Chem. Soc.*, 2011, **133**, 4250.
19 C. M. Amb, S. Chen, K. R. Graham, J. Subbiah, C. E. Small, F. So and J. R. Reynolds, *J. Am. Chem. Soc.*, 2011, **133**, 10062.
20 Y.-R. Hong, H.-K. Wong, L. C. H. Moh, H.-S. Tan and Z.-K. Chen, *Chem. Commun.*, 2011, **47**, 4920.
21 X. Guo, N. Zhou, S. J. Lou, J. W. Hennek, R. P. Ortiz, M. R. Butler, P.-L. T. Boudreault, J. Strzalka, P.-O. Morin, M. Leclerc, J. T. L. Navarrete, M. A. Ratner, L. X. Chen, R. P. H. Chang, A. Facchetti and T. J. Marks, *J. Am. Chem. Soc.*, 2012, **134**, 18427.
22 C. M. Cardona, W. Li, A. E. Kaifer, D. Stockdale and G. C. Bazan, *Adv. Mater.*, 2011, **23**, 2367.
23 L. E. Polander, L. Pandey, S. Barlow, S. P. Tiwari, C. Risko, B. Kippelen, J.-L. Bredas and S. R. Marder, *J. Phys. Chem. C*, 2011, **115**, 23149.
24 I. W. Hwang, C. Soci, D. Moses, Z. Zhu, D. Waller, R. Gaudiana, C. J. Brabec and A. J. Heeger, *Adv. Mater.*, 2007, **19**, 2307.
25 I. W. Hwang, S. Cho, J. Y. Kim, K. Lee, N. Coates, D. Moses and A. J. Heeger, *J. Appl. Phys.*, 2008, **104**, 033706.
26 C. Soci, I. W. Hwang, D. Moses, Z. Zhu, D. Waller, R. Gaudiana, C. J. Brabec and A. J. Heeger, *Adv. Funct. Mater.*, 2007, **17**, 632.
27 M. Zhang, H. N. Tsao, W. Pisula, C. Yang, A. K. Mishra and K. Mullen, *J. Am. Chem. Soc.*, 2007, **129**, 3472.
28 H.-Y. Chen, J. Hou, A. E. Hayden, H. Yang, K. N. Houk and Y. Yang, *Adv. Mater.*, 2010, **22**, 371.
29 M. Tong, S. Cho, J. T. Rogers, K. Schmidt, B. B. Y. Hsu, D. Moses, R. C. Coffin, E. J. Kramer, G. C. Bazan and A. J. Heeger, *Adv. Funct. Mater.*, 2010, **20**, 3959.
30 P. M. Beaujuge, C. M. Amb and J. R. Reynolds, *Acc. Chem. Res.*, 2010, **43**, 1396.
31 E. Iizuka, M. Wakioka and F. Ozawa, *Macromolecules*, 2015, **48**, 2989.

Table S1. Cartesian coordinates (Å) of the DFT optimized structures: the 2-unit models of **1**-**3**.

1		x (Å)	y (Å)	z (Å)	**2**		x (Å)	y (Å)	z (Å)	**3**		x (Å)	y (Å)	z (Å)
C	1	4.015938	1.842031	-0.051031	C	1	-9.353063	2.357998	0.021003	Si	1	9.361064	0.676925	-0.032995
C	2	2.696940	1.072028	-0.019031	N	2	-9.013058	0.945999	-0.041997	C	2	9.873053	-1.147078	-0.038995
C	3	1.330939	1.404024	-0.039031	C	3	-7.738056	0.408005	-0.016997	C	3	8.715048	-1.914071	-0.031995
C	4	0.497942	0.294021	0.009969	C	4	-6.422058	0.918010	-0.020997	S	4	9.051037	-3.619073	-0.037995
S	5	1.458946	-1.202976	0.088969	C	5	-5.473054	-0.086986	-0.004997	C	5	10.764039	-3.304084	-0.049995
C	6	2.924944	-0.292972	0.047969	C	6	-4.027054	0.018020	-0.004997	C	6	11.040048	-1.963086	-0.049995
C	7	4.337944	-0.532968	0.070969	C	7	-3.331059	1.283022	-0.009997	H	7	12.053050	-1.580092	-0.055995
S	8	5.419948	-1.875965	0.142969	N	8	-3.903064	2.488020	-0.012997	H	8	11.452034	-4.136088	-0.056995
C	9	6.820945	-0.780961	0.103969	S	9	-2.707068	3.606025	-0.017997	C	9	7.457053	-1.192063	-0.020995
C	10	6.405941	0.540038	0.029969	N	10	-1.414064	2.601030	-0.014997	S	10	5.824049	-1.772053	-0.009995
C	11	5.005941	0.680034	0.013969	C	11	-1.873059	1.349028	-0.009997	C	11	5.195059	-0.114049	-0.002995
H	12	7.113939	1.354040	-0.010031	C	12	-1.066055	0.153032	-0.005997	C	12	6.246065	0.788944	-0.009995
C	13	8.168947	-1.323957	0.159969	C	13	-1.791050	-1.030971	-0.000997	C	13	7.529061	0.193936	-0.019995
C	14	9.338944	-0.504954	-0.062031	C	14	-3.197049	-1.094977	0.000003	H	14	6.068072	1.852946	-0.006995
N	15	9.357941	0.801046	-0.340031	H	15	-3.640045	-2.083979	0.003003	C	15	3.762061	0.121960	0.007005
S	16	10.928939	1.243050	-0.501031	H	16	-1.261046	-1.975969	0.004003	C	16	3.186069	1.444964	0.015005
N	17	11.647943	-0.202948	-0.228031	C	17	0.383945	0.179037	-0.008997	N	17	3.866076	2.591959	0.013005
C	18	10.669946	-1.086950	0.000969	S	18	1.289952	-1.364959	-0.018997	S	18	2.778084	3.814966	0.023005
C	19	10.850950	-2.466950	0.277969	C	19	2.801948	-0.507953	-0.010997	N	19	1.398078	2.933975	0.030005
C	20	9.725952	-3.219953	0.482969	C	20	4.190949	-0.709947	-0.009997	C	20	1.741070	1.644973	0.025005
C	21	8.420950	-2.659957	0.428969	S	21	5.395954	-1.961942	-0.016997	C	21	0.828063	0.527978	0.028005
H	22	7.587952	-3.326959	0.618969	C	22	6.702949	-0.740937	-0.006997	C	22	1.440056	-0.717025	0.021005
H	23	9.817955	-4.276953	0.700969	C	23	8.090951	-1.175931	-0.003997	C	23	2.835054	-0.910034	0.011005
H	24	11.847951	-2.884947	0.321969	C	24	9.195947	-0.242927	0.005003	H	24	3.184048	-1.936036	0.006005
C	25	-0.950058	0.223017	0.000969	N	25	9.115942	1.089073	0.013003	H	25	0.825050	-1.609022	0.023005
C	26	-1.791061	1.393015	0.060969	S	26	10.649939	1.671079	0.021003	C	26	-0.614936	0.689987	0.037005
N	27	-1.368065	2.656016	0.127969	N	27	11.475945	0.257082	0.016003	S	27	-1.670944	-0.734006	0.036005
S	28	-2.689067	3.621013	0.177969	C	28	10.567949	-0.724921	0.007003	C	28	-3.084938	0.269003	0.048005
N	29	-3.853064	2.471009	0.115969	C	29	10.854955	-2.114920	0.000003	C	29	-2.775930	1.625001	0.053005
C	30	-3.246061	1.285011	0.055969	C	30	9.789958	-2.974924	-0.007997	Si	30	-4.404924	2.594011	0.065005
C	31	-3.905057	0.002009	-0.010031	C	31	8.445956	-2.515930	-0.009997	C	31	-5.393934	0.977017	0.061005
C	32	-5.348057	-0.140995	-0.017031	H	32	7.666959	-3.268933	-0.016997	C	32	-4.487940	-0.077988	0.053005
S	33	-6.076052	-1.754997	-0.214031	H	33	9.962962	-4.044924	-0.013997	S	33	-5.269950	-1.624983	0.043005
C	34	-7.661054	-1.081001	-0.107031	H	34	11.880956	-2.456916	0.001003	C	34	-6.866945	-0.857973	0.057005
C	35	-9.026053	-1.531005	-0.146031	C	35	6.198944	0.546061	-0.000997	C	35	-6.730937	0.520026	0.061005
S	36	-9.902049	-3.013008	-0.320031	C	36	4.788944	0.563055	-0.006997	H	36	-7.595933	1.166031	0.065005
C	37	-11.415051	-2.147012	-0.191031	N	37	3.807940	1.537051	-0.019997	C	37	-8.071950	-1.674966	0.067005
C	38	-11.237055	-0.797011	-0.023031	C	38	2.591943	0.883046	-0.007997	C	38	-9.393947	-1.100958	-0.060995
C	39	-9.865056	-0.441007	0.001969	C	39	1.234941	1.269041	-0.003997	N	39	-9.692939	0.192044	-0.200995
C	40	-9.060060	0.847995	0.154969	H	40	0.866937	2.283039	0.005003	S	40	-11.324938	0.307055	-0.303995
C	41	-7.639058	0.291999	0.065969	C	41	4.015934	2.974052	0.071003	N	41	-11.717948	-1.276943	-0.175995
C	42	-6.337059	0.823002	0.114969	H	42	3.212932	3.491049	-0.454997	C	42	-10.571952	-1.952950	-0.047995
H	43	-6.093062	1.867003	0.241969	H	43	4.960933	3.233056	-0.405997	C	43	-10.453961	-3.361951	0.089005
C	44	-9.319061	1.517994	1.521969	H	44	4.036933	3.311052	1.112003	C	44	-9.191964	-3.876959	0.207005
H	45	-9.114059	0.826995	2.342969	H	45	6.840940	1.412064	0.008003	C	45	-8.033959	-3.053966	0.199005
H	46	-8.680064	2.395996	1.642969	S	46	-6.235047	-1.706989	0.017003	H	46	-7.074962	-3.546972	0.308005
H	47	-10.361062	1.841991	1.596969	C	47	-7.819050	-0.993996	0.009003	H	47	-9.054971	-4.946960	0.315005
C	48	-9.352062	1.837994	-0.992031	C	48	-9.188049	-1.326001	0.014003	H	48	-11.339965	-3.980945	0.097005
H	49	-10.394063	2.168991	-0.956031	S	49	-10.277043	-2.684006	0.032003	C	49	-4.652917	3.617013	1.623005
H	50	-9.171061	1.375994	-1.965031	C	50	-11.655047	-1.594011	0.017003	H	50	-5.664915	4.030019	1.654005
H	51	-8.713065	2.720996	-0.906031	C	51	-11.312053	-0.272010	-0.002997	H	51	-4.501921	3.012012	2.521005
H	52	-12.064057	-0.106014	0.074969	C	52	-9.898053	-0.114004	-0.008997	H	52	-3.946912	4.452008	1.650005
H	53	-12.340050	-2.700014	-0.248031	H	53	-12.037056	0.529987	-0.010997	C	53	-4.665917	3.631013	-1.480995
C	54	-3.043054	-1.084988	-0.065031	H	54	-12.647046	-2.018015	0.027003	H	54	-5.678915	4.044019	-1.499995
C	55	-1.640054	-0.979985	-0.064031	H	55	-6.151062	1.962011	-0.032997	H	55	-3.960912	4.467008	-1.505995
H	56	-1.082052	-1.907983	-0.120031	H	56	-10.307064	2.523994	-0.478997	H	56	-4.522921	3.035012	-2.384995
H	57	-3.457051	-2.084990	-0.113031	H	57	-8.589066	2.938001	-0.497997	C	57	-1.380928	1.845992	0.047005
H	58	0.932936	2.406023	-0.085031	H	58	-9.426065	2.708998	1.055003	H	58	-0.917922	2.820989	0.050005
C	59	4.154935	2.775032	1.170969						C	59	9.901070	1.597922	1.515005
H	60	4.048937	2.219031	2.103969						H	60	9.453076	2.595924	1.544005
H	61	5.133934	3.263034	1.167969						H	61	9.602067	1.061923	2.418005
H	62	3.387933	3.553029	1.143969						H	62	10.989071	1.717915	1.532005
C	63	4.170935	2.644032	-1.361031						C	63	9.879070	1.600922	-1.586995
H	64	3.405933	3.422029	-1.424031						H	64	9.430076	2.597925	-1.609995
H	65	4.072937	1.993031	-2.233031						H	65	10.966071	1.721915	-1.618995
H	66	5.150934	3.126034	-1.399031						H	66	9.568067	1.064924	-2.486995

Table S2. Cartesian coordinates (Å) of the DFT optimized structures: the 2-unit models of **4**-**6**.

4		x (Å)	y (Å)	z (Å)	**5**		x (Å)	y (Å)	z (Å)	**6**		x (Å)	y (Å)	z (Å)
C	1	3.665896	5.686031	-0.019974	C	1	-9.935047	0.991906	0.037005	Si	1	3.995963	2.871989	-0.002035
N	2	3.405909	4.256028	-0.015974	N	2	-9.132033	-0.219084	-0.033995	C	2	2.264965	2.092985	-0.001035
C	3	4.416918	3.280038	-0.013974	C	3	-7.750032	-0.288068	-0.012995	C	3	2.414968	0.707986	-0.001035
C	4	3.704930	1.988031	-0.008974	C	4	-6.692043	0.638944	-0.010995	S	4	0.894970	-0.125018	-0.001035
C	5	2.307927	2.250018	-0.007974	C	5	-5.459036	0.005958	-0.002995	C	5	0.021967	1.410980	-0.001035
C	6	1.502937	1.129011	-0.004974	S	6	-5.617015	-1.771044	0.004005	C	6	0.910964	2.478982	-0.001035
S	7	2.551950	-0.297979	-0.001974	C	7	-7.347016	-1.637064	0.001005	H	7	0.553962	3.499981	-0.001035
C	8	4.047942	0.649034	-0.004974	C	8	-8.519007	-2.415077	0.002005	C	8	-1.414034	1.448977	-0.000035
C	9	5.323948	-0.003954	-0.002974	S	9	-9.079988	-4.063084	0.008005	C	9	-2.300036	2.506974	-0.000035
S	10	5.442964	-1.775953	0.016026	C	10	-10.744995	-3.507103	0.001005	C	10	-3.674035	2.140971	-0.000035
C	11	7.162963	-1.678937	0.010026	C	11	-10.875011	-2.147105	-0.007995	C	11	-3.915032	0.780971	-0.000035
C	12	8.286971	-2.572927	0.018026	C	12	-9.600018	-1.517090	-0.010995	C	12	-5.141030	0.032968	-0.000035
S	13	8.595987	-4.275924	0.037026	H	13	-11.830016	-1.640116	-0.008995	S	13	-5.136026	-1.735032	-0.000035
C	14	10.315984	-3.972909	0.031026	H	14	-11.533986	-4.244112	0.007005	C	14	-6.868026	-1.768036	-0.000035
C	15	10.618972	-2.635906	0.016026	C	15	-4.165043	0.621973	-0.000995	C	15	-7.788023	-2.886038	-0.000035
C	16	9.453964	-1.828917	0.008026	C	16	-3.784058	1.949978	-0.001995	S	16	-7.500019	-4.599038	-0.001035
C	17	9.147951	-0.331919	-0.007974	C	17	-2.380061	2.172994	0.000005	C	17	-9.213019	-4.908042	-0.000035
C	18	7.620951	-0.368933	-0.004974	C	18	-1.608047	1.029003	0.001005	C	18	-9.946021	-3.751043	0.000965
C	19	6.586942	0.579057	-0.011974	S	19	-2.697031	-0.367010	0.002005	C	19	-9.142024	-2.577042	0.000965
H	20	6.709933	1.654058	-0.022974	C	20	-0.184045	0.842020	0.000005	Si	20	-9.313029	-0.689042	0.001965
C	21	9.693945	0.343086	-1.284974	S	21	0.507974	-0.801972	-0.000995	C	21	-7.427029	-0.493038	0.000965
H	22	9.308949	-0.144918	-2.181974	C	22	2.113966	-0.143954	0.001005	C	22	-6.443031	0.515965	0.000965
H	23	9.402935	1.396083	-1.311974	C	23	3.463971	-0.521938	0.000005	H	23	-6.641034	1.579964	0.001965
H	24	10.785945	0.291095	-1.305974	S	24	4.491987	-1.919926	-0.002995	C	24	-10.129030	-0.012044	-1.551035
C	25	9.698944	0.372086	1.251026	C	25	5.936975	-0.876909	-0.003995	H	25	-10.059033	1.078956	-1.575035
H	26	10.790945	0.322095	1.268026	C	26	5.614959	0.470087	-0.004995	H	26	-9.653029	-0.406043	-2.451035
H	27	9.317949	-0.095918	2.161026	C	27	4.221957	0.667071	-0.006995	H	27	-11.189029	-0.282046	-1.577035
H	28	9.406935	1.425083	1.256026	N	28	3.374944	1.758061	-0.021995	C	28	-10.128030	-0.013044	1.554965
H	29	11.634968	-2.264897	0.010026	C	29	2.084950	1.266046	-0.004995	H	29	-10.058033	1.077956	1.579965
H	30	10.992991	-4.813903	0.040026	C	30	0.792943	1.824031	-0.000995	H	30	-11.188029	-0.283046	1.580965
C	31	0.074939	0.986998	-0.002974	H	31	0.546931	2.877028	0.002005	H	31	-9.652029	-0.408043	2.454965
S	32	-0.680047	-0.618009	-0.015974	C	32	3.766928	3.158066	0.052005	H	32	-11.028021	-3.751046	0.000965
C	33	-2.246053	0.101977	-0.005974	H	33	3.021921	3.768057	-0.457995	H	33	-9.563016	-5.929043	-0.000035
C	34	-2.194066	1.489977	0.006026	H	34	4.723926	3.292077	-0.450995	S	34	-2.353030	-0.050026	-0.000035
C	35	-0.885070	1.993989	0.007026	H	35	3.855924	3.492067	1.089005	C	35	-4.479038	3.377969	-0.000035
H	36	-0.606080	3.038992	0.015026	H	36	6.373950	1.240096	-0.001995	N	36	-3.547041	4.424972	-0.000035
C	37	-3.601071	2.085965	0.014026	C	37	7.255981	-1.449894	-0.000995	C	37	-2.216040	3.982975	-0.000035
C	38	-4.434060	0.805957	0.003026	C	38	8.501974	-0.849879	-0.000995	O	38	-1.251041	4.724977	-0.000035
C	39	-3.614049	-0.316035	-0.008974	C	39	9.585985	-1.768867	0.001005	C	39	-3.933044	5.826971	-0.000035
S	40	-4.510036	-1.789044	-0.020974	C	40	9.224000	-3.075871	0.003005	H	40	-3.020045	6.419973	0.002965
C	41	-6.033044	-0.881057	-0.011974	S	41	7.490002	-3.205891	0.003005	H	41	-4.520044	6.060969	-0.890035
C	42	-7.301038	-1.558069	-0.017974	H	42	9.834011	-3.965864	0.005005	H	42	-4.525044	6.058969	0.886965
C	43	-8.592043	-1.062081	-0.000974	C	43	10.858976	-1.008852	0.000005	O	43	-5.684038	3.551967	0.000965
C	44	-9.599034	-2.066090	-0.015974	N	44	10.464961	0.339144	-0.001995	C	44	3.765969	0.201989	-0.001035
C	45	-9.132022	-3.339086	-0.043974	C	45	9.068959	0.513127	-0.002995	S	45	4.363973	-1.425010	-0.001035
S	46	-7.392022	-3.327070	-0.054974	O	46	8.531946	1.605121	-0.005995	C	46	6.029972	-0.841006	-0.001035
H	47	-9.667013	-4.275091	-0.059974	C	47	11.399948	1.452155	-0.003995	C	47	6.062969	0.546994	-0.002035
C	48	-10.927040	-1.409102	0.007026	H	48	12.405952	1.037166	-0.001995	C	48	4.788967	1.147991	-0.002035
N	49	-10.646052	-0.037099	0.035026	H	49	11.257940	2.068153	-0.893995	H	49	7.002967	1.081996	-0.002035
C	50	-9.266055	0.251913	0.032026	H	50	11.255940	2.072153	0.883005	C	50	7.145974	-1.750003	-0.001035
O	51	-8.811065	1.378917	0.052026	O	51	12.003981	-1.403838	0.002005	C	51	8.506973	-1.508000	-0.000035
C	52	-11.681061	0.982891	0.064026	C	52	-2.143078	3.629997	-0.001995	C	52	9.303976	-2.685998	-0.000035
H	53	-11.190070	1.953896	0.082026	N	53	-3.421085	4.208982	-0.003995	C	53	8.601979	-3.847000	-0.003035
H	54	-12.314061	0.907885	-0.820974	C	54	-4.456073	3.261970	-0.003995	S	54	6.897978	-3.504004	-0.004035
H	55	-12.302060	0.868886	0.955026	O	55	-5.637077	3.559956	-0.005995	H	55	8.949981	-4.868999	-0.003035
O	56	-12.040035	-1.889112	0.004026	C	56	-3.659101	5.642979	-0.005995	C	56	10.733975	-2.297995	0.001965
C	57	-5.801057	0.489945	0.002026	H	57	-2.691107	6.137991	-0.002995	N	57	10.718972	-0.893995	0.003965
H	58	-6.617063	1.200937	0.010026	H	58	-4.218105	5.934973	-0.895995	C	58	9.422971	-0.347998	0.002965
C	59	-3.860079	2.939962	-1.245974	H	59	-4.225105	5.935973	0.880005	O	59	9.200968	0.847002	0.003965
H	60	-3.684074	2.360964	-2.155974	O	60	-1.106085	4.268009	-0.000995	C	60	11.919970	-0.073992	0.006965
H	61	-4.894082	3.293953	-1.257974	H	61	-6.781056	1.716943	-0.012995	H	61	12.775972	-0.745990	0.009965
H	62	-3.201087	3.810968	-1.257974	H	62	-10.882045	0.828895	-0.476995	H	62	11.951969	0.558008	-0.882035
C	63	-3.856079	2.914962	1.291026	H	63	-9.409057	1.803912	-0.463995	H	63	11.945969	0.560008	0.894965
H	64	-3.197087	3.785968	1.317026	H	64	-10.135050	1.279904	1.073005	O	64	11.728977	-2.987993	0.002965
H	65	-3.676073	2.318964	2.188026						C	65	4.365961	3.857990	-1.557035
H	66	-4.890082	3.268953	1.313026						H	66	5.419960	4.148993	-1.583035
C	67	2.114914	3.715017	-0.011974						H	67	4.148962	3.275990	-2.455035
O	68	1.101908	4.390007	-0.010974						H	68	3.763959	4.769989	-1.585035
O	69	5.606916	3.535048	-0.016974						C	69	4.366961	3.857990	1.552965
H	70	4.744895	5.825041	-0.020974						H	70	5.420960	4.148993	1.578965
H	71	3.235892	6.149027	-0.909974						H	71	3.764959	4.770989	1.580965
H	72	3.234892	6.154027	0.867026						H	72	4.149962	3.276990	2.451965

Table S3. Cartesian coordinates (Å) of the optimized structures: the stacked dimer models of **1**.

FFY		x (Å)	y (Å)	z (Å)	**FFXS**		x (Å)	y (Å)	z (Å)	**FF**		x (Å)	y (Å)	z (Å)
S	1	0.03711	-0.02189	-0.04328	S	1	-0.01125	-0.05997	0.04118	S	1	0.43543	0.04424	0.28287
C	2	-0.92686	-0.03224	1.39602	C	2	1.02559	-1.05834	-0.92375	C	2	1.68706	1.22968	0.08945
C	3	-0.17334	-0.03600	2.53505	C	3	0.33249	-1.89438	-1.75132	C	3	0.54637	2.49375	0.30214
C	4	1.21387	-0.02279	2.24553	C	4	-1.06710	-1.73042	-1.60649	C	4	-0.72515	2.02026	0.50375
C	5	1.47097	0.00010	0.89672	C	5	-1.39333	-0.77817	-0.67427	C	5	-0.79105	0.60484	0.49454
C	6	2.90184	0.01223	0.69735	C	6	-2.83208	-0.67772	-0.59885	C	6	-1.69133	0.02068	0.63327
S	7	4.01674	0.05003	-0.59874	S	7	-4.00606	0.20975	0.26797	S	7	-1.71475	3.15962	0.67544
C	8	5.36962	0.06225	0.52582	C	8	-5.30071	-0.59632	-0.59841	C	8	-0.77114	4.34630	0.58932
C	9	4.92640	0.01407	1.82630	C	9	-4.80173	-1.52192	-1.48612	C	9	0.51699	3.93877	0.35340
C	10	3.52032	-0.00861	1.92027	C	10	-3.39108	-1.56203	-1.48595	C	10	1.60483	5.25535	0.22937
C	11	2.50455	-0.09114	3.04640	C	11	-2.31425	-2.34446	-2.22161	C	11	0.30246	6.39611	0.51109
C	12	2.61508	-1.45127	3.75836	C	12	-2.40973	-3.84447	-1.90458	C	12	0.56504	7.83219	0.51311
C	13	2.64599	1.05439	4.05365	C	13	-2.36479	-2.10460	-3.73635	C	13	-0.32397	8.75307	1.17233
S	14	9.42060	-0.12151	2.70356	S	14	-9.26767	-2.51123	-1.90363	S	14	-1.42186	8.44393	1.85597
N	15	7.87452	-0.09178	2.21271	N	15	-7.73871	-2.06828	-1.58692	N	15	-2.04701	9.83582	2.40578
N	16	10.17093	0.02370	1.27588	N	16	-10.06936	-1.33796	-1.12556	N	16	-0.97250	10.88807	1.80037
C	17	7.88374	0.04473	0.88947	C	17	-7.79814	-0.96446	-0.84708	C	17	-0.06466	10.17137	1.14126
C	18	9.22017	0.10514	0.34811	C	18	-9.15189	-0.54312	-0.57990	C	18	1.07435	10.69009	0.46907
C	19	9.43900	0.24071	-1.04842	C	19	-9.41766	0.61682	0.19746	C	19	1.25966	11.75595	0.46358
C	20	8.34051	0.32672	-1.84388	C	20	-8.34539	1.30842	0.66608	C	20	1.90580	9.79496	-0.12620
C	21	7.01887	0.27861	-1.31642	C	21	-7.00615	0.90867	0.39161	C	21	2.79283	10.14746	-0.63974
C	22	6.73696	0.12856	0.01942	C	22	-6.68282	-0.20880	-0.33759	C	22	1.65221	8.39272	-0.10851
H	23	-2.00247	-0.02240	1.30869	H	23	2.09527	-0.95953	-0.81923	H	23	2.34910	7.74814	-0.63260
H	24	-0.60509	-0.04396	3.52718	H	24	0.81364	-2.58694	-2.42929	H	24	-0.89743	5.74784	0.67978
H	25	5.60712	-0.00533	2.66275	H	25	-5.44836	-2.12872	-2.10242	H	25	-1.81773	6.28245	0.86362
H	26	2.51602	-2.27028	3.04275	H	26	-2.37208	-4.01354	-0.82637	H	26	-2.72774	3.18526	-0.48069
H	27	3.58447	-1.54168	4.25642	H	27	-3.34712	-4.25756	-2.28758	H	27	-3.38356	4.05603	-0.39303
H	28	1.83055	-1.55186	4.51386	H	28	-1.58158	-4.38677	-2.36999	H	28	-2.21381	3.23356	-1.44311
H	29	1.88043	0.97307	4.83145	H	29	-1.54715	-2.63376	-4.23412	H	29	-3.34977	2.28573	-0.46437
H	30	2.53396	2.01966	3.56054	H	30	-2.27362	-1.04094	-3.96217	H	30	-2.43477	3.09344	2.02695
H	31	3.62647	1.01384	4.53715	H	31	-3.30965	-2.46633	-4.15190	H	31	-1.71093	3.07271	2.84204
H	32	10.44866	0.28411	-1.43416	H	32	-10.44000	0.91833	0.38084	H	32	-3.08319	3.96428	2.15910
H	33	8.45815	0.44190	-2.91511	H	33	-8.49740	2.20277	1.25901	H	33	-3.05495	2.19400	2.08393
H	34	6.20110	0.36662	-2.02271	H	34	-6.21091	1.54043	0.77052	H	34	0.68683	-1.00364	0.21905
S	35	9.27297	3.65923	-0.05409	S	35	-0.01163	1.62586	-3.43199	S	35	2.45885	3.10657	3.38898
C	36	10.23702	3.67799	1.38506	C	36	1.02493	2.62465	-2.46720	C	36	1.14025	2.18401	4.02954
C	37	9.48356	3.68832	2.52409	C	37	0.33160	3.46044	-1.63956	C	37	1.15530	1.10910	3.93298
C	38	8.09634	3.67324	2.23474	C	38	-1.06794	3.29599	-1.78431	C	38	0.18010	2.96780	4.60256
C	39	7.83916	3.64246	0.88610	C	39	-1.39391	2.34362	-2.71648	C	39	-0.71248	2.56354	5.06201
C	40	6.40829	3.62900	0.68690	C	40	-2.83262	2.24264	-2.79178	C	40	0.50013	4.34575	4.50710
S	41	5.29332	3.58361	-0.60890	S	41	-4.00635	1.35472	-3.65848	S	41	1.69912	4.56423	3.87700
C	42	3.94050	3.57785	0.51578	C	42	-5.30121	2.16032	-2.79199	C	42	1.93783	5.98689	3.81303
C	43	4.38378	3.63363	1.81593	C	43	-4.80250	3.08614	-1.90436	C	43	3.12127	7.06227	3.20453
C	44	5.78987	3.65691	1.90971	C	44	-3.39187	3.12676	-1.90464	C	44	2.17319	8.44625	3.72938
C	45	6.80570	3.74607	3.03527	C	45	-2.31525	3.90958	-1.16908	C	45	2.63674	9.79625	3.43104
C	46	6.69505	5.11022	3.73945	C	46	-2.41131	5.40956	-1.48606	C	46	3.79310	10.04018	2.73114
C	47	6.66451	2.60628	4.04906	C	47	-2.36557	3.66967	0.34566	C	47	4.40885	9.20430	2.41861
S	48	-0.11045	3.77421	2.69253	S	48	-9.26866	4.07380	-1.48640	S	48	4.22456	11.34272	2.35578
N	49	1.43562	3.74143	2.20185	N	49	-7.73957	3.63140	-1.80323	N	49	5.14957	11.43328	1.79771
N	50	-0.86081	3.62100	1.26571	N	50	-10.07006	2.90026	-2.26434	N	50	3.50924	12.45813	2.66335
C	51	1.42637	3.59745	0.87940	C	51	-7.79873	2.52758	-2.54307	C	51	3.81971	13.45372	2.37518
C	52	0.08993	3.53415	0.33841	C	52	-9.15237	2.10576	-2.81010	C	52	2.31333	12.27758	3.40864
C	53	-0.12893	3.39064	-1.05732	C	53	-9.41781	0.94572	-3.58742	C	53	1.87999	10.96241	3.80951
C	54	0.96953	3.29995	-1.85229	C	54	-8.34535	0.25449	-4.05614	C	54	0.75275	10.98818	4.51779
C	55	2.29119	3.35096	-1.32514	C	55	-7.00623	0.65470	-3.78180	C	55	0.29830	12.53798	4.63657
C	56	2.57314	3.50862	0.00982	C	56	-6.68320	1.77230	-3.05267	C	56	1.49835	13.24936	3.81616
H	57	11.31263	3.66776	1.29773	H	57	2.09464	2.52625	-2.57183	H	57	1.01416	8.04423	4.35147
H	58	9.91537	3.70213	3.51614	H	58	0.81257	4.15318	-0.96164	H	58	0.29978	8.75334	4.74198
H	59	3.70309	3.65789	2.65228	H	59	-5.44931	3.69271	-1.28802	H	59	0.88488	6.64117	4.39761
H	60	6.79395	5.92514	3.01915	H	60	-2.37383	5.57868	-2.56427	H	60	-0.13771	5.65640	4.93825
H	61	5.72568	5.20336	4.23705	H	61	-3.34881	5.82231	-1.10296	H	61	-1.51703	5.86913	4.30478
H	62	7.47962	5.21525	4.49431	H	62	-1.58331	5.95215	-1.02073	H	62	-1.91668	6.84627	4.58978
H	63	7.43008	2.69216	4.82634	H	63	-1.54808	4.19912	0.84337	H	63	-1.44967	5.83761	3.21746
H	64	6.77668	1.63824	3.56145	H	64	-2.27397	2.60604	0.57144	H	64	-2.21728	5.09880	4.64173
H	65	5.68404	2.64940	4.53237	H	65	-3.31052	4.03103	0.76130	H	65	-0.22193	5.74373	6.47066
H	66	-1.13860	3.34516	-1.44279	H	66	-10.44007	0.64385	-3.77070	H	66	-0.90428	4.98202	6.85905
H	67	0.85187	3.17866	-2.92284	H	67	-8.49711	-0.63993	-4.64903	H	67	-0.59560	6.72518	6.77560
H	68	3.10894	3.25890	-2.03093	H	68	-6.21080	0.02319	-4.16075	H	68	0.76062	5.59161	6.92269

Table S3. Cartesian coordinates (Å) of the optimized structures: the stacked dimer models of **1** (Continued).

FFX		x (Å)	y (Å)	z (Å)	**FFYS**		x (Å)	y (Å)	z (Å)	**FFZ**		x (Å)	y (Å)	z (Å)
S	1	0.02987	0.02386	0.00470	S	1	0.09864	0.03284	-0.23243	S	1	-0.04976	0.10479	0.04691
C	2	-1.46268	0.43901	0.78581	C	2	-1.29465	0.99062	-0.61971	C	2	-0.76383	1.66042	0.32063
C	3	-1.28250	1.25979	1.86146	C	3	-1.05021	2.33125	-0.54241	C	3	0.66650	2.43293	-0.22652
C	4	0.08636	1.56529	2.06420	C	4	0.28908	2.59897	-0.16416	C	4	1.62492	1.53592	-0.62446
C	5	0.90491	0.96741	1.13906	C	5	1.02114	1.45541	0.03627	C	5	1.21529	0.18904	-0.45801
C	6	2.26661	1.38593	1.38210	C	6	2.36925	1.82523	0.40510	C	6	1.81528	-0.68000	-0.69367
S	7	3.82689	1.12285	0.73187	S	7	3.83344	1.06237	0.85776	S	7	2.83766	2.25150	-1.19773
C	8	4.53874	2.16120	1.95332	C	8	4.62057	2.62329	1.05306	C	8	2.41230	3.69744	-1.00463
C	9	3.57676	2.69229	2.77995	C	9	3.74850	3.65120	0.78329	C	9	1.15972	3.77243	-0.45020
C	10	2.28133	2.24032	2.45582	C	10	2.46652	3.19223	0.41438	C	10	0.64502	5.38530	-0.21351
C	11	0.88719	2.41991	3.03261	C	11	1.13228	3.83894	0.08169	C	11	2.14216	5.99302	-0.89989
C	12	0.81313	1.85215	4.45917	C	12	0.61001	4.63188	1.29116	C	12	2.97792	4.96299	-1.26229
C	13	0.43724	3.88479	3.00856	C	13	1.20405	4.73714	-1.15925	C	13	3.95542	5.14078	-1.68487
S	14	7.10215	5.35311	4.00936	S	14	7.41182	6.22179	1.65723	S	14	2.35100	7.43266	-1.01461
N	15	5.96453	4.38492	3.37925	N	15	6.21579	5.15850	1.39635	N	15	3.65358	7.99715	-1.25940
N	16	8.43940	4.57188	3.52768	N	16	8.61920	5.20159	2.01855	N	16	4.78805	7.32819	-1.44802
C	17	6.59721	3.39774	2.75175	C	17	6.72299	3.94281	1.57884	C	17	5.95231	8.42858	-1.70235
C	18	8.03286	3.50663	2.84112	C	18	8.11943	3.97112	1.94292	C	18	5.08378	9.79195	-1.59015
C	19	8.87623	2.54319	2.22572	C	19	8.83656	2.76794	2.18188	C	19	3.82844	9.42663	-1.34018
C	20	8.27454	1.52144	1.56118	C	20	8.15409	1.60141	2.05069	C	20	2.72735	10.30829	-1.16922
C	21	6.85705	1.40115	1.47811	C	21	6.77705	1.56559	1.68844	C	21	2.88299	11.37756	-1.21839
C	22	5.98837	2.30424	2.03919	C	22	6.02692	2.68760	1.44209	C	22	1.50747	9.74764	-0.96083
H	23	-2.38721	0.03525	0.40203	H	23	-2.21789	0.49553	-0.87977	H	23	0.63556	10.38003	-0.83928
H	24	-2.09896	1.62354	2.47122	H	24	-1.80188	3.08151	-0.74929	H	24	1.32416	8.33626	-0.90270
H	25	3.82204	3.37152	3.58276	H	25	4.04524	4.68700	0.84978	H	25	0.31277	7.96931	-0.76806
H	26	1.13373	0.80824	4.47813	H	26	0.55694	3.99585	2.17745	H	26	3.00179	1.92250	-2.69029
H	27	1.45922	2.42634	5.12907	H	27	1.27460	5.47279	1.50781	H	27	3.23244	0.86166	-2.82423
H	28	-0.21038	1.90927	4.84050	H	28	-0.38843	5.02884	1.08707	H	28	2.08542	2.14930	-3.23932
H	29	-0.58429	3.98137	3.38748	H	29	0.22318	5.17456	-1.36694	H	29	3.81901	2.50755	-3.12124
H	30	0.46590	4.28932	1.99702	H	30	1.52170	4.17446	-2.03809	H	30	4.12356	1.93003	-0.42806
H	31	1.09186	4.49596	3.63619	H	31	1.92133	5.54717	-1.01018	H	31	4.00487	2.17595	0.62717
H	32	9.95068	2.64627	2.29566	H	32	9.88442	2.80193	2.44581	H	32	4.96305	2.50602	-0.82716
H	33	8.87971	0.76778	1.07133	H	33	8.66232	0.65868	2.21427	H	33	4.36576	0.86653	-0.51233
H	34	6.45606	0.53905	0.95746	H	34	6.31487	0.58900	1.59682	H	34	-0.61472	-0.78132	0.29244
S	35	0.05995	7.49231	1.92938	S	35	12.94918	0.03276	-0.16083	S	35	5.21698	8.74908	1.85328
C	36	-1.43108	7.08794	1.13978	C	36	14.34243	0.99022	0.22734	C	36	4.50299	10.30482	2.12662
C	37	-1.25079	6.26530	0.06556	C	37	14.09808	2.33091	0.15082	C	37	5.06811	11.19085	1.88117
C	38	0.11692	5.94950	-0.12909	C	38	12.75884	2.59894	-0.22739	C	38	3.23768	10.22075	2.63092
C	39	0.93451	6.54164	0.80059	C	39	12.02674	1.45555	-0.42862	C	39	2.63768	11.08989	2.86618
C	40	2.29445	6.11297	0.56556	C	40	10.67871	1.82566	-0.79747	C	40	2.82771	8.87393	2.79704
S	41	3.85279	6.36427	1.22496	S	41	9.21449	1.06315	-1.25060	S	41	3.78615	7.97678	2.39947
C	42	4.56384	5.31971	0.00837	C	42	8.42746	2.62422	-1.44503	C	42	3.29287	6.63736	2.62340
C	43	3.60273	4.79586	-0.82389	C	43	9.29959	3.65193	-1.17465	C	43	3.80755	5.02445	2.38712
C	44	2.30901	5.25814	-0.50780	C	44	10.58153	3.19267	-0.80597	C	44	2.31019	4.41688	3.07320
C	45	0.91689	5.08821	-1.09225	C	45	11.91577	3.83910	-0.47272	C	45	1.47443	5.44704	3.43527
C	46	0.85456	5.65438	-2.51993	C	46	12.43832	4.63257	-1.68172	C	46	0.49682	5.26936	3.85765
C	47	0.45659	3.62658	-1.06805	C	47	11.84389	4.73674	0.76863	C	47	2.04016	6.71251	3.17754
S	48	7.11305	2.10604	-2.03110	S	48	5.63656	6.22329	-2.04737	S	48	1.61498	8.15851	3.37054
N	49	5.97973	3.08390	-1.40819	N	49	6.83250	5.15975	-1.78709	N	49	0.32870	8.48024	2.60170
N	50	8.45379	2.87596	-1.54096	N	50	4.42905	5.20338	-2.40908	N	50	0.44648	8.23438	1.54635
C	51	6.61678	4.06586	-0.77693	C	51	6.32516	3.94420	-1.97010	C	51	0.08675	9.54379	2.68621
C	52	8.05198	3.94480	-0.85722	C	52	4.92870	3.97283	-2.33407	C	52	-0.51066	7.90447	3.00140
C	53	8.89956	4.90114	-0.23653	C	53	4.21143	2.76982	-2.57358	C	53	1.45172	8.48754	4.86324
C	54	8.30235	5.92787	0.42435	C	54	4.89380	1.60317	-2.44299	C	54	2.36835	8.26058	5.41175
C	55	6.88543	6.06017	0.49849	C	55	6.27085	1.56703	-2.08083	C	55	0.63463	7.90263	5.29462
C	56	6.01271	5.16457	-0.06830	C	56	7.02112	2.68886	-1.83400	C	56	1.22133	9.54843	4.99729
H	57	-2.35480	7.49871	1.51803	H	57	15.26559	0.49493	0.48728	H	57	2.10114	2.97728	3.18798
H	58	-2.06638	5.90731	-0.54874	H	58	14.84975	3.08102	0.35828	H	58	0.79852	2.41300	3.43319
H	59	3.84745	4.11429	-1.62488	H	59	9.00291	4.68778	-1.24054	H	59	-0.33584	3.08212	3.62187
H	60	1.18266	6.69596	-2.53870	H	60	12.49146	3.99698	-2.56832	H	60	-1.50023	1.98194	3.87640
H	61	1.50013	5.07462	-3.18551	H	61	11.77387	5.47367	-1.89806	H	61	-0.63192	0.61843	3.76418
H	62	-0.16726	5.60395	-2.90671	H	62	13.43678	5.02930	-1.47729	H	62	0.62346	0.98355	3.51412
H	63	-0.56393	3.53625	-1.45120	H	63	12.82484	5.17376	0.97680	H	63	1.72435	0.10168	3.34301
H	64	0.47826	3.22414	-0.05554	H	64	11.52581	4.17376	1.64712	H	64	1.56855	-0.96755	3.39235
H	65	1.10983	3.00974	-1.69156	H	65	11.12693	5.54708	0.61971	H	65	2.94423	0.66211	3.13409
H	66	9.97353	4.78903	-0.29971	H	66	3.16357	2.80405	-2.83746	H	66	3.81601	0.02958	3.01225
H	67	8.91076	6.67630	0.91816	H	67	4.38546	0.66056	-2.60698	H	67	3.12775	2.07345	3.07572
H	68	6.48844	6.92558	1.01674	H	68	6.73293	0.59035	-1.98967	H	68	4.13915	2.44009	2.94029

Table S3. Cartesian coordinates (Å) of the optimized structures: the stacked dimer models of **1** (Continued).

CF		x (Å)	y (Å)	z (Å)
S	1	0.03574	0.05503	-0.16232
C	2	0.11691	-1.67592	-0.25803
C	3	-1.11664	-2.25933	-0.27560
C	4	-2.15387	-1.29599	-0.20817
C	5	-1.68017	-0.00907	-0.14183
C	6	-2.80354	0.89902	-0.07145
S	7	-3.10187	2.58450	-0.02372
C	8	-4.82910	2.30219	0.03656
C	9	-5.12216	0.96163	-0.01999
C	10	-3.96242	0.16399	-0.08146
C	11	-3.67290	-1.31970	-0.22530
C	12	-4.26550	-2.15428	0.91555
C	13	-4.19097	-1.82384	-1.58394
S	14	-9.20763	2.71974	-1.20078
N	15	-7.65993	2.32049	-0.92454
N	16	-9.24693	4.19393	-0.52562
C	17	-7.10562	3.34327	-0.27885
C	18	-8.02560	4.42840	-0.04987
C	19	-7.60671	5.60381	0.63220
C	20	-6.31465	5.65509	1.05480
C	21	-5.40379	4.57806	0.84760
C	22	-5.75090	3.42071	0.19839
H	23	1.08253	-2.15675	-0.29637
H	24	-1.26344	-3.32974	-0.33489
H	25	-6.13598	0.58904	-0.01400
H	26	-3.85816	-1.83665	1.87516
H	27	-5.35264	-2.04150	0.94924
H	28	-4.03658	-3.21435	0.77399
H	29	-3.91627	-2.87192	-1.73339
H	30	-3.77020	-1.23446	-2.40142
H	31	-5.28077	-1.74537	-1.62724
H	32	-8.31117	6.40831	0.79715
H	33	-5.95496	6.53033	1.58387
H	34	-4.40902	4.67239	1.26731
S	35	-6.38012	-2.39409	4.22208
C	36	-8.09022	-2.14377	4.37363
C	37	-8.43858	-0.82664	4.29082
C	38	-7.30641	0.00368	4.10064
C	39	-6.13257	-0.70503	4.04424
C	40	-5.04148	0.22058	3.84003
S	41	-3.33741	0.18434	3.69841
C	42	-3.28812	1.92741	3.49409
C	43	-4.54966	2.47011	3.56835
C	44	-5.54696	1.49291	3.76239
C	45	-7.05496	1.49408	3.94668
C	46	-7.44543	2.25753	5.22207
C	47	-7.78551	2.06924	2.72798
S	48	-2.20580	6.38391	3.14591
N	49	-2.86593	4.91162	3.33135
N	50	-0.66759	5.96554	2.85346
C	51	-1.89030	4.02006	3.17193
C	52	-0.61513	4.63630	2.89287
C	53	0.54814	3.84763	2.68041
C	54	0.40257	2.49789	2.74556
C	55	-0.85371	1.88217	3.01347
C	56	-2.01112	2.58530	3.23969
H	57	-8.73677	-2.99612	4.51725
H	58	-9.46093	-0.47994	4.36507
H	59	-4.72699	3.53036	3.47484
H	60	-6.92016	1.85518	6.09085
H	61	-7.19265	3.31668	5.12201
H	62	-8.52170	2.17828	5.39974
H	63	-8.86876	2.00201	2.86485
H	64	-7.51665	1.52246	1.82262
H	65	-7.52397	3.12196	2.58751
H	66	1.49463	4.32883	2.47393
H	67	1.25811	1.85323	2.58235
H	68	-0.88196	0.79824	3.01485

Table S4. Cartesian coordinates (Å) of the optimized structures: the stacked dimer models of **4**.

FFY		x (Å)	y (Å)	z (Å)	FFXS		x (Å)	y (Å)	z (Å)	FF		x (Å)	y (Å)	z (Å)
C	1	-0.01442	0.08174	-0.04869	C	1	-0.02554	-0.06338	0.04082	C	1	0.00575	-0.76431	0.74977
N	2	-0.93739	0.02062	-1.15912	N	2	1.02833	0.76968	0.58359	N	2	1.10874	-1.36189	0.02787
C	3	-2.31327	-0.14194	-0.98627	C	3	2.39163	0.47144	0.45507	C	3	2.18312	-0.62271	-0.46315
C	4	-2.88360	-0.14060	-2.35014	C	4	3.09804	1.59197	1.11371	C	4	3.07861	-1.62445	-1.08604
C	5	-1.80708	-0.01349	-3.26339	C	5	2.11793	2.49474	1.59733	C	5	2.50522	-2.90824	-0.91694
C	6	-2.17052	-0.01759	-4.56400	C	6	2.61672	3.58511	2.21982	C	6	3.27098	-3.92948	-1.41268
S	7	-3.88724	-0.18138	-4.68643	S	7	4.34186	3.51617	2.21634	S	7	3.02416	-5.35362	-1.41720
C	8	-4.11295	-0.23696	-2.95040	C	8	4.38720	1.98655	1.36605	C	8	4.32283	-6.50668	-1.65120
C	9	-5.43051	-0.33795	-2.36704	C	9	5.64073	1.35897	1.02177	C	9	3.22432	-7.80781	-1.48016
S	10	-6.87023	-0.35354	-3.36818	S	10	7.17006	2.03448	1.54949	S	10	3.24710	-9.25237	-1.48105
C	11	-7.85961	-0.43346	-1.97574	C	11	8.01968	0.79171	0.74084	C	11	4.38470	-10.52679	-1.63770
C	12	-9.26515	-0.49677	-1.65132	C	12	9.38778	0.39658	0.50311	C	12	3.12736	-11.69801	-1.40531
S	13	-10.77631	-0.54526	-2.46305	S	13	10.97067	0.90336	0.92593	S	13	1.90113	-11.12634	-1.22221
C	14	-11.60460	-0.63819	-0.94385	C	14	11.64763	-0.41637	0.02981	C	14	1.97191	-9.71185	-1.26782
C	15	-10.75260	-0.64494	0.12345	C	15	10.69630	-1.20227	-0.55537	C	15	0.98528	-8.56306	-1.14880
C	16	-9.39810	-0.56620	-0.28629	C	16	9.38886	-0.73248	-0.27879	C	16	1.93573	-7.38421	-1.26416
C	17	-8.04065	-0.61560	0.39632	C	17	7.97278	-1.17718	-0.60534	C	17	1.81513	-5.98244	-1.22817
C	18	-7.13153	-0.46592	-0.81103	C	18	7.18191	-0.09459	0.10782	C	18	0.90216	-5.42856	-1.05442
C	19	-5.74260	-0.40861	-1.02787	C	19	5.82079	0.21931	0.26935	C	19	-0.00693	-8.57132	-2.32374
C	20	-7.83006	-1.99764	1.04220	C	20	4.98444	-0.33777	-0.13305	C	20	-0.63853	-9.46328	-2.28321
C	21	-7.84176	0.49480	1.43252	C	21	7.67504	-2.56107	-0.00783	C	21	-0.65547	-7.69215	-2.27975
C	22	-0.54271	0.10615	-2.49981	C	22	7.86618	-2.56841	1.06733	C	22	0.52318	-8.56538	-3.27855
O	23	0.58736	0.24735	-2.88501	O	23	6.62829	-2.82887	-0.17542	O	23	0.24021	-8.57661	0.19021
O	24	-2.83734	-0.27246	0.09552	O	24	8.30360	-3.32302	-0.47734	O	24	-0.40359	-7.69722	0.27855
C	25	-12.13399	2.78005	-0.05415	C	25	7.70410	-1.16841	-2.11649	C	25	-0.38839	-9.46859	0.26674
N	26	-11.21073	2.84040	-1.16441	N	26	8.32691	-1.91300	-2.62020	N	26	0.94706	-8.57330	1.02017
C	27	-9.83515	3.00612	-0.99200	C	27	7.92223	-0.18839	-2.54496	C	27	0.99819	-11.70127	-1.06486
C	28	-9.26492	3.00288	-2.35589	C	28	6.65591	-1.40730	-2.31643	C	28	3.37691	-12.74809	-1.42688
C	29	-10.34137	2.87276	-3.26877	C	29	10.93467	-2.07245	-1.15253	C	29	4.71412	-3.24264	-2.12761
C	30	-9.97804	2.87402	-4.56941	C	30	12.72026	-0.53001	-0.01164	C	30	4.27528	-1.62344	-1.71338
S	31	-8.26141	3.03842	-4.69242	S	31	2.09972	4.42259	2.66109	S	31	4.92466	-0.79445	-1.94889
C	32	-8.03562	3.09818	-2.95646	C	32	0.77674	1.96446	1.26166	C	32	1.21944	-2.73888	-0.20634
C	33	-6.71804	3.20085	-2.37337	C	33	-0.31677	2.41515	1.48798	C	33	0.38370	-3.54780	0.11679
S	34	-5.27824	3.21349	-3.37450	S	34	2.81621	-0.51514	-0.09791	S	34	2.30353	0.57285	-0.36368
C	35	-4.28900	3.29615	-1.98222	C	35	0.40926	-1.03210	-0.20090	C	35	-0.79021	-1.50501	0.81046
C	36	-2.88348	3.35993	-1.65815	C	36	-0.81286	-0.17855	0.78634	C	36	0.32650	-0.48362	1.75455
S	37	-1.37261	3.40735	-2.47026	S	37	-0.44595	0.39371	-0.85765	S	37	-0.34391	0.11895	0.21414
C	38	-0.54390	3.50365	-0.95141	C	38	-0.03513	4.91331	-0.72417	C	38	5.15680	-8.48881	1.57196
C	39	-1.39577	3.51261	0.11602	C	39	1.01832	4.08252	-1.27142	C	39	3.84508	-9.41874	2.21532
C	40	-2.75032	3.43262	-0.29330	C	40	2.38161	4.38309	-1.14807	C	40	2.86577	-8.64051	2.76238
C	41	-4.10766	3.48457	0.38931	C	41	3.08730	3.26363	-1.80937	C	41	3.16561	-7.25991	2.64609
C	42	-5.01697	3.33118	-0.81753	C	42	2.10686	2.35963	-2.28996	C	42	4.36807	-7.03421	2.02505
C	43	-6.40593	3.27381	-1.03430	C	43	2.60517	1.26982	-2.91390	C	43	4.58349	-5.61003	1.94089
C	44	-4.31770	4.86996	1.02852	C	44	4.33025	1.34090	-2.91550	C	44	5.78069	-4.53255	1.36842
C	45	-4.30652	2.37947	1.43105	C	45	4.37620	2.87055	-2.06537	C	45	4.81274	-3.15941	1.87212
C	46	-11.60546	2.75212	-2.50488	C	46	5.62984	3.49864	-1.72249	C	46	3.63043	-3.55832	2.45707
O	47	-12.73541	2.60832	-2.88942	O	47	7.15924	2.82413	-2.25143	O	47	3.50900	-4.96013	2.49897
O	48	-9.31101	3.13987	0.08937	O	48	8.00858	4.06545	-1.44007	O	48	2.49970	-5.95453	3.04851
H	49	-4.97774	-0.42540	-0.26273	H	49	9.37664	4.45802	-1.19803	H	49	1.11716	-5.79037	2.41021
H	50	-7.95974	-2.79426	0.30625	H	50	10.95979	3.95038	-1.61885	H	50	0.43434	-6.56163	2.77890
H	51	-6.82268	-2.07114	1.46069	H	51	11.63658	5.26467	-0.71468	H	51	0.69432	-4.81217	2.65060
H	52	-8.54959	-2.15141	1.85126	H	52	10.68505	6.04964	-0.12859	H	52	1.17931	-5.86605	1.32547
H	53	-8.54969	0.37273	2.25754	H	53	9.37756	5.58354	-0.41100	H	53	2.41035	-5.83822	4.57934
H	54	-8.00201	1.47797	0.99198	H	54	7.96140	6.02849	-0.08520	H	54	2.00038	-4.86486	4.86207
H	55	-6.82966	0.44556	1.84387	H	55	7.17075	4.95034	-0.80524	H	55	1.75375	-6.61490	4.98119
H	56	-11.09100	-0.70678	1.14947	H	56	5.80974	4.63701	-0.96817	H	56	3.39663	-5.94597	5.03608
H	57	-12.68338	-0.67748	-0.93733	H	57	4.97335	5.19343	-0.56505	H	57	2.90502	-2.84432	2.82697
H	58	-1.55832	0.06192	-5.44888	H	58	7.66632	7.41617	-0.67502	H	58	5.26568	-1.80856	1.63785
H	59	0.06311	-0.88951	0.44443	H	59	7.86004	7.43021	-1.74964	H	59	6.81693	-1.49098	0.88772
H	60	0.95782	0.36800	-0.44757	H	60	6.61940	7.68376	-0.50823	H	60	6.58516	0.22340	0.89010
H	61	-0.35647	0.82481	0.67166	H	61	8.29426	8.17470	-0.19917	H	61	5.39145	0.51828	1.44802
H	62	-7.17082	3.29255	-0.26925	H	62	7.68938	6.01169	1.42541	H	62	4.64794	-0.60811	1.87873
H	63	-4.18738	5.66265	0.28849	H	63	8.31310	6.75159	1.93482	H	63	3.37823	-0.11098	2.44996
H	64	-5.32514	4.94610	1.44640	H	64	7.90348	5.02860	1.84880	H	64	3.44208	1.27648	2.35367
H	65	-3.59823	5.02722	1.83697	H	65	6.64141	6.25231	1.62426	H	65	4.60535	1.74442	1.72908
H	66	-3.59914	2.50652	2.25578	H	66	10.92334	6.91654	0.47332	H	66	4.85880	2.89546	1.50038
H	67	-4.14524	1.39395	0.99610	H	67	12.70929	5.37623	-0.66981	H	67	2.31183	2.12759	2.65136
H	68	-5.31888	2.43010	1.84159	H	68	2.08790	0.43181	-3.35382	H	68	2.67446	3.15055	2.73859
H	69	-1.05723	3.57656	1.14189	H	69	0.76608	2.88756	-1.94885	H	69	1.58010	2.06810	1.84205
H	70	0.53489	3.54256	-0.94516	H	70	-0.32755	2.43480	-2.17026	H	70	1.85467	1.80827	3.58751
H	71	-10.59037	2.79189	-5.45397	H	71	2.80672	5.37019	-0.59647	H	71	2.43426	-0.71340	2.91190
H	72	-12.24037	3.75994	0.41626	H	72	0.40389	5.87566	-0.46475	H	72	7.33951	0.88536	0.49375
H	73	-13.09724	2.45695	-0.44666	H	73	-0.81683	5.04479	-1.47302	H	73	1.97535	-9.04995	3.22109
H	74	-11.77134	2.06408	0.68312	H	74	-0.46366	4.44500	0.16459	H	74	3.87759	-10.49523	2.14230

Table S4. Cartesian coordinates (Å) of the optimized structures: the stacked dimer models of **4** (Continued).

FFX		x (Å)	y (Å)	z (Å)	**FFYS**		x (Å)	y (Å)	z (Å)	**FFZ**		x (Å)	y (Å)	z (Å)
C	1	-0.00014	0.00020	-0.00050	C	1	-0.03210	0.00455	-0.06964	C	1	-0.08145	-0.19278	-0.09615
N	2	0.88947	0.81802	0.91986	N	2	0.07266	-1.42309	-0.27760	N	2	-1.21399	-0.94431	0.58604
C	3	2.27738	1.08137	1.02812	C	3	1.20654	-2.15491	0.07579	C	3	-1.56768	-2.30340	0.78373
C	4	2.55572	1.88486	2.09592	C	4	0.84798	-3.57036	-0.14420	C	4	-2.78983	-2.42634	1.37881
C	5	1.13692	2.33473	2.98528	C	5	-0.49563	-3.60727	-0.59243	C	5	-3.53810	-0.89472	1.68972
C	6	0.15684	1.42908	1.90712	C	6	-0.96566	-4.84781	-0.84761	C	6	-2.17090	-0.07746	1.05221
S	7	-1.22980	1.05640	1.75206	S	7	0.26242	-6.01418	-0.51828	S	7	-1.72885	1.27607	0.81184
C	8	-2.73337	1.37999	2.49982	C	8	1.43560	-4.80528	-0.04273	C	8	-2.27247	2.87133	1.10137
C	9	-3.55660	0.39343	1.30788	C	9	2.77159	-5.17675	0.36306	C	9	-0.82776	3.51720	0.34830
S	10	-2.67369	-0.17178	0.41429	S	10	3.31200	-6.84384	0.26793	S	10	0.01529	2.51771	-0.08292
C	11	-1.34593	0.21527	0.67072	C	11	4.85215	-6.39652	0.86392	C	11	-0.50658	1.23890	0.18339
C	12	-3.00419	-0.82475	-0.38340	C	12	6.13419	-7.01662	1.10452	C	12	0.97127	2.73216	-0.54279
S	13	-4.99712	0.29683	1.28271	S	13	6.84721	-8.57674	1.04133	S	13	-0.60429	4.94118	0.26036
C	14	-5.99675	1.32069	2.29214	C	14	8.36452	-7.91799	1.56087	C	14	-1.89429	6.08488	0.55725
C	15	-7.47427	0.64886	1.69696	C	15	8.31258	-6.56996	1.76912	C	15	-0.87396	7.46074	0.32450
C	16	-7.20010	-0.28679	0.76154	C	16	7.02226	-6.04884	1.50161	C	16	0.36986	7.04978	-0.00283
C	17	-5.81907	-0.48765	0.51569	C	17	6.35808	-4.68380	1.56689	C	17	0.53256	5.64222	-0.04495
C	18	-5.69232	-1.53045	-0.52419	C	18	4.95092	-5.05015	1.12169	C	18	1.94522	5.36225	-0.37751
C	19	-7.00532	-1.90549	-0.82939	C	19	3.76535	-4.34684	0.83254	C	19	2.54436	6.61836	-0.52449
C	20	-7.97683	-1.22161	-0.08759	C	20	3.61762	-3.27980	0.93957	C	20	1.67310	7.68988	-0.29580
C	21	-9.16258	-1.40499	-0.16054	C	21	6.99433	-3.69247	0.58121	C	21	1.97601	8.85355	-0.33462
C	22	-7.31245	-2.95061	-1.77876	C	22	6.96056	-4.08430	-0.43773	C	22	3.95202	6.78163	-0.80952
O	23	-8.39596	-2.99717	-1.87953	O	23	6.46020	-2.73896	0.60590	O	23	4.13848	7.84660	-0.94072
O	24	-6.85603	-2.72910	-2.74426	O	24	8.03840	-3.50601	0.84728	O	24	4.55702	6.40119	0.01633
C	25	-6.93123	-3.91121	-1.42397	C	25	6.39511	-4.12743	2.99765	C	25	4.21610	6.24134	-1.71950
N	26	-4.72036	-2.01019	-1.05674	N	26	7.42412	-3.88481	3.27803	N	26	2.53728	4.31855	-0.51461
C	27	-8.42797	0.97403	2.08369	C	27	6.02406	-4.87013	3.70756	C	27	-1.25838	8.46163	0.44257
C	28	3.51668	2.25790	2.41640	C	28	5.79097	-3.22282	3.09345	C	28	-3.30408	-3.32807	1.67389
C	29	3.03781	0.70277	0.35815	C	29	9.16507	-5.98924	2.09557	C	29	-0.95851	-3.15363	0.50664
C	30	0.40945	-1.47633	-0.02456	C	30	9.21095	-8.57770	1.67761	C	30	-0.12197	-0.46169	-1.61267
S	31	0.45300	-1.88962	0.98273	S	31	-1.93915	-5.15884	-1.19051	S	31	-1.10912	-0.23183	-2.01923
C	32	-0.30879	-2.06310	-0.60381	C	32	-1.01455	-2.22132	-0.64435	C	32	0.61898	0.15619	-2.12696
C	33	1.39495	-1.59328	-0.48424	C	33	-2.11235	-1.81065	-0.91980	C	33	0.10263	-1.51182	-1.81948
S	34	-0.01005	0.58447	-1.42256	S	34	2.22991	-1.65405	0.48602	S	34	1.30467	-0.52461	0.46338
C	35	0.98265	0.50376	-1.87419	C	35	0.88106	0.48779	-0.41640	C	35	1.54430	-1.57733	0.28735
C	36	-0.30075	1.63716	-1.40808	C	36	-0.88776	0.36426	-0.63899	C	36	1.35000	-0.33087	1.53459
S	37	-0.71671	0.03657	-2.05170	S	37	-0.18312	0.21431	0.99150	S	37	2.06774	0.08417	-0.02897
C	38	1.14065	-5.08249	1.06710	C	38	2.00256	0.00411	3.32631	C	38	2.14660	7.05450	2.96694
C	39	2.55957	-4.63187	1.95589	C	39	1.89768	-1.42355	3.53402	C	39	1.39797	8.58603	3.27743
C	40	2.28127	-3.82828	3.02363	C	40	0.76371	-2.15521	3.18053	C	40	0.17563	8.46295	3.87209
C	41	0.89329	-3.56545	3.13230	C	41	1.12213	-3.57073	3.40030	C	41	-0.17791	7.10383	4.06978
C	42	0.16058	-4.17702	2.14541	C	42	2.46574	-3.60784	3.84852	C	42	0.77930	6.23708	3.60404
C	43	-1.22622	-3.80516	2.30109	C	43	2.93566	-4.84846	4.10348	C	43	0.33735	4.88351	3.84431
C	44	-2.72992	-4.12959	1.55394	C	44	1.70749	-6.01467	3.77391	C	44	0.88130	3.28830	3.55511
C	45	-3.55320	-3.14340	2.74616	C	45	0.53441	-4.80558	3.29859	C	45	-0.56355	2.64229	4.30782
C	46	-2.67023	-2.57761	3.63931	C	46	-0.80162	-5.17688	2.89276	C	46	-1.40688	3.64169	4.73867
O	47	-1.34235	-2.96397	3.38237	O	47	-1.34213	-6.84395	2.98753	O	47	-0.88513	4.92055	4.47237
O	48	0.00364	-2.74797	4.05290	O	48	-2.88224	-6.39642	2.39160	O	48	-1.31065	6.35219	4.75153
H	49	0.41236	-1.27118	4.07635	H	49	-4.16429	-7.01641	2.15078	H	49	-2.69648	6.68357	4.19099
H	50	0.45526	-0.85820	3.06889	H	50	-4.87736	-8.57653	2.21353	H	50	-2.74101	6.48913	3.11987
H	51	-0.30599	-0.68465	4.65570	H	51	-6.39463	-7.91759	1.69410	H	51	-3.45979	6.07500	4.68322
H	52	1.39798	-1.15350	4.53559	H	52	-6.34263	-6.56950	1.48621	H	52	-2.93632	7.73638	4.36620
H	53	-0.00521	-3.33186	5.47512	H	53	-5.05230	-6.04850	1.75391	H	53	-1.27111	6.62137	6.26800
H	54	0.98767	-3.25045	5.92623	H	54	-4.38808	-4.68347	1.68900	H	54	-1.49608	7.67148	6.47449
H	55	-0.29530	-4.38473	5.46107	H	55	-2.98095	-5.04999	2.13417	H	55	-0.28414	6.39181	6.67520
H	56	-0.71188	-2.78420	6.10447	H	56	-1.79536	-4.34679	2.42352	H	56	-2.01222	6.00341	6.78195
H	57	-3.00076	-1.92478	4.43712	H	57	-1.64756	-3.27974	2.31672	H	57	-2.36297	3.42714	5.19827
H	58	-4.99378	-3.04782	2.77208	H	58	-5.02433	-3.69237	2.67490	H	58	-0.78690	1.21828	4.39566
H	59	-5.81589	-2.26402	3.53964	H	59	-4.99062	-4.08447	3.69375	H	59	0.50303	0.07473	4.09792
H	60	-5.68936	-1.22124	4.57957	H	60	-4.49016	-2.73887	2.65049	H	60	-0.51708	-1.30124	4.33098
H	61	-7.00250	-0.84749	4.88580	H	61	-6.06838	-3.50581	2.40884	H	61	-1.76078	-0.89044	4.65892
H	62	-7.97389	-1.53201	4.14446	H	62	-4.42504	-4.12673	0.25837	H	62	-1.92358	0.51711	4.70136
H	63	-7.19691	-2.46600	3.29464	H	63	-5.45405	-3.88410	-0.02201	H	63	-3.33610	0.79689	5.03459
H	64	-7.47090	-3.40181	2.35932	H	64	-4.05390	-4.86922	-0.45171	H	64	-3.93504	-0.45929	5.18178
H	65	-5.99321	-4.07240	1.76318	H	65	-3.82094	-3.22206	0.16284	H	65	-3.06381	-1.53070	4.95245
H	66	-8.42457	-3.72778	1.97321	H	66	-7.19508	-5.98867	1.15987	H	66	-3.36658	-2.69441	4.99127
H	67	-9.15976	-1.34966	4.21817	H	67	-7.24107	-8.57724	1.57715	H	67	-5.34249	-0.62270	5.46776
H	68	-7.30991	0.19715	5.83561	H	68	3.90911	-5.15964	4.44633	H	68	-5.52903	-1.68783	5.59756
H	69	-8.39342	0.24309	5.93669	H	69	2.98480	-2.22195	3.90064	H	69	-5.60573	-0.08375	6.37879
H	70	-6.85312	-0.02443	6.80092	H	70	4.08264	-1.81143	4.17617	H	70	-5.94809	-0.24086	4.64301
H	71	-6.92929	1.15805	5.48101	H	71	-0.25960	-1.65419	2.77037	H	71	-3.92823	1.84051	5.17216
H	72	-4.71748	-0.74074	5.11156	H	72	1.08941	0.48736	3.67310	H	72	-0.13259	-2.30209	4.21267
H	73	3.04177	-3.44925	3.69327	H	73	2.85821	0.36365	3.89579	H	73	-0.43379	9.31310	4.14886
H	74	3.52058	-5.00455	1.63514	H	74	2.15367	0.21405	2.26522	H	74	1.91220	9.48782	2.98244

Table S4. Cartesian coordinates (Å) of the optimized structures: the stacked dimer models of **4** (Continued).

CF		x (Å)	y (Å)	z (Å)
C	1	0.02652	-0.00770	0.09051
N	2	0.27576	-1.29512	-0.51832
C	3	1.55400	-1.72386	-0.88587
C	4	1.34983	-2.99087	-1.61646
C	5	-0.04488	-3.23922	-1.66029
C	6	-0.39479	-4.37828	-2.29755
S	7	1.02556	-5.18537	-2.85811
C	8	2.10569	-3.95908	-2.22761
C	9	3.53646	-4.08450	-2.37503
S	10	4.23566	-5.51195	-3.11793
C	11	5.81033	-4.92453	-2.80672
C	12	7.17375	-5.37364	-2.95875
S	13	8.02985	-6.71275	-3.60666
C	14	9.53583	-5.99390	-3.13609
C	15	9.37596	-4.78756	-2.51750
C	16	8.00857	-4.43149	-2.41331
C	17	7.22457	-3.24851	-1.87159
C	18	5.80606	-3.70081	-2.18043
C	19	4.50843	-3.21115	-1.93632
C	20	4.25899	-2.27714	-1.44808
C	21	7.58910	-1.97190	-2.63775
C	22	7.44679	-2.11836	-3.70954
O	23	6.96244	-1.13537	-2.32303
O	24	8.63414	-1.70204	-2.46202
C	25	7.43180	-3.06357	-0.36232
N	26	8.47487	-2.81402	-0.14880
C	27	7.17541	-3.97622	0.18006
C	28	6.80238	-2.25051	0.01010
C	29	10.20519	-4.19347	-2.15699
C	30	10.45680	-6.51530	-3.34868
S	31	-1.37388	-4.79538	-2.47755
C	32	-0.74520	-2.13637	-0.96072
C	33	-1.92244	-1.95581	-0.78253
S	34	2.56674	-1.11918	-0.61971
C	35	0.80641	0.19970	0.82211
C	36	0.02137	0.77413	-0.67277
S	37	-0.94750	-0.04477	0.57594
C	38	-2.74092	-1.18946	-3.85691
C	39	-1.54422	-1.76401	-4.43939
C	40	-0.25763	-1.28105	-4.18897
C	41	0.64871	-2.16476	-4.95316
C	42	-0.14528	-3.15048	-5.58910
C	43	0.54903	-4.02458	-6.35018
C	44	2.23380	-3.64594	-6.27910
C	45	1.98826	-2.26853	-5.22681
C	46	3.09128	-1.43542	-4.80913
O	47	4.65141	-1.53436	-5.60454
O	48	5.24550	-0.25777	-4.63202
H	49	6.44269	0.54151	-4.51221
H	50	8.00627	0.64011	-5.21164
H	51	8.41564	1.94776	-4.14916
H	52	7.39454	2.28299	-3.30741
H	53	6.25261	1.47142	-3.52099
H	54	4.86301	1.35806	-2.91762
H	55	4.31331	0.19952	-3.73185
H	56	3.07512	-0.46072	-3.83848
H	57	2.18624	-0.23158	-3.26765
H	58	4.04200	2.63339	-3.16218
H	59	3.99010	2.86282	-4.22870
H	60	3.02387	2.50500	-2.78499
H	61	4.49434	3.48417	-2.64499
H	62	4.92241	1.03211	-1.41844
H	63	5.38804	1.85775	-0.87242
H	64	5.50722	0.12754	-1.23622
H	65	3.92125	0.86302	-1.01883
H	66	7.46706	3.07711	-2.57623
H	67	9.39332	2.39918	-4.22335
H	68	0.19452	-4.85807	-6.93645
H	69	-1.56546	-2.91151	-5.23948
H	70	-2.55305	-3.52914	-5.53845
H	71	-0.01695	-0.33986	-3.46709
H	72	-2.98481	-1.67532	-2.91082
H	73	-2.55782	-0.13158	-3.67407
H	74	-3.56193	-1.31644	-4.56167