Electronic Supplementary Material (ESI) for ChemComm.

- Supporting Information -

Molecular design of two-dimensional donor-acceptor covalent organic frameworks for intramolecular singlet fission

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Section S1. Monomers characterization

Table S1.1 S_1, T_1, HOMO and LUMO energies (in eV) obtained at DFT and TDDFT(TDA) level with ωb97xd/6-31g* for selected acceptors as previously reported.[1]

Acceptors_R1	S_1	T_1	HOMO	LUMO
DPP_OMe	3.684	1.7695	-7.68939	-0.66205
DPP_Me	3.8528	1.7786	-7.45592	-0.39701
II_COOMe	3.1111	1.7845	-7.80858	-1.39921
DPP_H	4.0952	1.8454	-7.68041	-0.48762
II_H	3.1899	1.9691	-7.59742	-1.02831
II_Me	3.1298	1.9733	-7.49265	-0.95076
II_OMe	3.1683	2.042	-7.66436	-1.08002
DPP_COOMe	4.1485	2.0824	-8.29403	-0.83239

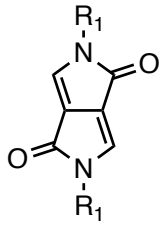
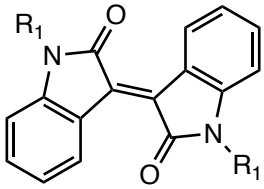
DPP	II
	

Figure S1.1 Molecular structure of selected DPP (diketopyrrolopyrrole) and II (isoindigo) acceptors.

Table S1.2 S_1, T_1, HOMO and LUMO energies (in eV) obtained at DFT and TDDFT(TDA) level with ωb97xd/6-31g* for selected donors as previously reported.[1]

Donors_R1_R2	S1	T1	HOMO	LUMO
2,2'-bithiophene_H_OH	4.519	2.7303	-6.72094	1.10505
BDT_OMe_OH	4.2371	2.8725	-6.77346	0.80191
2,2'-bithiophene_OH_OH	4.622	2.8086	-6.77482	1.1573
BDT_H_OH	4.3288	2.955	-6.82271	0.86804

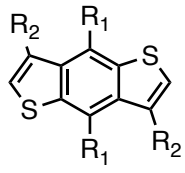
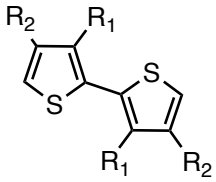
BDT	2,2'-bithiophene
	

Figure S1.2 Molecular structure of selected BDT (benzodithiophene) and 2-2'-bithiophene donors.

[1] J. T. Blaskovits, M. Fumanal, S. Vela, R. Fabregat, C. Corminboeuf, *Chem. Mater.* 2021, **33**, 2567.

Section S2. Tetramer model excited state characterization

Table S2.1 Excited state characterization of S_1 and T_1 of the DPP-BDT-DPP-TTE tetramer obtained at ωb97xD/6-31g* level using the ωb97xD/6-31g* optimized geometry in gas phase.

S_1 2.600 eV

A→A 0.225	A→D_1 0.086	A→D_2 0.048
D_1→A 0.222	D_1→D_1 0.144	D_1→D_2 0.022
D_2→ A 0.109	D_2→D_1 0.023	D_2→D_2 0.113

T_1 1.486 eV

A→A 0.454	A→D_1 0.096	A→D_2 0.077
D_1→A 0.095	D_1→D_1 0.061	D_1→D_2 0.013
D_2→ A 0.102	D_2→D_1 0.017	D_2→D_2 0.081

Table S2.2 Excited state characterization of S_1 and T_1 of the DPP-BDT-DPP-TTE tetramer obtained at ωb97xD/6-31g* level using the PBE-D3 optimized geometry of the Kagome lattice.

S_1 2.306 eV

A→A 0.211	A→D_1 0.102	A→D_2 0.054
D_1→A 0.162	D_1→D_1 0.127	D_1→D_2 0.020
D_2→ A 0.123	D_2→D_1 0.034	D_2→D_2 0.157

T_1 1.235 eV

A→A 0.389	A→D_1 0.114	A→D_2 0.076
D_1→A 0.094	D_1→D_1 0.077	D_1→D_2 0.014
D_2→ A 0.101	D_2→D_1 0.023	D_2→D_2 0.108

Table S3.2 Excited state characterization of S_1 and T_1 of the DPP-BDT-DPP-TTE tetramer obtained at ωb97xd/6-31g* level using the PBE-D3 optimized geometry of the Rhombic lattice.

S_1 2.120 eV

A→A 0.161	A→D_1 0.087	A→D_2 0.042
D_1→A 0.226	D_1→D_1 0.195	D_1→D_2 0.029
D_2→ A 0.093	D_2→D_1 0.029	D_2→D_2 0.131

T_1 1.162 eV

A→A 0.284	A→D_1 0.116	A→D_2 0.057
D_1→A 0.132	D_1→D_1 0.139	D_1→D_2 0.017
D_2→ A 0.085	D_2→D_1 0.026	D_2→D_2 0.140

Section S3. Optimized unit cell characterization

Table S3. Cell parameters of the optimized Kagome and rhombic unit cells.

	Kagome	Rhombic
a	55.752852	44.378063
b	56.015658	31.523305
c	21.726400	22.000000
α	90.910405	90.000000
β	90.950982	90.000000
γ	120.110730	88.623700
PBE-D3 total energy (a.u.)	-3506.5930861147	-3506.33134281630[a]
S_1 energy (eV) (tetramer)	1.20708 (1.44129)	1.18289 (1.58054)
T_1 energy (eV) (tetramer)	0.54586 (0.40297)	0.54364 (0.53335)

[a] Multiplied by 1.5 to be comparable to the Kagome unit cell

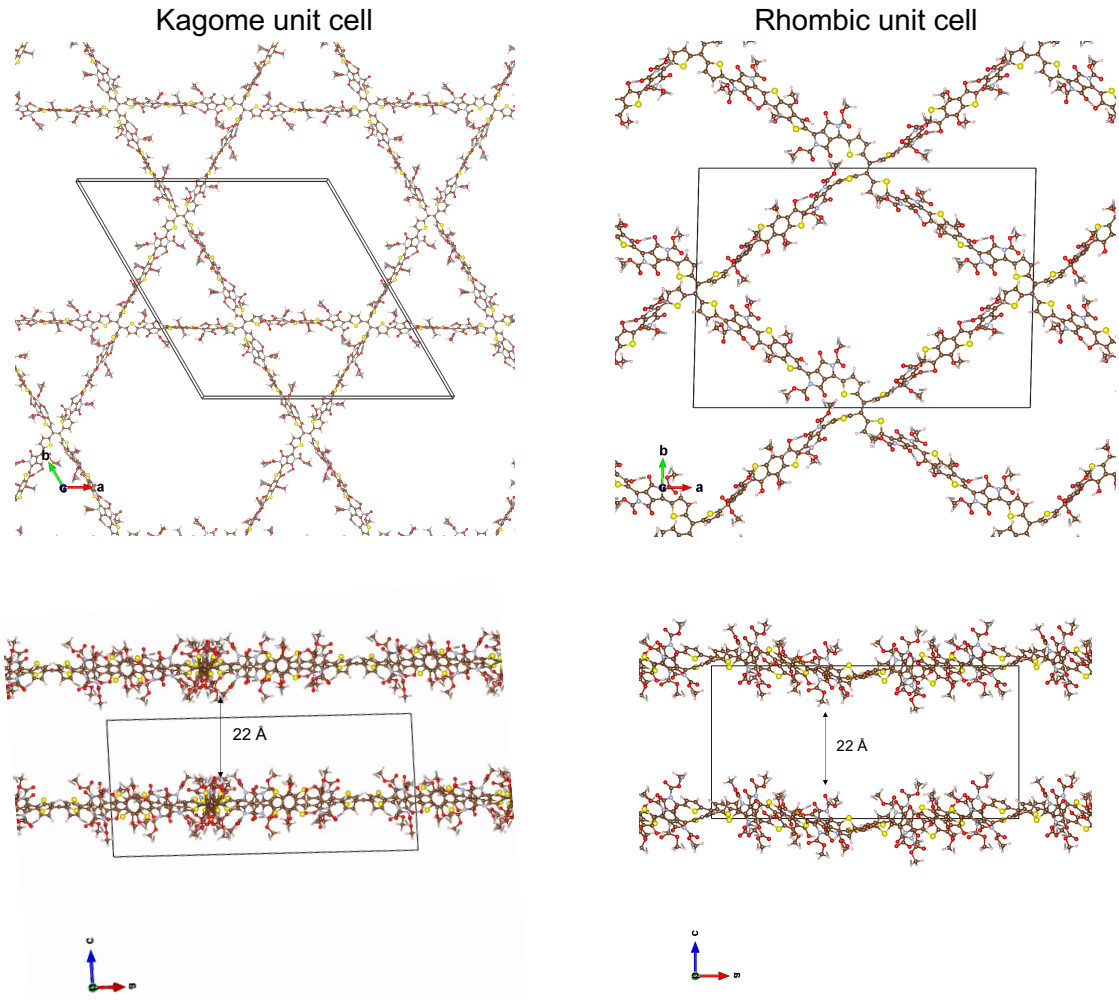


Figure S3. Representation of the front and side view of the Kagome and rhombic 2D COF monolayers.

Cif file of the optimized Kagome monolayer

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_cell_length_a    55.75285
_cell_length_b    56.01566
_cell_length_c    21.72640
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 'x,y,z'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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C        C      0.34193  -0.16703   0.37199
C        C      0.83017   0.34575   0.37476
C        C      0.34176   0.34670   0.36136
C        C      0.31773  -0.16543   0.37209
C        C      0.82947   0.32074   0.37555
C        C      0.28936   0.31559   0.36330
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C        C      0.37021   0.35161   0.36381
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C        C      0.80289   0.29428   0.36932
C        C      0.26748   0.29599   0.32558
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C        C      0.39111   0.36984   0.32552
C        C      0.79428   0.27849   0.31489
C        C      0.24253   0.29589   0.33217
C        C     -0.11086   0.41057   0.31522
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C        C      0.34005   0.76152   0.36606
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C        C      0.32997   0.78913   0.43044
C        C      0.33299  -0.11941   0.42927
C        C      0.32002   0.29593   0.35165
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```

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C	C	0.76077	0.34882	0.36614
C	C	0.34319	0.41775	0.36069
C	C	0.24511	0.76552	0.35783
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C	C	0.33515	0.26657	0.31417
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C	C	0.33663	0.29209	0.30997
C	C	0.32172	0.37426	0.31089
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H	H	0.22373	0.28301	0.30474
H	H	0.34627	0.25958	0.28512
H	H	0.34947	0.30779	0.27776
H	H	0.32366	0.74874	0.45805
H	H	0.32241	0.79482	0.47064
H	H	0.39195	-0.16034	0.42087
H	H	0.43803	-0.11344	0.40829
H	H	-0.14829	0.37654	0.26925
H	H	-0.10112	0.42385	0.27653
H	H	0.82617	0.39097	0.41886
H	H	0.77832	0.38910	0.41370
H	H	0.38744	0.38189	0.29188
H	H	0.43433	0.38207	0.30532
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H	H	0.22247	0.78202	0.40755
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H	H	-0.11755	0.27903	0.41875
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C	C	0.31501	0.18298	0.36816
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C	C	0.28225	0.20963	0.46770
C	C	0.32426	0.16779	0.33473
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H	H	0.27238	0.24452	0.53046
C	C	0.38766	0.19093	0.17038
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H	H	0.40647	0.20796	0.19232
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H	H	0.37369	0.06348	0.52817
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C	C	0.31453	0.12569	0.39611
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C	C	0.31550	0.10070	0.38675
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C	C	0.31723	0.07241	0.29904
C	C	0.31419	0.05790	0.40547
O	O	0.31251	0.08295	0.49220
C	C	0.31561	0.05273	0.34141
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H	H	0.34091	0.12518	0.51092
H	H	0.33337	0.10171	0.57256
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O	O	0.42502	0.35419	0.51903
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C	C	0.51723	0.37799	0.25157
C	C	0.40888	0.34962	0.57401
C	C	0.53907	0.34995	0.41286
S	S	0.53766	0.33910	0.29338
O	O	0.53934	0.39710	0.27002
O	O	0.50829	0.37044	0.19284
H	H	0.42028	0.34842	0.61433

H	H	0.40592	0.36746	0.57803
H	H	0.38889	0.33040	0.56857
C	C	0.56417	0.34942	0.40147
O	O	0.53309	0.35410	0.46989
C	C	0.56537	0.34260	0.33830
C	C	0.52734	0.38903	0.14795
C	C	0.58660	0.35448	0.44197
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H	H	0.51692	0.38065	0.10321
H	H	0.53099	0.40997	0.15620
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C	C	0.60788	0.34228	0.35548
O	O	0.58518	0.33326	0.25210
S	S	0.63681	0.35714	0.46100
C	C	0.59358	0.39016	0.51414
C	C	0.63259	0.34094	0.34412
C	C	0.57678	0.30490	0.23488
C	C	0.65113	0.35035	0.39579
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H	H	0.57474	0.39085	0.50231
H	H	0.59836	0.39438	0.56360
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H	H	0.59200	0.29948	0.25207
H	H	0.55613	0.29075	0.25241
H	H	0.57601	0.30403	0.18442
C	C	0.67921	0.35661	0.39740
H	H	0.64863	0.32377	0.29039
C	C	0.69275	0.34531	0.36456
N	N	0.69910	0.37583	0.43985
C	C	0.72090	0.35735	0.38542
C	C	0.68642	0.32318	0.32167
C	C	0.72613	0.37758	0.43449
C	C	0.69767	0.39779	0.47122
C	C	0.73309	0.34362	0.35679
N	N	0.71183	0.32241	0.31866
O	O	0.66518	0.30818	0.28924
O	O	0.70085	0.40170	0.52640
O	O	0.69334	0.41317	0.42983
C	C	0.71561	0.30629	0.27207
C	C	0.68865	0.43420	0.45780
O	O	0.73484	0.31558	0.23715
O	O	0.69489	0.27999	0.27410
H	H	0.70658	0.44847	0.48701
H	H	0.68572	0.44481	0.41909
H	H	0.67000	0.42429	0.48554
C	C	0.69608	0.26181	0.22690
H	H	0.71456	0.25997	0.23498
H	H	0.67712	0.24195	0.23200
H	H	0.69675	0.27004	0.18111
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C	C	0.46192	-0.05766	0.37599
N	N	0.43821	-0.05370	0.29589
C	C	0.47865	-0.03119	0.35093
C	C	0.47487	-0.05893	0.43354
C	C	0.46415	-0.02793	0.30001
C	C	0.41975	-0.05875	0.24492
C	C	0.50207	-0.01509	0.38868
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O	O	0.47118	-0.00885	0.26315
O	O	0.41462	-0.04158	0.22580
O	O	0.41015	-0.08459	0.22179
C	C	0.52386	0.01253	0.38339

C	C	0.52338	-0.02911	0.47284
C	C	0.38822	-0.09303	0.17465
C	C	0.53464	0.02723	0.32851
S	S	0.54271	0.03140	0.44980
O	O	0.54381	-0.02664	0.44808
O	O	0.51852	-0.03109	0.53337
H	H	0.39611	-0.07947	0.13523
H	H	0.38239	-0.11425	0.16169
H	H	0.37053	-0.09218	0.19362
C	C	0.56028	0.05263	0.34039
O	O	0.52441	0.01916	0.27120
C	C	0.56668	0.05752	0.40484
C	C	0.54016	-0.03173	0.57061
C	C	0.57889	0.07261	0.29958
H	H	0.50294	0.00785	0.26869
C	C	0.58947	0.08099	0.43075
H	H	0.55991	-0.01248	0.56567
H	H	0.53308	-0.03395	0.61790
H	H	0.54242	-0.04931	0.55597
C	C	0.60179	0.09602	0.32548
O	O	0.57617	0.07108	0.23659
C	C	0.60797	0.10104	0.39002
O	O	0.59276	0.08173	0.49355
S	S	0.62643	0.12193	0.28086
C	C	0.58003	0.04993	0.20675
C	C	0.63406	0.12594	0.40212
C	C	0.58887	0.10234	0.52609
C	C	0.64716	0.13891	0.34721
H	H	0.60026	0.05251	0.22070
H	H	0.56325	0.02922	0.21752
H	H	0.57957	0.05323	0.15727
O	O	0.64445	0.13333	0.45935
H	H	0.60463	0.12325	0.51367
H	H	0.56793	0.09883	0.51617
H	H	0.59121	0.09938	0.57509
C	C	0.67433	0.16173	0.34132
H	H	0.65627	0.15445	0.46694
C	C	0.69102	0.18422	0.38125
N	N	0.68901	0.16692	0.28634
C	C	0.71602	0.20327	0.35254
C	C	0.69003	0.19508	0.44019
C	C	0.71551	0.19296	0.29037
C	C	0.68489	0.14657	0.23977
C	C	0.73188	0.22612	0.39214
N	N	0.71586	0.22115	0.44586
O	O	0.67262	0.18523	0.48151
O	O	0.73178	0.20137	0.24804
O	O	0.68302	0.14964	0.18523
O	O	0.68450	0.12471	0.26659
C	C	0.72466	0.23748	0.50126
C	C	0.67728	0.10159	0.22412
O	O	0.74834	0.24888	0.52221
O	O	0.70337	0.23847	0.52600
H	H	0.69211	0.10803	0.18683
H	H	0.67817	0.08597	0.25205
H	H	0.65626	0.09388	0.20483
C	C	0.70962	0.25271	0.58589
H	H	0.72551	0.27446	0.58154
H	H	0.68994	0.25064	0.60004
H	H	0.71695	0.24288	0.61855
C	C	0.34845	0.44507	0.37377
C	C	0.33690	0.45879	0.34277
N	N	0.36735	0.46450	0.41854
C	C	0.34778	0.48592	0.36838
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C	C	0.36728	0.49010	0.41689

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C	C	0.33720	0.50021	0.33564
N	N	0.31992	0.48184	0.28817
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O	O	0.38080	0.50967	0.45455
O	O	0.40703	0.47527	0.47771
O	O	0.36450	0.43851	0.50012
C	C	0.34260	0.52776	0.34088
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C	C	0.37779	0.43131	0.54883
C	C	0.35210	0.54564	0.39383
S	S	0.33515	0.54260	0.27776
O	O	0.27851	0.48296	0.29256
O	O	0.29630	0.48000	0.20035
H	H	0.38895	0.44881	0.58145
H	H	0.36080	0.41366	0.57095
H	H	0.39232	0.42569	0.52900
C	C	0.35084	0.57043	0.38442
O	O	0.35988	0.54087	0.44822
C	C	0.34194	0.57127	0.32286
C	C	0.27166	0.47749	0.16962
C	C	0.35714	0.59305	0.42511
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C	C	0.33921	0.59287	0.29972
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H	H	0.27453	0.47542	0.12056
H	H	0.25307	0.45920	0.18562
C	C	0.35449	0.61472	0.40193
O	O	0.36600	0.59553	0.48538
C	C	0.34550	0.61542	0.34042
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S	S	0.36095	0.64348	0.44670
C	C	0.34499	0.57724	0.52721
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C	C	0.34891	0.60742	0.19607
C	C	0.34885	0.65579	0.38621
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H	H	0.35493	0.58304	0.57318
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H	H	0.34101	0.66342	0.26752
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N	N	0.34841	0.73068	0.29076
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O	O	0.30948	0.64582	0.49615
C	C	0.34789	0.74278	0.23398
C	C	0.30073	0.62665	0.54644
O	O	0.33190	0.75107	0.22217
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H	H	0.28212	0.60812	0.52867
H	H	0.31721	0.62209	0.55829
C	C	0.36594	0.75245	0.13465
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C	C	0.19713	0.31055	0.35496
N	N	0.21795	0.33175	0.44462
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C	C	0.15674	0.31277	0.34655
N	N	0.16053	0.30213	0.29052
O	O	0.19265	0.29013	0.25149
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O	O	0.23867	0.31857	0.51616
C	C	0.13452	0.31790	0.35431
C	C	0.13763	0.28165	0.25286
C	C	0.25660	0.32493	0.57057
C	C	0.12203	0.31897	0.40995
S	S	0.11727	0.32091	0.28892
O	O	0.11712	0.26233	0.27367
O	O	0.14356	0.28730	0.19326
H	H	0.24710	0.32871	0.61058
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H	H	0.27688	0.34322	0.56302
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C	C	0.07313	0.28943	0.52436
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C	C	0.07468	0.34961	0.22190
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H	H	0.01467	0.58327	0.47835
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O	O	0.13324	0.70956	0.51430
O	O	0.11527	0.70069	0.41513
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C	C	0.08959	0.69789	0.43786
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H	H	0.25728	0.69057	0.19452
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S	S	0.27765	0.33312	0.40990
S	S	0.35921	0.40139	0.39594
S	S	0.38310	0.33573	0.41198
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Cif file of the optimized rhombic monolayer

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H	H	-0.33667	0.03708	-0.10993
H	H	-0.05381	-0.30288	-0.21619
H	H	-0.02869	-0.28003	-0.16235
H	H	-0.05973	-0.24846	-0.19255
H	H	-0.15575	-0.29659	-0.09090
H	H	-0.24734	-0.24902	-0.20162
H	H	-0.23461	-0.19552	-0.19478
H	H	-0.20995	-0.23607	-0.22507
H	H	-0.33237	-0.13404	-0.30418
H	H	-0.35097	-0.08250	-0.30553
H	H	-0.31341	-0.08895	-0.27481
H	H	0.15146	-0.45033	-0.03767
H	H	0.15723	-0.47721	-0.10869
H	H	0.12598	-0.49096	-0.06142
H	H	0.25815	-0.28368	-0.12194
H	H	0.29295	-0.31163	-0.10543
H	H	0.25974	-0.34064	-0.12245
H	H	0.34340	-0.24977	-0.22754
H	H	0.34903	-0.19923	-0.26243
H	H	0.38068	-0.23538	-0.25168
H	H	-0.46977	-0.16177	-0.01974
H	H	-0.48138	0.10852	-0.07089
H	H	0.16331	0.41582	-0.22173
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N	N	0.41042	0.17604	-0.09622
N	N	-0.36915	0.10421	-0.09201
N	N	-0.13524	0.34395	-0.03426
N	N	-0.08777	-0.34076	-0.06010
N	N	-0.34905	-0.14039	-0.12810
N	N	0.12078	-0.38853	-0.02375
N	N	0.35335	-0.16685	-0.09214
O	O	0.10738	0.42200	-0.05917
O	O	0.18699	0.37221	-0.13361
O	O	0.15183	0.42499	-0.12973
O	O	0.28322	0.27632	-0.11493
O	O	0.31661	0.20322	-0.11480
O	O	0.37215	0.22918	-0.07421
O	O	0.44229	0.17460	-0.18101
O	O	0.42038	0.23676	-0.14795
O	O	-0.32777	0.14821	-0.11158
O	O	-0.39810	0.10926	-0.18085
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O	O	-0.28507	0.15380	-0.03708
O	O	-0.23105	0.18760	-0.05597
O	O	-0.09255	0.38793	-0.05208
O	O	-0.16290	0.33069	-0.12235
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O	O	-0.04623	-0.35444	-0.12232
O	O	-0.07227	-0.29153	-0.12939
O	O	-0.17798	-0.30726	-0.09649
O	O	-0.21477	-0.23954	-0.13359
O	O	-0.39447	-0.09895	-0.15219
O	O	-0.30934	-0.15089	-0.19639
O	O	-0.34985	-0.10957	-0.22202

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O	O	0.12191	-0.43437	-0.11038
O	O	0.25952	-0.31526	-0.03748
O	O	0.39235	-0.13039	-0.14436
O	O	0.31654	-0.19006	-0.15954
O	O	0.36663	-0.20586	-0.17421
S	S	0.21917	0.32300	-0.06869
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S	S	-0.44219	-0.05522	-0.04121
S	S	-0.43697	0.05412	-0.09946
C	C	0.09040	0.36319	0.05770
C	C	0.11357	0.36602	0.01490
C	C	0.13729	0.33589	0.02613
C	C	0.12974	0.31460	0.08145
C	C	0.08692	0.31409	0.15226
C	C	0.06283	0.33285	0.24404
C	C	0.19248	0.27257	0.00821
C	C	0.22222	0.25444	-0.00063
C	C	0.23556	0.21863	0.02933
C	C	0.26403	0.20523	0.00947
C	C	0.21831	0.21695	0.13209
C	C	0.32753	0.06884	0.02750
C	C	0.27728	0.05204	0.05124
C	C	-0.38207	0.12578	0.07083
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C	C	-0.23691	-0.28597	0.01196
C	C	-0.21834	-0.39821	0.16222
C	C	-0.26546	-0.26886	0.02433
C	C	-0.28220	-0.24841	0.12328
C	C	-0.36910	-0.16449	0.03152
C	C	-0.41492	-0.15219	0.09597
C	C	-0.45770	-0.13058	0.15234
C	C	0.06187	0.38515	0.06247
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C	C	0.01887	0.43964	0.06151
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C	C	-0.03353	0.46852	0.07181

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C	C	0.11021	-0.40291	0.03236
C	C	0.12634	-0.38135	0.07696
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C	C	0.12373	-0.37211	0.14077
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C	C	0.18316	-0.29718	0.08049
C	C	0.14750	-0.31899	0.20879
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C	C	0.40601	0.01179	0.12451
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H	H	0.05667	0.36227	0.26782
H	H	0.04272	0.31493	0.23254
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H	H	0.24036	0.22465	0.15134
H	H	0.20424	0.24587	0.12767
H	H	0.20693	0.19440	0.16166
H	H	0.28379	0.04676	0.09876
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H	H	-0.33369	0.17236	0.25743
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H	H	0.23918	-0.19228	0.18055
H	H	0.23216	-0.13617	0.17477
H	H	0.30734	-0.12843	0.07062
H	H	0.42347	0.03110	0.10407
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O	O	0.08505	0.27651	0.16283
O	O	0.07799	0.34636	0.18892
O	O	0.17227	0.24994	0.03694
O	O	0.22224	0.19543	0.07430
O	O	0.38900	0.05162	-0.00383
O	O	0.33698	0.03668	0.05213
O	O	0.29817	0.08041	0.02179
O	O	-0.39999	0.11200	0.10754
O	O	-0.37965	0.17484	0.18136
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O	O	-0.26861	0.31766	0.10341
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O	O	-0.17586	0.36495	0.15258
O	O	-0.15004	0.41162	0.23731
O	O	-0.10565	0.44235	0.21141
O	O	-0.11479	-0.44043	0.07450
O	O	-0.16639	-0.43791	0.13656
O	O	-0.19821	-0.38298	0.11533
O	O	-0.27952	-0.28109	0.07714
O	O	-0.32775	-0.23465	0.01822
O	O	-0.35366	-0.17949	0.07456
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O	O	0.10926	-0.38811	0.18159
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O	O	0.17055	-0.29166	0.21088
O	O	0.21103	-0.34709	0.01474
O	O	0.23318	-0.16638	0.09311
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O	O	0.33528	-0.11454	0.09665
O	O	0.37028	-0.05467	0.14807
O	O	0.40173	-0.02242	0.08140
S	S	0.28500	0.16368	0.04147
S	S	-0.31503	0.24321	0.07285
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S	S	0.05465	0.43478	0.02836
S	S	-0.05368	0.42511	0.04771
S	S	0.18777	-0.24491	0.10716
S	S	-0.55343	0.05610	-0.07600
H	H	0.19344	-0.36417	0.02416
H	H	-0.30162	0.15198	-0.07005