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Packing effect on the transfer integrals and mobility in α,α′-bis(dithieno[3,2-*b*:2′,3′- *d*]thiophene) (BDT) and its heteroatom-substituted analogues

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Methodology

In order to calculate the electronic coupling the single-crystal structures were considered to generate all the possible nearest-neighbor intermolecular hopping pathways. The electronic coupling was obtained either by Koopmans' theorem, which has been widely employed [S1], or by directly evaluating the coupling element for the frontier orbitals [S2, S3]. In the former case, the charge transfer integral corresponds to half of the splitting of the HOMO or LUMO levels for holes or electrons. Bredas and co-workers [S4] have extensively investigated the parameters governing the transport on many conjugated systems by frontier orbital splitting. Valeev *et al.* [S5] cautioned recently that when the dimer is not cofacially stacked, the site-energy

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correction due to the crystal environment should be taken into account.

In this work a direct approach was utilized to investigate the charge transport properties [S2, S3]. The electronic coupling for hole/electron transfer in this scheme can be written as

$$t_{e/h} = \langle \phi_{LUMO/HOMO}^{0,site1} \mid F^0 \mid \phi_{LUMO/HOMO}^{0,site2} \rangle = \langle \phi_{LUMO/HOMO}^{0,site1} \mid h_{core} \mid \phi_{LUMO/HOMO}^{0,site2} \rangle +$$
$$\sum_{l(occ)} (\langle \phi_{LUMO/HOMO}^{0,site1} \phi_l^0 \mid \phi_{LUMO/HOMO}^{0,site2} \phi_l^0 \rangle - \langle \phi_{LUMO/HOMO}^{0,site1} \phi_{LUMO/HOMO}^{0,site2} \phi_l^0 \phi_l^0 \rangle) \quad (4)$$

Where, $t_{e/h}$ is the charge transfer coupling integral for the electron/hole and $\phi_{LUMO/HOMO}^{0,site1}$ and $\phi_{LUMO/HOMO}^{0,site2}$ represent the LUMOs/HOMOs of the two independent adjacent molecules 1 and 2. F^0 is the Fock operator for the dimer for a fixed pathway and the suffix zero indicates that the molecular orbitals appearing in the operator (the density matrix, for instance) are unperturbed. The summation over '*l*' includes all of the occupied levels for both sites and represents the Coulomb and exchange interactions between the transferred electron/hole and the whole system. It has been shown that the exchange term can contribute to the spin dependence of the charge recombination rates in exciton formation [S6]. The non-interacting molecular orbitals of the two individual molecules are calculated individually by the standard self-consistent-field (SCF) procedure. These non-interacting orbitals are used to construct the dimer Fock matrix as well as the two-electron integrals (Eq. 4). Specifically, the non-interacting orbitals and associated density matrix are used in evaluating the Fock matrix of the dimer structure. The density matrix of F^0 is constructed from non-interacting molecular orbitals. In practice, the Fockmatrix is evaluated as

$F = SC\varepsilon C^{-1}$ (5)

Where, S is the overlap matrix for the dimer taken from the crystal structure the Kohn–Sham orbital C and eigenvalue ε are obtained by diagonalizing the zeroth-order Fock matrix without any self-consistent field iteration [S2]. The intermolecular electronic couplings have been obtained by directly evaluating the dimer Fock matrix with unperturbed monomer's molecular orbits at the DFT/pw91pw91 with 6-31g** basis set. More over Shuai et al. explained that the GGA functional is chosen to be pw91pw91/6-31g(d). It has been shown that this choice of functional gives the best description for the bandwidth of organic solid [S2a]. Intuitively, one would think of a Hartree–Fock orbital because by definition it is a real electronic orbital and the Kohn–Sham orbital is fictitious. However, it has been known that the Hartree–Fock bandwidth for a polymer is always about 20%–30% larger than the result from (photoemission) experiments [S2b]. And from previous studies, the electronic coupling from the DFT orbital is usually about 20% less than that of the Hartree–Fock orbital [S2c]. Thus, we can believe that the Kohn–Sham orbitals from DFT can give a better description for the orbital coupling, which is proportional to the bandwidth [S2d].

Huang and Kertesz [S7] have reported that this functional as best description for intermolecular coupling term. Yang *et al.* [S8] have mentioned that this direct method for the coupling is equivalent to the site-energy corrected frontier orbital splitting method and offers remarkable simplicity in computation. INDO based calculations using ‘‘energy-splitting-in-dimer’’ method [S5] often over estimate electronic

couplings and also ignore the orthogonalisation of the basis. Direct method has been proven to be good in generating accurate results [S2, S8-S11].

Transfer integrals and mobilities

Table S1. The electronic couplings V of BDT (experimental crystal) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.883	155.5	52.5
2	5.882	0.11307	-12.9
3	7.859	-0.010916	-0.20163
4	16.691	2	-0.61491
5	17.136	0.1158	-0.24825
6	16.956	-7	1.4
7	17.823	-0.017707	0.0078135

Table S2. The electronic couplings V of BDT (simulated in C2/c) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.883	155.6	52.3
2	7.859	0.0072794	-0.25761
3	5.622	0.049693	-11.2
4	16.601	1.3	-0.066405
5	17.049	0.12082	-0.22874
6	17.823	-0.0091411	0.0029418
7	16.956	-8.3	2.6

Table S3. The electronic couplings V of NHBDT (simulated in C2/c) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.883	129.8	21.1
2	8.048	-0.0016533	0.0032838
3	5.882	-0.79785	3.1
4	16.691	0.82874	-0.69106
5	17.136	-0.029291	0.025037
6	17.823	-0.012186	0.0066714
7	16.956	-0.45033	0.029889

Table S4. The electronic couplings V of OBDT (simulated in C2/c) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.883	112	10
2	8.048	-0.00222	0.00061294
3	5.882	-1.1	3.4
4	16.691	0.48973	-0.45558
5	17.136	-0.017903	0.015916
6	17.823	-0.0029575	0.0016311
7	16.956	-0.27119	-0.0038706

Table S5. The electronic couplings V of BHBDT (simulated in C2/c) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.883	163.3	116.7
2	8.023	-0.30407	-0.076346
3	5.882	-5.8	-0.9234
4	16.691	4.1	-5.5
5	15.776	-0.21738	0.25726
6	17.823	0.00028885	-0.00035474
7	16.956	-2.2	4

Table S6. The electronic couplings V of BDT (simulated in P1) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.676	206.4	180.6
2	6.267	-0.4773	-3.6
3	8.144	-0.013506	-0.48459
4	16.776	-0.17711	1
5	17.134	-0.15874	-0.35438
6	17.03	3.3	-0.38665
7	17.751	-0.010716	0.00088934

Table S7. The electronic couplings V of NHBDT (simulated in P1) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.703	180.4	62
2	8.211	-0.0012947	-0.018169
3	5.597	-0.53462	-13.6
4	16.198	-2.6	-2.2
5	16.595	-0.01499	-0.010585
6	16.342	-1.8	-0.75393
7	16.43	-0.22973	-0.21637

Table S8. The electronic couplings V of OBDT (simulated in P1) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	4.439	23.1	-6.2
2	9.971	0.00020164	0.0058574
3	4.286	-15.1	-12.2
4	16.438	2.7	2.1
5	16.393	-0.0040867	-0.0066685
6	16.395	-0.10612	-0.046155
7	16.382	-1	0.50175

Table S9. The electronic couplings V of BHBDT (simulated in P1) for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.889	-249.5	168.9
2	5.927	43.4	15.9
3	8.288	-0.07059	-0.016041
4	16.705	3.9	-5.7
5	17.157	0.17616	0.21458
6	16.949	-1.4	2.7
7	17.823	-0.001887	0.0027716

Table S10. The electronic couplings V of BDT opt P-1 for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.672	202.7	185.0
2	8.179	0.011467	-0.52312
3	6.243	-0.80913	-2.8
4	17.654	0.0022257	-0.00027438
5	17.055	1.5	-0.53181
6	19.314	1.5	-0.28586
7	19.056	-0.0000000000018747	-0.0000000000058520

Table S11. The electronic couplings V of NHBDT opt P-1 for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	V_h *(meV)*	V_e *(meV)*
1	3.603	230.8	132.4
2	5.670	-1.3	6.0
3	7.643	0.0020434	0.011075
4	16.512	2.1	-0.19843
5	16.506	1.2	-0.32374
6	17.268	0.0067709	-0.0026279
7	17.832	-0.000021141	0.000036111

Table S112. The electronic couplings V of OBDT opt P-1 for the seven pathways are

calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	*V_h (meV)*	*V_e (meV)*
1	3.690	172.3	129.3
2	5.402	-0.51552	9.0
3	7.039	-0.0073013	-0.011183
4	15.332	-1.5	-0.21396
5	15.610	0.17919	0.0088844
6	15.887	-0.020564	0.00040783
7	16.559	0.00067002	-0.0017179

Table S13. The electronic couplings V of BHBDT opt P-1 for the seven pathways are calculated at DFT/pw91pw91/ 6-31G** level.

Route	*Centre to centre Distance (A)*	*V_h (meV)*	*V_e (meV)*
1	3.636	-556.7	369.3
2	6.378	15.2	-4.1
3	8.108	-0.58155	-0.14897
4	16.926	0.027285	0.42417
5	16.946	0.0088533	0.17175
6	17.728	-0.00043505	0.0013512
7	19.386	-0.0000000000034775	0.00000000000181113

Table S14. Calculated hole and electron mobilities (cm^2/Vs)

Complexes	*External reorganization energy*	*Total hole reorganization energy*	*Hole mobility*	*Exp[b]*	*Total electron reorganization energy*	*Electron mobility*
BDT[a]	0.0	0.293	0.427	0.05	0.256	0.071
	0.05	0.343	0.243		0.306	0.040

	0.10	0.393	0.140	0.356	0.023
	0.15	0.443	0.081	0.406	0.013
	0.20	0.493	0.047	0.456	0.008
BDT[c]	0.0	0.293	0.427	0.256	0.071
	0.05	0.343	0.243	0.306	0.040
	0.10	0.393	0.140	0.356	0.023
	0.15	0.443	0.081	0.406	0.013
	0.20	0.493	0.047	0.456	0.008
BDT[d]	0.0	0.293	0.675	0.256	0.790
	0.05	0.343	0.385	0.306	0.446
	0.10	0.393	0.223	0.356	0.255
	0.15	0.443	0.129	0.406	0.147
	0.20	0.493	0.075	0.456	0.086
NHBDT[c]	0.0	0.293	0.298	0.696	0.0001
	0.05	0.343	0.150	0.746	0.0000540
	0.10	0.393	0.088	0.796	0.0000322
	0.15	0.443	0.052	0.846	0.0000193
	0.20	0.493	0.033	0.896	0.0000129
NHBDT[d]	0.0	0.293	0.523	0.696	0.000780
	0.05	0.343	0.279	0.746	0.000418
	0.10	0.393	0.152	0.796	0.000251
	0.15	0.443	0.098	0.846	0.000150

	0.20	0.493	0.058	0.896	0.0000994
OBDT[c]	0.0	0.282	0.251	0.289	0.002
	0.05	0.332	0.143	0.339	0.000972
	0.10	0.382	0.082	0.389	0.000559
	0.15	0.432	0.048	0.439	0.000325
	0.20	0.482	0.028	0.489	0.000190
OBDT[d]	0.0	0.282	0.011	0.289	0.003
	0.05	0.332	0.00646	0.339	0.00161
	0.10	0.382	0.00371	0.389	0.00092
	0.15	0.432	0.00215	0.439	0.00054
	0.20	0.482	0.00126	0.489	0.00031
BHBDT[c]	0.0	0.122	3.812	0.127	1.816
	0.05	0.172	1.980	0.177	0.948
	0.10	0.222	1.074	0.227	0.516
	0.15	0.272	0.598	0.277	0.288
	0.20	0.322	0.339	0.327	0.164
BHBDT[d]	0.0	0.122	8.699	0.127	3.79
	0.05	0.172	4.517	0.177	1.980
	0.10	0.222	2.452	0.227	1.078
	0.15	0.272	1.366	0.277	0.602
	0.20	0.322	0.774	0.327	0.341
BDTe	0.0	0.293	0.650	0.256	0.828

	0.05	0.343	0.370	0.306	0.459
	0.10	0.393	0.213	0.356	0.263
	0.15	0.443	0.123	0.406	0.158
	0.20	0.493	0.072	0.456	0.089
NHBDTe	0.0	0.293	0.811	0.696	0.0035
	0.05	0.343	0.462	0.746	0.0021
	0.10	0.393	0.266	0.796	0.0012
	0.15	0.443	0.148	0.846	0.00082
	0.20	0.493	0.090	0.896	0.000446
OBDTe	0.0	0.282	0.538	0.289	0.278
	0.05	0.332	0.328	0.339	0.158
	0.10	0.382	0.176	0.389	0.094
	0.15	0.432	0.101	0.439	0.053
	0.20	0.482	0.059	0.489	0.031
BHBDTe	0.0	0.122	38.889	0.127	15.996
	0.05	0.172	20.200	0.177	8.772
	0.10	0.222	10.766	0.227	4.549
	0.15	0.272	6.107	0.277	2.487
	0.20	0.322	3.460	0.327	1.441

[a] Mobility of exp crystal structure
[b] Experimental data from reference S12
c Mobility of simulated crystal C2/C
d Mobility of simulated crystal P1
e Mobility of simulated crystal $P\bar{1}$

Fig. S1. Selected dimers of BDT along OAC axis

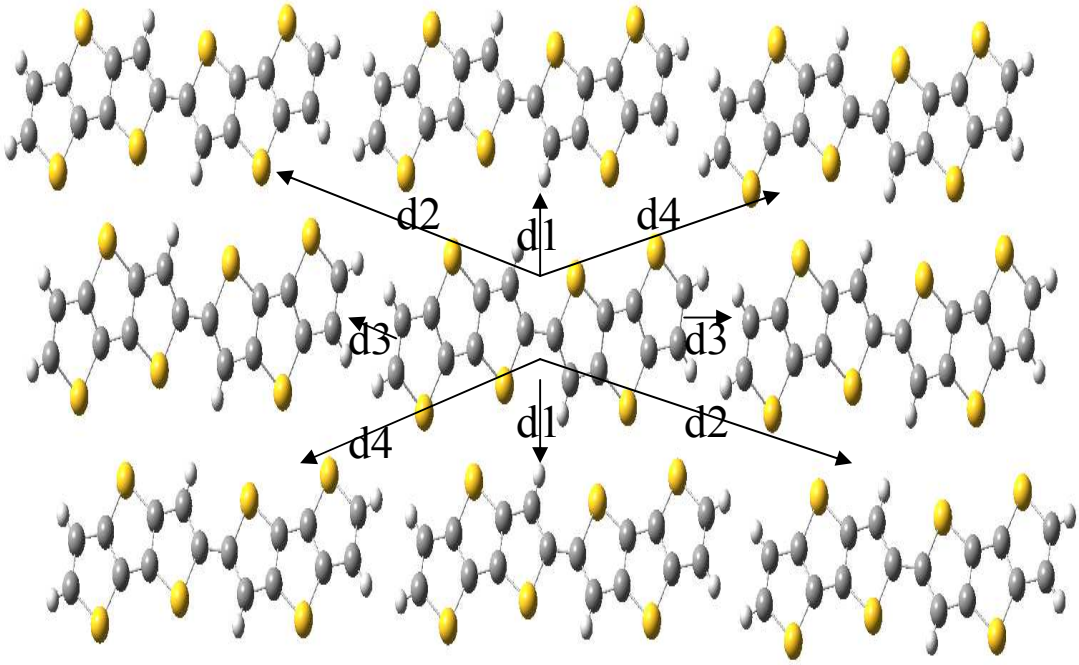
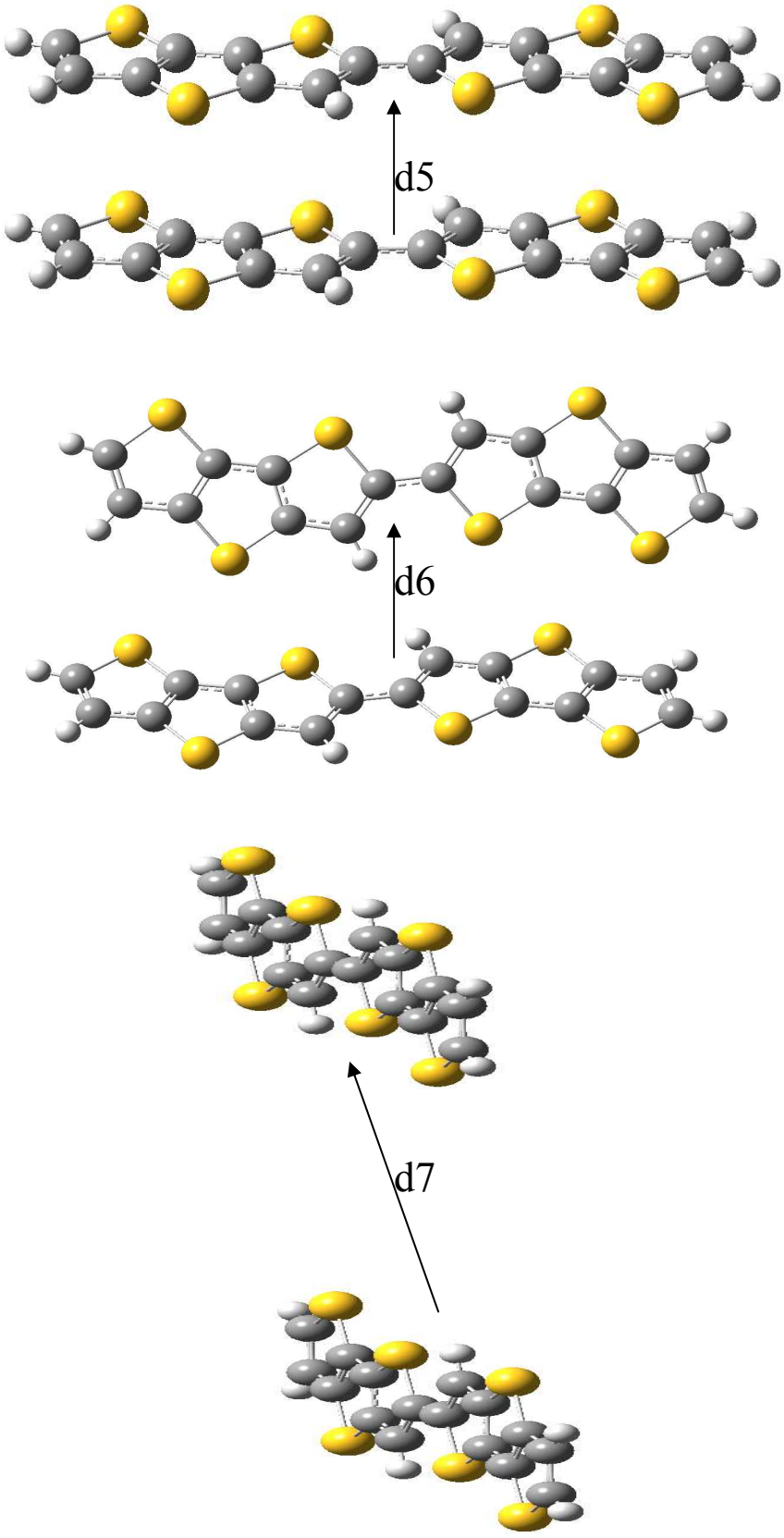


Fig S1 Selected dimers along OAB axis



Experimental crystal structure of BDT

Geometries of dimers of BDT

d1

Mode1 (first molecule)

S	35.67040000	2.09470000	12.59720000
S	34.38680000	3.71910000	8.96160000
C	38.48250000	2.42210000	11.98890000
H	38.83720000	2.06250000	12.79320000
C	33.27430000	2.71060000	11.07560000
H	32.62400000	2.40070000	11.69470000
C	37.10320000	2.53200000	11.71430000
C	34.68640000	2.66440000	11.28270000
C	36.82290000	3.09430000	10.47190000
C	35.41910000	3.16230000	10.22780000
C	32.99430000	3.26050000	9.86810000
H	32.10790000	3.38210000	9.54880000
S	38.27330000	3.50980000	9.63810000
C	39.25420000	2.89780000	10.95140000
S	44.27860000	3.73040000	9.19880000
S	45.56220000	2.10600000	12.83440000
C	41.46660000	3.40300000	9.80710000
H	41.11190000	3.76260000	9.00280000
C	46.67470000	3.11450000	10.72040000
H	47.32500000	3.42440000	10.10140000
C	42.84590000	3.29310000	10.08170000
C	45.26270000	3.16070000	10.51330000
C	43.12610000	2.73080000	11.32410000
C	44.52990000	2.66280000	11.56820000
C	46.95480000	2.56460000	11.92790000
H	47.84120000	2.44300000	12.24720000
S	41.67570000	2.31530000	12.15790000
C	40.69480000	2.92730000	10.84460000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000

C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000
C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

d2

Mode1 (first molecule)

S	45.34700000	7.91980000	3.74980000
S	46.63060000	9.54420000	7.38540000
C	42.53490000	8.24720000	4.35810000
H	42.18020000	7.88760000	3.55380000
C	47.74310000	8.53570000	5.27140000
H	48.39340000	8.22580000	4.65240000
C	43.91420000	8.35710000	4.63270000
C	46.33100000	8.48950000	5.06430000
C	44.19450000	8.91940000	5.87510000
C	45.59830000	8.98740000	6.11920000
C	48.02310000	9.08560000	6.47890000
H	48.90950000	9.20720000	6.79820000
S	42.74410000	9.33490000	6.70890000
C	41.76320000	8.72290000	5.39560000
S	36.73880000	9.55550000	7.14820000
S	35.45520000	7.93110000	3.51260000
C	39.55080000	9.22810000	6.53990000
H	39.90560000	9.58770000	7.34420000

C	34.34270000	8.93960000	5.62660000
H	33.69240000	9.24950000	6.24560000
C	38.17160000	9.11820000	6.26530000
C	35.75480000	8.98580000	5.83370000
C	37.89130000	8.55590000	5.02290000
C	36.48750000	8.48790000	4.77880000
C	34.06270000	8.38970000	4.41910000
H	33.17620000	8.26810000	4.09980000
S	39.34170000	8.14040000	4.18910000
C	40.32260000	8.75240000	5.50240000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000
C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000
C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

d3

Mode1 (first molecule)

S	45.34700000	0.15300000	3.74980000
S	46.63060000	1.77740000	7.38540000
C	42.53490000	0.48040000	4.35810000
H	42.18020000	0.12080000	3.55380000
C	47.74310000	0.76890000	5.27140000
H	48.39340000	0.45900000	4.65240000
C	43.91420000	0.59030000	4.63270000
C	46.33100000	0.72270000	5.06430000
C	44.19450000	1.15260000	5.87510000
C	45.59830000	1.22060000	6.11920000
C	48.02310000	1.31880000	6.47890000
H	48.90950000	1.44040000	6.79820000
S	42.74410000	1.56810000	6.70890000
C	41.76320000	0.95610000	5.39560000
S	36.73880000	1.78870000	7.14820000
S	35.45520000	0.16430000	3.51260000
C	39.55080000	1.46130000	6.53990000
H	39.90560000	1.82090000	7.34420000
C	34.34270000	1.17280000	5.62660000
H	33.69240000	1.48270000	6.24560000
C	38.17160000	1.35140000	6.26530000
C	35.75480000	1.21900000	5.83370000
C	37.89130000	0.78910000	5.02290000
C	36.48750000	0.72110000	4.77880000
C	34.06270000	0.62290000	4.41910000
H	33.17620000	0.50130000	4.09980000
S	39.34170000	0.37360000	4.18910000
C	40.32260000	0.98560000	5.50240000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000
C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000

C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

d4

Mode1 (first molecule)

S	60.05470000	5.97810000	14.64780000
S	61.33830000	7.60250000	18.28340000
C	57.24270000	6.30550000	15.25610000
H	56.88800000	5.94590000	14.45180000
C	62.45090000	6.59400000	16.16940000
H	63.10110000	6.28410000	15.55040000
C	58.62200000	6.41540000	15.53070000
C	61.03880000	6.54780000	15.96230000
C	58.90230000	6.97770000	16.77310000
C	60.30610000	7.04570000	17.01720000
C	62.73090000	7.14390000	17.37690000
H	63.61730000	7.26550000	17.69620000
S	57.45190000	7.39320000	17.60690000
C	56.47100000	6.78120000	16.29360000
S	51.44660000	7.61380000	18.04620000
S	50.16300000	5.98940000	14.41070000
C	54.25860000	7.28640000	17.43790000
H	54.61330000	7.64600000	18.24220000

C	49.05050000	6.99790000	16.52460000
H	48.40020000	7.30780000	17.14370000
C	52.87930000	7.17650000	17.16330000
C	50.46250000	7.04410000	16.73170000
C	52.59910000	6.61420000	15.92090000
C	51.19530000	6.54620000	15.67680000
C	48.77040000	6.44800000	15.31710000
H	47.88400000	6.32640000	14.99780000
S	54.04950000	6.19870000	15.08710000
C	55.03040000	6.81070000	16.40040000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000
C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000
C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

d5

Mode1 (first molecule)

S	60.05470000	2.09470000	14.64780000
S	61.33830000	3.71910000	18.28340000
C	57.24270000	2.42210000	15.25610000
H	56.88800000	2.06250000	14.45180000
C	62.45090000	2.71060000	16.16940000
H	63.10110000	2.40070000	15.55040000
C	58.62200000	2.53200000	15.53070000
C	61.03880000	2.66440000	15.96230000
C	58.90230000	3.09430000	16.77310000
C	60.30610000	3.16230000	17.01720000
C	62.73090000	3.26050000	17.37690000
H	63.61730000	3.38210000	17.69620000
S	57.45190000	3.50980000	17.60690000
C	56.47100000	2.89780000	16.29360000
S	51.44660000	3.73040000	18.04620000
S	50.16300000	2.10600000	14.41070000
C	54.25860000	3.40300000	17.43790000
H	54.61330000	3.76260000	18.24220000
C	49.05050000	3.11450000	16.52460000
H	48.40020000	3.42440000	17.14370000
C	52.87930000	3.29310000	17.16330000
C	50.46250000	3.16070000	16.73170000
C	52.59910000	2.73080000	15.92090000
C	51.19530000	2.66280000	15.67680000
C	48.77040000	2.56460000	15.31710000
H	47.88400000	2.44300000	14.99780000
S	54.04950000	2.31530000	15.08710000
C	55.03040000	2.92730000	16.40040000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000
C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000

C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

d6

Mode1 (first molecule)

S	52.51490000	4.03640000	12.59720000
S	51.23130000	5.66080000	8.96160000
C	55.32700000	4.36380000	11.98890000
H	55.68170000	4.00420000	12.79320000
C	50.11880000	4.65230000	11.07560000
H	49.46850000	4.34240000	11.69470000
C	53.94770000	4.47370000	11.71430000
C	51.53090000	4.60610000	11.28270000
C	53.66740000	5.03600000	10.47190000
C	52.26360000	5.10400000	10.22780000
C	49.83880000	5.20220000	9.86810000
H	48.95240000	5.32380000	9.54880000
S	55.11780000	5.45150000	9.63810000
C	56.09870000	4.83950000	10.95140000
S	61.12310000	5.67210000	9.19880000
S	62.40670000	4.04770000	12.83440000
C	58.31110000	5.34470000	9.80710000
H	57.95640000	5.70430000	9.00280000

C	63.51920000	5.05620000	10.72040000
H	64.16950000	5.36610000	10.10140000
C	59.69040000	5.23480000	10.08170000
C	62.10720000	5.10240000	10.51330000
C	59.97060000	4.67250000	11.32410000
C	61.37440000	4.60450000	11.56820000
C	63.79930000	4.50630000	11.92790000
H	64.68570000	4.38470000	12.24720000
S	58.52020000	4.25700000	12.15790000
C	57.53930000	4.86900000	10.84460000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000
C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000
C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

d7

Mode1 (first molecule)

S	52.51490000	0.15300000	12.59720000
S	51.23130000	1.77740000	8.96160000
C	55.32700000	0.48040000	11.98890000
H	55.68170000	0.12080000	12.79320000
C	50.11880000	0.76890000	11.07560000
H	49.46850000	0.45900000	11.69470000
C	53.94770000	0.59030000	11.71430000
C	51.53090000	0.72270000	11.28270000
C	53.66740000	1.15260000	10.47190000
C	52.26360000	1.22060000	10.22780000
C	49.83880000	1.31880000	9.86810000
H	48.95240000	1.44040000	9.54880000
S	55.11780000	1.56810000	9.63810000
C	56.09870000	0.95610000	10.95140000
S	61.12310000	1.78870000	9.19880000
S	62.40670000	0.16430000	12.83440000
C	58.31110000	1.46130000	9.80710000
H	57.95640000	1.82090000	9.00280000
C	63.51920000	1.17280000	10.72040000
H	64.16950000	1.48270000	10.10140000
C	59.69040000	1.35140000	10.08170000
C	62.10720000	1.21900000	10.51330000
C	59.97060000	0.78910000	11.32410000
C	61.37440000	0.72110000	11.56820000
C	63.79930000	0.62290000	11.92790000
H	64.68570000	0.50130000	12.24720000
S	58.52020000	0.37360000	12.15790000
C	57.53930000	0.98560000	10.84460000

Mode2 (second molecule)

S	35.67040000	5.97810000	12.59720000
S	34.38680000	7.60250000	8.96160000
C	38.48250000	6.30550000	11.98890000
H	38.83720000	5.94590000	12.79320000
C	33.27430000	6.59400000	11.07560000
H	32.62400000	6.28410000	11.69470000
C	37.10320000	6.41540000	11.71430000
C	34.68640000	6.54780000	11.28270000

C	36.82290000	6.97770000	10.47190000
C	35.41910000	7.04570000	10.22780000
C	32.99430000	7.14390000	9.86810000
H	32.10790000	7.26550000	9.54880000
S	38.27330000	7.39320000	9.63810000
C	39.25420000	6.78120000	10.95140000
S	44.27860000	7.61380000	9.19880000
S	45.56220000	5.98940000	12.83440000
C	41.46660000	7.28640000	9.80710000
H	41.11190000	7.64600000	9.00280000
C	46.67470000	6.99790000	10.72040000
H	47.32500000	7.30780000	10.10140000
C	42.84590000	7.17650000	10.08170000
C	45.26270000	7.04410000	10.51330000
C	43.12610000	6.61420000	11.32410000
C	44.52990000	6.54620000	11.56820000
C	46.95480000	6.44800000	11.92790000
H	47.84120000	6.32640000	12.24720000
S	41.67570000	6.19870000	12.15790000
C	40.69480000	6.81070000	10.84460000

C2/c simulated crystal structures

Geometries of dimers of BDT

d1

Mode1 (first molecule)

S	34.63590000	1.96950000	18.06090000
S	33.28700000	3.62470000	14.46840000
C	37.43490000	2.35420000	17.43170000
H	37.80430000	1.99020000	18.22640000
C	32.21410000	2.59140000	16.58480000
H	31.57560000	2.27580000	17.21050000
C	36.05160000	2.43520000	17.16860000
C	33.62880000	2.54820000	16.76950000
C	35.74880000	3.00720000	15.93800000
C	34.34160000	3.06880000	15.71480000
C	31.91210000	3.14750000	15.38770000
H	31.02070000	3.26430000	15.08160000
S	37.18300000	3.45070000	15.09420000
C	38.18720000	2.86560000	16.39890000

S	43.17640000	3.85560000	14.63310000
S	44.52540000	2.20040000	18.22560000
C	40.37750000	3.47090000	15.26230000
H	40.00810000	3.83490000	14.46760000
C	45.59830000	3.23370000	16.10920000
H	46.23670000	3.54930000	15.48360000
C	41.76070000	3.38990000	15.52540000
C	44.18350000	3.27690000	15.92450000
C	42.06350000	2.81790000	16.75600000
C	43.47070000	2.75630000	16.97920000
C	45.90020000	2.67760000	17.30640000
H	46.79160000	2.56080000	17.61240000
S	40.62930000	2.37440000	17.59980000
C	39.62520000	2.95950000	16.29510000

Mode2 (second molecule)

S	34.63590000	5.85290000	18.06090000
S	33.28700000	7.50810000	14.46840000
C	37.43490000	6.23760000	17.43170000
H	37.80430000	5.87360000	18.22640000
C	32.21410000	6.47480000	16.58480000
H	31.57560000	6.15920000	17.21050000
C	36.05160000	6.31860000	17.16860000
C	33.62880000	6.43160000	16.76950000
C	35.74880000	6.89060000	15.93800000
C	34.34160000	6.95220000	15.71480000
C	31.91210000	7.03090000	15.38770000
H	31.02070000	7.14770000	15.08160000
S	37.18300000	7.33410000	15.09420000
C	38.18720000	6.74900000	16.39890000
S	43.17640000	7.73900000	14.63310000
S	44.52540000	6.08380000	18.22560000
C	40.37750000	7.35430000	15.26230000
H	40.00810000	7.71830000	14.46760000
C	45.59830000	7.11710000	16.10920000
H	46.23670000	7.43270000	15.48360000
C	41.76070000	7.27330000	15.52540000
C	44.18350000	7.16030000	15.92450000
C	42.06350000	6.70130000	16.75600000
C	43.47070000	6.63970000	16.97920000
C	45.90020000	6.56100000	17.30640000
H	46.79160000	6.44420000	17.61240000

S	40.62930000	6.25780000	17.59980000
C	39.62520000	6.84290000	16.29510000

d2

Mode1 (first molecule)

S	34.63590000	5.85290000	18.06090000
S	33.28700000	7.50810000	14.46840000
C	37.43490000	6.23760000	17.43170000
H	37.80430000	5.87360000	18.22640000
C	32.21410000	6.47480000	16.58480000
H	31.57560000	6.15920000	17.21050000
C	36.05160000	6.31860000	17.16860000
C	33.62880000	6.43160000	16.76950000
C	35.74880000	6.89060000	15.93800000
C	34.34160000	6.95220000	15.71480000
C	31.91210000	7.03090000	15.38770000
H	31.02070000	7.14770000	15.08160000
S	37.18300000	7.33410000	15.09420000
C	38.18720000	6.74900000	16.39890000
S	43.17640000	7.73900000	14.63310000
S	44.52540000	6.08380000	18.22560000
C	40.37750000	7.35430000	15.26230000
H	40.00810000	7.71830000	14.46760000
C	45.59830000	7.11710000	16.10920000
H	46.23670000	7.43270000	15.48360000
C	41.76070000	7.27330000	15.52540000
C	44.18350000	7.16030000	15.92450000
C	42.06350000	6.70130000	16.75600000
C	43.47070000	6.63970000	16.97920000
C	45.90020000	6.56100000	17.30640000
H	46.79160000	6.44420000	17.61240000
S	40.62930000	6.25780000	17.59980000
C	39.62520000	6.84290000	16.29510000

Mode2 (second molecule)

S	33.56760000	1.91390000	23.50990000
S	32.21860000	0.25870000	19.91740000
C	36.36650000	1.52920000	22.88070000
H	36.73590000	1.89320000	23.67540000

C	31.14570000	1.29200000	22.03380000
H	30.50720000	1.60760000	22.65950000
C	34.98330000	1.44820000	22.61760000
C	32.56050000	1.33520000	22.21850000
C	34.68050000	0.87620000	21.38700000
C	33.27330000	0.81460000	21.16380000
C	30.84370000	0.73590000	20.83670000
H	29.95240000	0.61910000	20.53060000
S	36.11470000	0.43270000	20.54320000
C	37.11880000	1.01780000	21.84790000
S	42.10810000	0.02780000	20.08210000
S	43.45700000	1.68300000	23.67460000
C	39.30910000	0.41250000	20.71130000
H	38.93970000	0.04850000	19.91670000
C	44.52990000	0.64970000	21.55820000
H	45.16840000	0.33410000	20.93260000
C	40.69230000	0.49350000	20.97440000
C	43.11520000	0.60650000	21.37350000
C	40.99510000	1.06550000	22.20500000
C	42.40240000	1.12710000	22.42820000
C	44.83190000	1.20580000	22.75540000
H	45.72320000	1.32260000	23.06140000
S	39.56100000	1.50900000	23.04880000
C	38.55680000	0.92390000	21.74410000

d3

Mode1 (first molecule)

S	34.63590000	5.85290000	18.06090000
S	33.28700000	7.50810000	14.46840000
C	37.43490000	6.23760000	17.43170000
H	37.80430000	5.87360000	18.22640000
C	32.21410000	6.47480000	16.58480000
H	31.57560000	6.15920000	17.21050000
C	36.05160000	6.31860000	17.16860000
C	33.62880000	6.43160000	16.76950000
C	35.74880000	6.89060000	15.93800000
C	34.34160000	6.95220000	15.71480000
C	31.91210000	7.03090000	15.38770000
H	31.02070000	7.14770000	15.08160000
S	37.18300000	7.33410000	15.09420000
C	38.18720000	6.74900000	16.39890000

S	43.17640000	7.73900000	14.63310000
S	44.52540000	6.08380000	18.22560000
C	40.37750000	7.35430000	15.26230000
H	40.00810000	7.71830000	14.46760000
C	45.59830000	7.11710000	16.10920000
H	46.23670000	7.43270000	15.48360000
C	41.76070000	7.27330000	15.52540000
C	44.18350000	7.16030000	15.92450000
C	42.06350000	6.70130000	16.75600000
C	43.47070000	6.63970000	16.97920000
C	45.90020000	6.56100000	17.30640000
H	46.79160000	6.44420000	17.61240000
S	40.62930000	6.25780000	17.59980000
C	39.62520000	6.84290000	16.29510000

Mode2 (second molecule)

S	33.56760000	9.68070000	23.50990000
S	32.21860000	8.02550000	19.91740000
C	36.36650000	9.29600000	22.88070000
H	36.73590000	9.66000000	23.67540000
C	31.14570000	9.05880000	22.03380000
H	30.50720000	9.37440000	22.65950000
C	34.98330000	9.21500000	22.61760000
C	32.56050000	9.10200000	22.21850000
C	34.68050000	8.64300000	21.38700000
C	33.27330000	8.58140000	21.16380000
C	30.84370000	8.50270000	20.83670000
H	29.95240000	8.38590000	20.53060000
S	36.11470000	8.19950000	20.54320000
C	37.11880000	8.78460000	21.84790000
S	42.10810000	7.79460000	20.08210000
S	43.45700000	9.44980000	23.67460000
C	39.30910000	8.17930000	20.71130000
H	38.93970000	7.81530000	19.91670000
C	44.52990000	8.41650000	21.55820000
H	45.16840000	8.10090000	20.93260000
C	40.69230000	8.26030000	20.97440000
C	43.11520000	8.37330000	21.37350000
C	40.99510000	8.83230000	22.20500000
C	42.40240000	8.89390000	22.42820000
C	44.83190000	8.97260000	22.75540000
H	45.72320000	9.08940000	23.06140000

```
 S              39.56100000   9.27580000  23.04880000
 C              38.55680000   8.69070000  21.74410000
```

d4

Mode1 (first molecule)

```
S              34.63590000   5.85290000  18.06090000
 S              33.28700000   7.50810000  14.46840000
 C              37.43490000   6.23760000  17.43170000
 H              37.80430000   5.87360000  18.22640000
 C              32.21410000   6.47480000  16.58480000
 H              31.57560000   6.15920000  17.21050000
 C              36.05160000   6.31860000  17.16860000
 C              33.62880000   6.43160000  16.76950000
 C              35.74880000   6.89060000  15.93800000
 C              34.34160000   6.95220000  15.71480000
 C              31.91210000   7.03090000  15.38770000
 H              31.02070000   7.14770000  15.08160000
 S              37.18300000   7.33410000  15.09420000
 C              38.18720000   6.74900000  16.39890000
 S              43.17640000   7.73900000  14.63310000
 S              44.52540000   6.08380000  18.22560000
 C              40.37750000   7.35430000  15.26230000
 H              40.00810000   7.71830000  14.46760000
 C              45.59830000   7.11710000  16.10920000
 H              46.23670000   7.43270000  15.48360000
 C              41.76070000   7.27330000  15.52540000
 C              44.18350000   7.16030000  15.92450000
 C              42.06350000   6.70130000  16.75600000
 C              43.47070000   6.63970000  16.97920000
 C              45.90020000   6.56100000  17.30640000
 H              46.79160000   6.44420000  17.61240000
 S              40.62930000   6.25780000  17.59980000
 C              39.62520000   6.84290000  16.29510000
```

Mode2 (second molecule)

```
S              58.95260000   5.85290000  20.08210000
 S              60.30150000   7.50810000  23.67460000
 C              56.15360000   6.23760000  20.71130000
 H              55.78420000   5.87360000  19.91670000
```

C	61.37440000	6.47480000	21.55820000
H	62.01290000	6.15920000	20.93260000
C	57.53680000	6.31860000	20.97440000
C	59.95970000	6.43160000	21.37350000
C	57.83960000	6.89060000	22.20500000
C	59.24690000	6.95220000	22.42820000
C	61.67640000	7.03090000	22.75540000
H	62.56770000	7.14770000	23.06140000
S	56.40550000	7.33410000	23.04880000
C	55.40130000	6.74900000	21.74410000
S	50.41210000	7.73900000	23.50990000
S	49.06310000	6.08380000	19.91740000
C	53.21100000	7.35430000	22.88070000
H	53.58040000	7.71830000	23.67540000
C	47.99020000	7.11710000	22.03380000
H	47.35170000	7.43270000	22.65950000
C	51.82780000	7.27330000	22.61760000
C	49.40500000	7.16030000	22.21850000
C	51.52500000	6.70130000	21.38700000
C	50.11780000	6.63970000	21.16380000
C	47.68820000	6.56100000	20.83670000
H	46.79690000	6.44420000	20.53060000
S	52.95920000	6.25780000	20.54320000
C	53.96330000	6.84290000	21.84790000

d5

Mode1 (first molecule)

S	34.63590000	5.85290000	18.06090000
S	33.28700000	7.50810000	14.46840000
C	37.43490000	6.23760000	17.43170000
H	37.80430000	5.87360000	18.22640000
C	32.21410000	6.47480000	16.58480000
H	31.57560000	6.15920000	17.21050000
C	36.05160000	6.31860000	17.16860000
C	33.62880000	6.43160000	16.76950000
C	35.74880000	6.89060000	15.93800000
C	34.34160000	6.95220000	15.71480000
C	31.91210000	7.03090000	15.38770000
H	31.02070000	7.14770000	15.08160000
S	37.18300000	7.33410000	15.09420000
C	38.18720000	6.74900000	16.39890000

S	43.17640000	7.73900000	14.63310000
S	44.52540000	6.08380000	18.22560000
C	40.37750000	7.35430000	15.26230000
H	40.00810000	7.71830000	14.46760000
C	45.59830000	7.11710000	16.10920000
H	46.23670000	7.43270000	15.48360000
C	41.76070000	7.27330000	15.52540000
C	44.18350000	7.16030000	15.92450000
C	42.06350000	6.70130000	16.75600000
C	43.47070000	6.63970000	16.97920000
C	45.90020000	6.56100000	17.30640000
H	46.79160000	6.44420000	17.61240000
S	40.62930000	6.25780000	17.59980000
C	39.62520000	6.84290000	16.29510000

Mode2 (second molecule)

S	58.95260000	9.73630000	20.08210000
S	60.30150000	11.39150000	23.67460000
C	56.15360000	10.12100000	20.71130000
H	55.78420000	9.75700000	19.91670000
C	61.37440000	10.35820000	21.55820000
H	62.01290000	10.04260000	20.93260000
C	57.53680000	10.20200000	20.97440000
C	59.95970000	10.31500000	21.37350000
C	57.83960000	10.77400000	22.20500000
C	59.24690000	10.83560000	22.42820000
C	61.67640000	10.91430000	22.75540000
H	62.56770000	11.03110000	23.06140000
S	56.40550000	11.21750000	23.04880000
C	55.40130000	10.63240000	21.74410000
S	50.41210000	11.62240000	23.50990000
S	49.06310000	9.96720000	19.91740000
C	53.21100000	11.23770000	22.88070000
H	53.58040000	11.60170000	23.67540000
C	47.99020000	11.00050000	22.03380000
H	47.35170000	11.31610000	22.65950000
C	51.82780000	11.15670000	22.61760000
C	49.40500000	11.04370000	22.21850000
C	51.52500000	10.58470000	21.38700000
C	50.11780000	10.52310000	21.16380000
C	47.68820000	10.44440000	20.83670000
H	46.79690000	10.32760000	20.53060000

S	52.95920000	10.14120000	20.54320000
C	53.96330000	10.72630000	21.84790000

d6

Mode1 (first molecule)

S	34.63590000	5.85290000	18.06090000
S	33.28700000	7.50810000	14.46840000
C	37.43490000	6.23760000	17.43170000
H	37.80430000	5.87360000	18.22640000
C	32.21410000	6.47480000	16.58480000
H	31.57560000	6.15920000	17.21050000
C	36.05160000	6.31860000	17.16860000
C	33.62880000	6.43160000	16.76950000
C	35.74880000	6.89060000	15.93800000
C	34.34160000	6.95220000	15.71480000
C	31.91210000	7.03090000	15.38770000
H	31.02070000	7.14770000	15.08160000
S	37.18300000	7.33410000	15.09420000
C	38.18720000	6.74900000	16.39890000
S	43.17640000	7.73900000	14.63310000
S	44.52540000	6.08380000	18.22560000
C	40.37750000	7.35430000	15.26230000
H	40.00810000	7.71830000	14.46760000
C	45.59830000	7.11710000	16.10920000
H	46.23670000	7.43270000	15.48360000
C	41.76070000	7.27330000	15.52540000
C	44.18350000	7.16030000	15.92450000
C	42.06350000	6.70130000	16.75600000
C	43.47070000	6.63970000	16.97920000
C	45.90020000	6.56100000	17.30640000
H	46.79160000	6.44420000	17.61240000
S	40.62930000	6.25780000	17.59980000
C	39.62520000	6.84290000	16.29510000

Mode2 (second molecule)

S	60.02090000	1.91390000	14.63310000
S	61.36990000	0.25870000	18.22560000
C	57.22200000	1.52920000	15.26230000
H	56.85260000	1.89320000	14.46760000

C	62.44280000	1.29200000	16.10920000
H	63.08120000	1.60760000	15.48360000
C	58.60520000	1.44820000	15.52540000
C	61.02800000	1.33520000	15.92450000
C	58.90800000	0.87620000	16.75600000
C	60.31520000	0.81460000	16.97920000
C	62.74470000	0.73590000	17.30640000
H	63.63610000	0.61910000	17.61240000
S	57.47380000	0.43270000	17.59980000
C	56.46970000	1.01780000	16.29510000
S	51.48040000	0.02780000	18.06090000
S	50.13150000	1.68300000	14.46840000
C	54.27940000	0.41250000	17.43170000
H	54.64880000	0.04850000	18.22640000
C	49.05860000	0.64970000	16.58480000
H	48.42010000	0.33410000	17.21050000
C	52.89610000	0.49350000	17.16860000
C	50.47330000	0.60650000	16.76950000
C	52.59330000	1.06550000	15.93800000
C	51.18610000	1.12710000	15.71480000
C	48.75660000	1.20580000	15.38770000
H	47.86520000	1.32260000	15.08160000
S	54.02750000	1.50900000	15.09420000
C	55.03170000	0.92390000	16.39890000

d7

Mode1 (first molecule)

S	34.63590000	5.85290000	18.06090000
S	33.28700000	7.50810000	14.46840000
C	37.43490000	6.23760000	17.43170000
H	37.80430000	5.87360000	18.22640000
C	32.21410000	6.47480000	16.58480000
H	31.57560000	6.15920000	17.21050000
C	36.05160000	6.31860000	17.16860000
C	33.62880000	6.43160000	16.76950000
C	35.74880000	6.89060000	15.93800000
C	34.34160000	6.95220000	15.71480000
C	31.91210000	7.03090000	15.38770000
H	31.02070000	7.14770000	15.08160000
S	37.18300000	7.33410000	15.09420000
C	38.18720000	6.74900000	16.39890000

S	43.17640000	7.73900000	14.63310000
S	44.52540000	6.08380000	18.22560000
C	40.37750000	7.35430000	15.26230000
H	40.00810000	7.71830000	14.46760000
C	45.59830000	7.11710000	16.10920000
H	46.23670000	7.43270000	15.48360000
C	41.76070000	7.27330000	15.52540000
C	44.18350000	7.16030000	15.92450000
C	42.06350000	6.70130000	16.75600000
C	43.47070000	6.63970000	16.97920000
C	45.90020000	6.56100000	17.30640000
H	46.79160000	6.44420000	17.61240000
S	40.62930000	6.25780000	17.59980000
C	39.62520000	6.84290000	16.29510000

Mode2 (second molecule)

S	60.02090000	5.79730000	14.63310000
S	61.36990000	4.14210000	18.22560000
C	57.22200000	5.41260000	15.26230000
H	56.85260000	5.77660000	14.46760000
C	62.44280000	5.17540000	16.10920000
H	63.08120000	5.49100000	15.48360000
C	58.60520000	5.33160000	15.52540000
C	61.02800000	5.21860000	15.92450000
C	58.90800000	4.75960000	16.75600000
C	60.31520000	4.69800000	16.97920000
C	62.74470000	4.61930000	17.30640000
H	63.63610000	4.50250000	17.61240000
S	57.47380000	4.31610000	17.59980000
C	56.46970000	4.90120000	16.29510000
S	51.48040000	3.91120000	18.06090000
S	50.13150000	5.56640000	14.46840000
C	54.27940000	4.29590000	17.43170000
H	54.64880000	3.93190000	18.22640000
C	49.05860000	4.53310000	16.58480000
H	48.42010000	4.21750000	17.21050000
C	52.89610000	4.37690000	17.16860000
C	50.47330000	4.48990000	16.76950000
C	52.59330000	4.94890000	15.93800000
C	51.18610000	5.01050000	15.71480000
C	48.75660000	5.08920000	15.38770000
H	47.86520000	5.20600000	15.08160000

S	54.02750000	5.39240000	15.09420000
C	55.03170000	4.80730000	16.39890000

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