Supporting Information for

Interfacial states in donor-acceptor organic heterojunctions: computational insights into thiophene-oligomer/fullerene junctions

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I. Features of the density functionals

Table SI-1 characterizes the density functionals used in this work in terms of the long-range-definition parameter μ, and the fraction of Hartree-Fock exchange in the short ($c_{X,SR}^{HF}$) and long ($c_{X,LR}^{HF}$) range domains.

Table SI-1.

	μ (a_0^{-1})	$c_{X,SR}^{HF}$	$c_{X,LR}^{HF}$	Ref.
B3LYP	0	0.2	0.2	1,2
PBE0	0	0.25	0.25	3
M06-2X	0	0.54	0.54	4
M06-HF	0	$\lesssim 1$	1	5
LC-BLYP	0.47	0	1	6-8
LC-BLYP	0.29	0	1	9
LC-BLYP	0.20	0	1	10
CAM-B3LYP	0.33	0.19	0.65	11
ωB97X-D	0.30	0.157706	1	12

II. Practical hints for state classification

As described in the paper, our procedure for state classification requires the overlap integrals $S_{\mu\nu}$ and the molecular orbital coefficients $c_{\mu k}$. When using Gaussian 09, these quantities can be printed out by including the following keywords in the input:

```
gfprint pop=full IOP(3/33=3)
```

Optionally, the threshold for printing the TDDFT coefficients can be reduced to10^{-n} with

```
IOP(9/40=n)
```

A copy of the program for state classification can be obtained by contacting the corresponding author.

III. Parameters for spectrum simulation

The number of points in the Wigner distribution (N_p), the number of excited states (N_{fs}), the width of the normalized Gaussian line shapes (δ) and the refractive index of the medium (n_r) are given in Table SI-2. These parameters were used in the spectrum simulation of 6T and C_{60} using the nuclear ensemble approach,[13] as discussed in the paper.

Table SI-2.

	N_p	N_{fs}	δ (eV)	n_r
6T	200	40	0.3	1.51
C_{60}	200	40	0.05	1.38

IV. Asymptotic limit of the vertical excitations

The vertical excitation energies of the nT-C_{60} complexes are plotted in Fig. SI-1 as a function of the number of monomers n. The results are fitted with reciprocal function $E = E_\infty + \Delta E$ / n, where E_∞ is the asymptotic limit when n$\rightarrow \infty$, and ΔE is the energy increment. The fitting parameters are given in Table SI-3. Experimental results[14] for the band maximum of nT oligomers in benzene are shown as well.

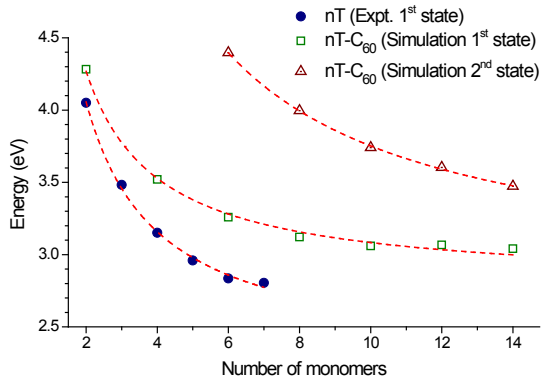

Fig. SI-1.

Table SI-3.

	State	Solvent	E_∞ (eV)	ΔE (eV.mol)
Simulation	1st	Gas	2.8	3.6
	2nd	Gas	2.8	9.7
Expt.[14]	1st	Benzene	2.3	3.0
Expt.[15]	1st	DCM[a]	2.14	4.11
Expt.[15]	1st	DMSO[a]	2.14	3.76

[a] DCM: dichloromethane; DMSO dimethylsulfoxide

V. Collection of experimental data

Table SI-4 lists experimental results for the band maximum of several molecular systems that are of interest to our investigations.

Table SI-4.

Molecule	Phase	ΔE (eV)	Ref.
6T	benzene	2.9	14
	DCM	2.78	15
	DMSO	2.72	15
	solution	2.9	16
	film	2.26	15
	film	2.3	17
	film	2.4,2.9,3.4	16
C_{60}	n-hexane	3.8	18
	film	3.4	19
P3HT	film	2.2	20
	film (rr)[b]	2.37	21
	film (rr)	2.4	22
	film (rr)	2.4	23
	film (rra)[b]	2.7	22
	solution	2.7	23
P3HT-C_{60}	film (50 wt.% C60)	2.9	24
P3HT-PCBM	film	2.4, 3.7	25
	film (spin coated)	2.7	20
	film (annealing)	2.2	20
	film (50 wt.% PCBM)	2.6	24
	film (75 wt.% PCBM)	3.1	24

[a] DCM: dichloromethane; DMSO dimethylsulfoxide. [b] rr: regioregular, rra: regiorandom.

VI. Bright CT states

The bright states of 6T-C_{60} are characterized as CT D→A. This is an odd situation, since CT states usually have small transition dipole moments with the ground state, due to the small overlap between the donor and acceptor orbitals involved in the excitation. To understand how a bright CT state can arise, we analyze here the excited state 18 of 6T-C_{60} computed at the TD-ωB97X-D/6-31G(d) level. This state is characterized in Table SI-5.

Table SI-5.

St	E(eV)	Osc	ΔP_A	ΣP_A	Class
18	3.244	0.672	0.66	0.73	CTB→A

The TDDFT characterization of the two main configurations contributing to this state is given in Table SI-6. Both configurations give important contributions to the state (46% and 29%). The first configuration has CT character while the second one has LOC(B) character. While the first one should not contribute to the oscillator strength, due to the small overlap between orbitals 307 (6T) and 309 (C_{60}), the second configuration, with both orbitals localized in 6T, does. As a consequence, even though the average amount of charge transfer from 6T to C_{60} (0.66) is large enough to characterize the state as a CT state, the oscillator strength is large due to the contributions from the second configuration to the transition dipole moment.

Table SI-6.

$i \rightarrow j$	$C_{i\rightarrow j}$	$C^2_{i\rightarrow j}$	$\Delta P_A^{i\rightarrow j}$	$\Sigma P_A^{i\rightarrow j}$	Class
307→309	0.678	0.46	0.99	1.01	CTB→A
307→311	-0.542	0.29	0.28	0.30	LOC(B)
…	…	…	…	…	…
Average			**0.66**	**0.73**	**CTB→A**

VII. Bright C_{60}-localized states

For n = 8, important oscillator-strength contributions to the first bright band are made by states classified as LOC(A). This occurs because, for these long oligomers, the bright LOC(D) state mixes with many LOC(A) states in the second C_{60} band. The contribution of LOC(D) configuration for each of these mixed states is small, usually about 10%, and these states are mostly characterized as LOC(A). Take, for instance, the 10T-C_{60} complex. The low-energy states with the largest oscillator strength are shown in Table SI-7. In this Table, C^2 is the total weight of the LOC(D) configuration for the state. The six states listed in this table have between 3% and 36% of LOC(D) configuration. The oscillator strength f of each state is linearly correlated with C^2: the larger the LOC(D) contribution, the higher the oscillator strength (Fig. SI-2). Over these six states centered at 3.06 eV, f sums to 3.09, while C^2 sums to 0.74. For comparison, the oscillator strength of the bright state (3.08 eV) of the isolated 10T computed with the same geometry as in the complex is 3.49.

Table SI-7.

State	E (eV)	C^2	f
10T-C_{60}			
12	3.03	0.03	0.16
16	3.09	0.04	0.21
13	3.06	0.07	0.34
11	3.00	0.09	0.34
15	3.08	0.15	0.63
17	3.10	0.36	1.41
Total	**3.06**[a]	**0.74**	**3.09**
10T			
	3.08		**3.49**

[a] Average.

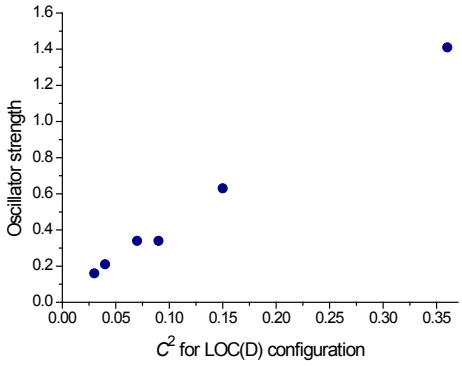

Fig. SI-2.

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IX. Distances and Dihedrals

Here we tabulate the values of distances and dihedral angles plotted as a figure in the paper (the figure is reproduced below, Fig. SI-3). Distances are in Angstrom and dihedral angles in degrees. 6 = 6T-C_{60}; 6i = 6T; 6s = S3HT-C_{60}.

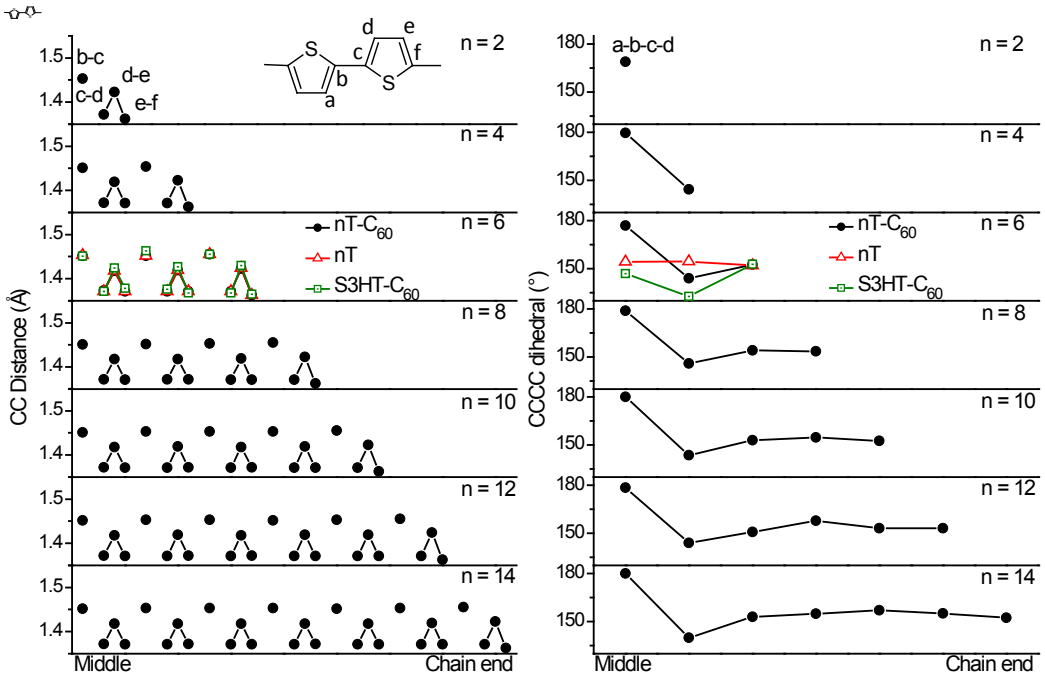

Fig. SI-3.

Distances

14	12	10	8	6	6i	6s	4	2
1.452	1.452	1.451	1.451	1.452	1.453	1.451	1.451	1.453
1.372	1.372	1.372	1.372	1.373	1.371	1.371	1.372	1.372
1.418	1.418	1.418	1.418	1.418	1.418	1.424	1.419	1.423
1.371	1.371	1.371	1.371	1.371	1.371	1.378	1.371	1.362
1.453	1.453	1.453	1.452	1.452	1.452	1.463	1.454	
1.371	1.371	1.371	1.372	1.371	1.371	1.376	1.371	
1.418	1.419	1.419	1.418	1.419	1.419	1.427	1.423	
1.372	1.372	1.372	1.372	1.371	1.371	1.368	1.363	
1.453	1.453	1.453	1.453	1.455	1.455	1.455		
1.371	1.371	1.371	1.371	1.371	1.371	1.368		
1.418	1.418	1.418	1.419	1.423	1.424	1.430		
1.371	1.372	1.372	1.371	1.363	1.363	1.365		
1.453	1.452	1.453	1.455					
1.371	1.371	1.371	1.371					
1.418	1.419	1.419	1.423					
1.372	1.371	1.371	1.363					
1.452	1.453	1.455						

```
1.371  1.371  1.371
1.418  1.419  1.423
1.371  1.371  1.363

1.453  1.455

1.371  1.371
1.419  1.424
1.371  1.363

1.455

1.371
1.423
1.363
```

Dihedral angles

```
 14     12     10      8      6      6i     6s     4      2
-180.0  178.3  180.0 -178.8 -176.8 -154.2 -146.9 -179.5 -168.8
 139.9  144.0  143.7  145.9  143.9  154.5  132.7  144.3
-153.0  150.8  152.9 -154.1 -152.5  151.9 -152.7
-154.9 -157.7  154.7  153.5
 157.1  153.2  152.6
 155.1 -153.1
-152.3
```

X. Electronic states of the complexes

TDDFT calculations in the gas phase (ε=1). Other dielectric constants used with PCM. Osc – oscillator strength. ΔP_A and ΣP_A are defined in the paper. cR, cA and cB are defined in Ref.[13]. A – acceptor; B – donor.

2T-C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6592	0.0000	0.0247	1.9687	0.0000	0.9505	0.0000	loc(A)
2	2.6754	0.0000	0.2010	1.7955	0.0000	0.5001	0.0000	loc(A)
3	2.6808	0.0000	0.0115	1.9835	0.0000	0.9614	0.0000	loc(A)
4	2.7187	0.0000	0.0215	1.9752	0.0000	0.9565	0.0000	loc(A)
5	2.7264	0.0000	0.1938	1.8023	0.0000	0.5156	0.0000	loc(A)
6	2.7357	0.0000	0.0479	1.9492	0.0000	0.8874	0.0000	loc(A)
7	2.7607	0.0001	0.1519	1.8436	0.0000	0.6044	0.0000	loc(A)
8	2.7749	0.0000	0.0785	1.9180	0.0000	0.8024	0.0000	loc(A)
9	2.7767	0.0000	0.0005	1.9919	0.0000	1.0000	0.0000	loc(A)
10	2.7832	0.0000	0.0144	1.9794	0.0000	0.9382	0.0000	loc(A)
11	3.0479	0.0004	0.1053	1.8909	0.0000	0.7805	0.0000	loc(A)
12	3.0678	0.0003	0.0556	1.9402	0.0000	0.8783	0.0000	loc(A)
13	3.0813	0.0001	0.0927	1.9038	0.0000	0.7521	0.0000	loc(A)
14	3.0880	0.0014	0.1697	1.8241	0.0000	0.5966	0.0000	loc(A)
15	3.0952	0.0001	0.0070	1.9862	0.0000	0.9673	0.0000	loc(A)
16	3.5322	0.0053	0.4767	1.5166	0.0000	0.2186	0.0000	loc(A)
17	3.5637	0.0001	0.0774	1.9168	0.0000	0.8789	0.0000	loc(A)
18	3.5772	0.0000	0.0816	1.9122	0.0000	0.8749	0.0000	loc(A)
19	3.6027	0.0280	0.5387	1.4565	0.0000	0.1159	0.0000	CTB->A
20	3.6367	0.0336	0.3668	1.6251	0.0000	0.2907	0.0000	loc(A)
21	3.7684	0.0001	0.0859	1.9062	0.0000	0.9386	0.0000	loc(A)
22	3.7753	0.0009	0.0857	1.9071	0.0000	0.7975	0.0000	loc(A)
23	3.7854	0.0000	0.0570	1.9366	0.0000	0.9189	0.0000	loc(A)
24	3.7905	0.0009	0.1176	1.8761	0.0000	0.7492	0.0000	loc(A)
25	3.8018	0.0003	0.1218	1.8726	0.0000	0.7047	0.0000	loc(A)
26	3.8307	0.0000	0.1926	1.8030	0.0000	0.7055	0.0000	loc(A)
27	3.8605	0.0003	0.1659	1.8283	0.0000	0.7070	0.0000	loc(A)

28	3.8626	0.0003	0.0786	1.9156	0.0000	0.8265	0.0000	loc(A)
29	3.8726	0.0030	0.0978	1.8962	0.0000	0.7659	0.0000	loc(A)
30	3.8898	0.0005	0.4176	1.5785	0.0000	0.3169	0.0000	loc(A)
31	4.2497	0.0010	0.1494	1.8463	0.0000	0.8284	0.0000	loc(A)
32	4.2567	0.0007	0.1991	1.7955	0.0000	0.6909	0.0000	loc(A)
33	4.2783	0.0001	0.0747	1.9189	0.0000	0.8690	0.0000	loc(A)
34	4.2822	0.1091	-0.3033	0.3774	0.0000	0.0000	0.0000	loc(B)
35	4.2897	0.0028	0.0148	1.9300	0.0000	0.9740	0.0000	loc(A)
36	4.3921	0.0006	0.2677	1.7287	0.0000	0.6918	0.0000	loc(A)
37	4.4207	0.0006	0.2066	1.7898	0.0000	0.6240	0.0000	loc(A)
38	4.4381	0.0139	0.2017	1.7924	0.0000	0.8093	0.0000	loc(A)
39	4.4418	0.0341	0.1372	1.8584	0.0000	0.9192	0.0000	loc(A)
40	4.4519	0.2399	0.1034	1.8892	0.0000	0.7710	0.0000	loc(A)

4T- C_{60} ε=1 singlet B3LYP 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	1.7231	0.0009	0.9782	1.0108	0.0000	0.0000	1.0000	CTB->A
2	1.7547	0.0000	0.9820	1.0146	0.0000	0.0000	1.0000	CTB->A
3	1.7564	0.0167	0.9779	1.0105	0.0000	0.0000	1.0000	CTB->A
4	2.1114	0.0000	0.0621	1.9271	0.0000	1.0000	0.0000	loc(A)
5	2.1243	0.0001	0.0525	1.9361	0.0000	1.0000	0.0000	loc(A)
6	2.1308	0.0000	0.0386	1.9550	0.0000	1.0000	0.0000	loc(A)
7	2.1499	0.0000	0.0009	1.9932	0.0000	1.0000	0.0000	loc(A)
8	2.1504	0.0000	0.0020	1.9916	0.0000	1.0000	0.0000	loc(A)
9	2.1575	0.0000	-0.0009	1.9914	0.0000	1.0000	0.0000	loc(A)
10	2.1598	0.0000	-0.0027	1.9909	0.0000	1.0000	0.0000	loc(A)
11	2.1598	0.0001	0.0010	1.9895	0.0000	1.0000	0.0000	loc(A)
12	2.1706	0.0000	0.0018	1.9933	0.0000	1.0000	0.0000	loc(A)
13	2.1723	0.0000	-0.0003	1.9915	0.0000	1.0000	0.0000	loc(A)
14	2.3027	0.0000	0.0306	1.9623	0.0000	1.0000	0.0000	loc(A)
15	2.3139	0.0001	0.0145	1.9760	0.0000	1.0000	0.0000	loc(A)
16	2.3305	0.0001	0.0010	1.9924	0.0000	1.0000	0.0000	loc(A)
17	2.3373	0.0003	0.0013	1.9884	0.0000	1.0000	0.0000	loc(A)
18	2.3388	0.0000	-0.0004	1.9890	0.0000	1.0000	0.0000	loc(A)
19	2.6882	0.0006	0.9307	1.0517	0.0000	0.0000	1.0000	CTB->A
20	2.7146	0.0014	0.9365	1.0601	0.0000	0.0000	1.0000	CTB->A
21	2.7164	0.0017	0.9323	1.0560	0.0000	0.0000	1.0000	CTB->A
22	2.9270	0.0003	0.9767	1.0092	0.0000	0.0000	1.0000	CTB->A
23	2.9322	0.0556	0.8644	0.8989	0.0000	0.0000	1.0000	CTB->A
24	2.9476	0.0104	0.9744	1.0069	0.0000	0.0000	1.0000	CTB->A
25	3.1339	0.5940	0.1096	0.1421	0.0000	0.0000	1.0000	loc(B)
26	3.2389	0.0001	0.0380	1.7391	0.0000	0.8594	0.0484	loc(A)
27	3.2491	0.0031	0.0271	1.9224	0.0000	1.0000	0.0000	loc(A)
28	3.2620	0.0024	0.1559	1.7896	0.0000	0.8460	0.1540	loc(A)
29	3.2677	0.0002	-0.0136	1.8322	0.0000	0.9044	0.0379	loc(A)
30	3.2799	0.0000	0.0021	1.9837	0.0000	1.0000	0.0000	loc(A)
31	3.2817	0.0039	0.0624	1.8976	0.0000	0.9067	0.0382	loc(A)
32	3.2851	0.0018	0.0086	1.9454	0.0000	0.9627	0.0000	loc(A)
33	3.2860	0.0003	0.0966	1.8350	0.0000	0.8590	0.0915	loc(A)
34	3.3259	0.0010	0.1051	1.8711	0.0000	0.8968	0.1032	loc(A)
35	3.3406	0.0002	-0.0182	1.9265	0.0000	0.9687	0.0000	loc(A)
36	3.3450	0.0001	-0.0051	1.9698	0.0000	1.0000	0.0000	loc(A)
37	3.3487	0.0002	0.0666	1.8661	0.0000	0.8934	0.1066	loc(A)
38	3.3884	0.0005	0.7545	1.2090	0.0000	0.1411	0.8589	CTB->A
39	3.4027	0.0020	0.7407	1.2294	0.0000	0.1637	0.8363	CTB->A
40	3.4102	0.0014	0.7387	1.2458	0.0000	0.0779	0.5763	CTB->A
41	3.4429	0.0042	0.5930	1.3835	0.0000	0.2871	0.5359	CTB->A
42	3.4436	0.0002	0.4279	1.5385	0.0000	0.4346	0.2671	loc(A)
43	3.4535	0.0012	0.3746	1.5855	0.0000	0.5482	0.2987	loc(A)
44	3.4621	0.0001	0.4061	1.5673	0.0000	0.5338	0.3108	loc(A)
45	3.4849	0.0003	0.2371	1.7521	0.0000	0.7859	0.2141	loc(A)
46	3.4955	0.0004	0.3812	1.6103	0.0000	0.6165	0.3835	loc(A)
47	3.4968	0.0002	0.4555	1.5288	0.0000	0.5248	0.4358	loc(A)

48	3.5005	0.0054	0.1836	1.7787	0.0000	0.8248	0.1752	loc(A)
49	3.5045	0.0000	0.5119	1.4802	0.0000	0.4092	0.4270	CTB->A
50	3.5171	0.0013	0.2298	1.7222	0.0000	0.7240	0.2039	loc(A)

4T- C_{60} ε=1 singlet PBE0 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	1.8180	0.0007	0.9797	1.0099	0.0000	0.0000	1.0000	CTB->A
2	1.8532	0.0177	0.9794	1.0096	0.0000	0.0000	1.0000	CTB->A
3	1.8586	0.0000	0.9833	1.0134	0.0000	0.0000	1.0000	CTB->A
4	2.1952	0.0000	0.0770	1.9126	0.0000	1.0000	0.0000	loc(A)
5	2.2092	0.0001	0.0594	1.9300	0.0000	1.0000	0.0000	loc(A)
6	2.2205	0.0000	0.0448	1.9492	0.0000	1.0000	0.0000	loc(A)
7	2.2383	0.0000	0.0025	1.9918	0.0000	1.0000	0.0000	loc(A)
8	2.2394	0.0001	0.0009	1.9923	0.0000	1.0000	0.0000	loc(A)
9	2.2425	0.0000	0.0017	1.9915	0.0000	1.0000	0.0000	loc(A)
10	2.2430	0.0000	-0.0015	1.9913	0.0000	1.0000	0.0000	loc(A)
11	2.2446	0.0000	-0.0017	1.9913	0.0000	1.0000	0.0000	loc(A)
12	2.2527	0.0000	0.0013	1.9940	0.0000	1.0000	0.0000	loc(A)
13	2.2573	0.0000	-0.0009	1.9913	0.0000	1.0000	0.0000	loc(A)
14	2.4047	0.0000	0.0363	1.9569	0.0000	1.0000	0.0000	loc(A)
15	2.4161	0.0001	0.0184	1.9726	0.0000	1.0000	0.0000	loc(A)
16	2.4334	0.0001	0.0011	1.9927	0.0000	1.0000	0.0000	loc(A)
17	2.4408	0.0003	0.0023	1.9880	0.0000	1.0000	0.0000	loc(A)
18	2.4424	0.0000	-0.0005	1.9898	0.0000	1.0000	0.0000	loc(A)
19	2.8192	0.0013	0.9200	1.0648	0.0000	0.0000	1.0000	CTB->A
20	2.8522	0.0016	0.9237	1.0729	0.0000	0.0000	1.0000	CTB->A
21	2.8528	0.0022	0.9199	1.0691	0.0000	0.0000	1.0000	CTB->A
22	3.0843	0.0002	0.9783	1.0084	0.0000	0.0000	1.0000	CTB->A
23	3.0851	0.1129	0.8846	0.9178	0.0000	0.0000	1.0000	CTB->A
24	3.1061	0.0110	0.9749	1.0082	0.0000	0.0000	1.0000	CTB->A
25	3.2434	0.5585	0.0929	0.1230	0.0000	0.0000	1.0000	loc(B)
26	3.3546	0.0022	0.0452	1.9261	0.0000	1.0000	0.0000	loc(A)
27	3.3549	0.0001	0.1260	1.7786	0.0000	0.8169	0.0402	loc(A)
28	3.3674	0.0051	0.1646	1.7957	0.0000	0.8491	0.1509	loc(A)
29	3.3808	0.0037	0.0739	1.8962	0.0000	0.8577	0.0000	loc(A)
30	3.3817	0.0002	0.0323	1.8803	0.0000	0.9088	0.0280	loc(A)
31	3.3842	0.0002	0.1046	1.8590	0.0000	0.8779	0.0929	loc(A)
32	3.3943	0.0000	0.0245	1.9632	0.0000	0.9681	0.0000	loc(A)
33	3.3951	0.0003	-0.0056	1.9839	0.0000	1.0000	0.0000	loc(A)
34	3.4465	0.0009	0.1180	1.8640	0.0000	0.8927	0.1073	loc(A)
35	3.4636	0.0001	0.0121	1.9398	0.0000	0.9549	0.0000	loc(A)
36	3.4673	0.0002	0.0008	1.9730	0.0000	1.0000	0.0000	loc(A)
37	3.4711	0.0001	0.0719	1.8880	0.0000	0.9073	0.0927	loc(A)
38	3.5299	0.0005	0.7854	1.1927	0.0000	0.1503	0.8497	CTB->A
39	3.5419	0.0022	0.7874	1.1937	0.0000	0.1529	0.8471	CTB->A
40	3.5560	0.0017	0.7221	1.2668	0.0000	0.1248	0.5040	CTB->A
41	3.5927	0.0050	0.6328	1.3536	0.0000	0.2670	0.4864	CTB->A
42	3.5942	0.0004	0.4375	1.5409	0.0000	0.4284	0.2086	loc(A)
43	3.6042	0.0012	0.2915	1.6985	0.0000	0.7083	0.2065	loc(A)
44	3.6206	0.0007	0.4936	1.4728	0.0000	0.4168	0.3471	deloc
45	3.6423	0.0001	0.2167	1.7756	0.0000	0.7900	0.2100	loc(A)
46	3.6512	0.0001	0.3682	1.6187	0.0000	0.6101	0.3314	loc(A)
47	3.6547	0.0004	0.6808	1.3085	0.0000	0.2841	0.6898	CTB->A
48	3.6553	0.0002	0.6514	1.3374	0.0000	0.2927	0.6040	CTB->A
49	3.6668	0.0008	0.7112	1.2789	0.0000	0.2667	0.7333	CTB->A
50	3.6758	0.0005	0.5230	1.4677	0.0000	0.4410	0.4692	CTB->A

4T-C_{60} ε=1 singlet M06-2X 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.5560	0.0001	0.0427	1.9475	0.0000	1.0000	0.0000	loc(A)
2	2.5647	0.0005	0.2351	1.7557	0.0000	0.7627	0.2373	loc(A)

3	2.5860	0.0000	0.0885	1.9056	0.0000	0.9154	0.0846	loc(A)
4	2.5917	0.0000	0.0087	1.9828	0.0000	1.0000	0.0000	loc(A)
5	2.6004	0.0000	0.0050	1.9901	0.0000	1.0000	0.0000	loc(A)
6	2.6033	0.0005	0.1011	1.8928	0.0000	0.8961	0.1039	loc(A)
7	2.6207	0.0005	0.2004	1.7934	0.0000	0.8126	0.1874	loc(A)
8	2.6389	0.0000	0.0149	1.9758	0.0000	1.0000	0.0000	loc(A)
9	2.6522	0.0000	0.0444	1.9481	0.0000	0.9544	0.0456	loc(A)
10	2.6621	0.0000	0.0019	1.9918	0.0000	1.0000	0.0000	loc(A)
11	2.7048	0.0004	0.5624	1.4287	0.0000	0.4322	0.5678	CTB->A
12	2.7286	0.0190	0.8919	1.0995	0.0000	0.0914	0.9086	CTB->A
13	2.8096	0.0007	0.8282	1.1677	0.0000	0.1574	0.8426	CTB->A
14	2.9050	0.0001	0.0228	1.9711	0.0000	1.0000	0.0000	loc(A)
15	2.9152	0.0002	0.0496	1.9426	0.0000	0.9625	0.0375	loc(A)
16	2.9238	0.0000	0.0026	1.9913	0.0000	1.0000	0.0000	loc(A)
17	2.9343	0.0003	-0.0003	1.9922	0.0000	1.0000	0.0000	loc(A)
18	2.9433	0.0006	0.0256	1.9660	0.0000	0.9756	0.0244	loc(A)
19	3.5262	0.6301	0.1921	0.2231	0.0000	0.0000	1.0000	loc(B)
20	3.5939	0.0075	0.0549	1.9266	0.0000	0.9279	0.0000	loc(A)
21	3.6213	0.0001	0.0217	1.9415	0.0000	0.9734	0.0000	loc(A)
22	3.6220	0.0225	0.0184	1.8806	0.0000	0.9364	0.0300	loc(A)
23	3.6949	0.0019	0.1915	1.7902	0.0000	0.8072	0.1680	loc(A)
24	3.7077	0.0000	0.0964	1.8465	0.0000	0.7773	0.0000	loc(A)
25	3.7250	0.0000	0.0188	1.9280	0.0000	0.9400	0.0000	loc(A)
26	3.7301	0.0000	0.0280	1.9463	0.0000	0.9600	0.0000	loc(A)
27	3.7347	0.0009	0.0023	1.9778	0.0000	1.0000	0.0000	loc(A)
28	3.8037	0.0055	0.5611	1.3856	0.0000	0.3996	0.6004	CTB->A
29	3.8505	0.0062	0.3570	1.6225	0.0000	0.6395	0.3605	loc(A)
30	3.8528	0.0001	0.1139	1.8624	0.0000	0.8829	0.0778	loc(A)
31	3.8607	0.0000	0.0360	1.9220	0.0000	0.9070	0.0000	loc(A)
32	3.8679	0.0001	0.1153	1.8529	0.0000	0.8877	0.1123	loc(A)
33	3.8884	0.0032	0.9325	1.0633	0.0000	0.0333	0.9667	CTB->A
34	3.8998	0.0004	0.9610	1.0305	0.0000	0.0000	1.0000	CTB->A
35	4.1401	0.0036	0.9771	1.0082	0.0000	0.0000	1.0000	CTB->A
36	4.1512	0.0010	0.1925	1.8008	0.0000	0.7540	0.0959	loc(A)
37	4.1559	0.0001	0.2680	1.7251	0.0000	0.5687	0.0855	loc(A)
38	4.1673	0.0108	0.3602	1.6319	0.0000	0.6289	0.3368	loc(A)
39	4.1895	0.0242	0.7110	1.2789	0.0000	0.2836	0.7164	CTB->A
40	4.1929	0.0006	0.0311	1.9607	0.0000	1.0000	0.0000	loc(A)

4T-C_{60} ε=1 singlet M06-HF 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	3.0101	0.0002	0.0599	1.9304	0.0000	1.0000	0.0000	loc(A)
2	3.0370	0.0000	0.0039	1.9868	0.0000	1.0000	0.0000	loc(A)
3	3.0404	0.0000	0.0151	1.9763	0.0000	1.0000	0.0000	loc(A)
4	3.0441	0.0000	0.0002	1.9919	0.0000	1.0000	0.0000	loc(A)
5	3.0561	0.0000	0.0026	1.9928	0.0000	1.0000	0.0000	loc(A)
6	3.0571	0.0000	0.0011	1.9939	0.0000	1.0000	0.0000	loc(A)
7	3.1990	0.0000	0.0232	1.9673	0.0000	1.0000	0.0000	loc(A)
8	3.2038	0.0000	0.0256	1.9673	0.0000	1.0000	0.0000	loc(A)
9	3.2191	0.0000	0.0010	1.9916	0.0000	1.0000	0.0000	loc(A)
10	3.2241	0.0000	0.0014	1.9925	0.0000	1.0000	0.0000	loc(A)
11	3.6038	0.0008	0.1074	1.8869	0.0000	0.9230	0.0770	loc(A)
12	3.6195	0.0028	0.0153	1.9757	0.0000	1.0000	0.0000	loc(A)
13	3.6332	0.0032	0.0668	1.9240	0.0000	0.9346	0.0654	loc(A)
14	3.6387	0.0000	0.0031	1.9913	0.0000	1.0000	0.0000	loc(A)
15	3.6436	0.0044	0.0041	1.9877	0.0000	1.0000	0.0000	loc(A)
16	3.7526	0.0001	0.8843	1.1053	0.0000	0.0972	0.9028	CTB->A
17	3.8619	0.0344	0.8791	1.1109	0.0000	0.1026	0.8974	CTB->A
18	3.8765	0.6429	0.0819	0.1166	0.0000	0.0000	1.0000	loc(B)
19	3.9169	0.0000	0.0641	1.9213	0.0000	0.9726	0.0274	loc(A)
20	3.9440	0.0234	0.0464	1.8675	0.0000	0.8895	0.0310	loc(A)
21	3.9568	0.0001	0.0547	1.9215	0.0000	0.8654	0.0260	loc(A)
22	4.0824	0.0023	0.9829	1.0139	0.0000	0.0000	1.0000	CTB->A

23	4.1385	0.0000	0.0256	1.9581	0.0000	1.0000	0.0000	loc(A)
24	4.1464	0.0002	0.0782	1.8934	0.0000	0.9460	0.0540	loc(A)
25	4.1606	0.0000	0.0374	1.9396	0.0000	0.8589	0.0000	loc(A)
26	4.1631	0.0001	0.0211	1.9581	0.0000	1.0000	0.0000	loc(A)
27	4.1676	0.0007	0.0416	1.9430	0.0000	0.9660	0.0340	loc(A)
28	4.3556	0.0001	0.0220	1.9659	0.0000	1.0000	0.0000	loc(A)
29	4.3742	0.0009	0.0228	1.9581	0.0000	1.0000	0.0000	loc(A)
30	4.3819	0.0000	0.0880	1.8884	0.0000	0.8679	0.0421	loc(A)
31	4.3832	0.0008	0.0409	1.9374	0.0000	0.8814	0.0000	loc(A)
32	4.8225	0.0253	0.0248	1.3278	0.0000	0.6350	0.3079	deloc
33	4.8317	0.0345	-0.0044	0.6404	0.0000	0.2808	0.6751	deloc
34	4.8350	0.0012	0.1354	1.8504	0.0000	0.8966	0.1034	loc(A)
35	4.8517	0.0001	0.0480	1.9424	0.0000	0.8672	0.0000	loc(A)
36	4.8636	0.0001	0.0110	1.9798	0.0000	1.0000	0.0000	loc(A)
37	4.9714	0.4114	0.0201	1.9556	0.0000	1.0000	0.0000	loc(A)
38	4.9846	0.5671	0.0177	1.9567	0.0000	0.9233	0.0000	loc(A)
39	4.9996	0.5770	0.0420	1.8733	0.0000	0.8799	0.0298	loc(A)
40	5.0671	0.0152	0.9409	1.0429	0.0000	0.0000	1.0000	CTB->A
41	5.1604	0.0001	0.2370	1.7579	0.0000	0.7606	0.1958	loc(A)
42	5.1952	0.0094	0.3539	1.5466	0.0000	0.5689	0.3997	loc(A)
43	5.1969	0.0002	0.2640	1.7279	0.0000	0.5562	0.1420	loc(A)
44	5.2092	0.0003	0.2856	1.7034	0.0000	0.7011	0.2404	loc(A)
45	5.2295	0.0000	0.0912	1.8992	0.0000	0.6955	0.0257	loc(A)
46	5.2353	0.0163	0.3887	1.3891	0.0000	0.4619	0.5094	deloc
47	5.2819	0.0683	0.1004	0.8038	0.0000	0.2605	0.7395	deloc
48	5.2826	0.0023	-0.0168	0.4975	0.0000	0.2131	0.7869	loc(B)
49	5.3151	0.0004	0.5359	1.1501	0.0000	0.2419	0.7280	CTB->A
50	5.3485	0.0141	0.3569	1.4368	0.0000	0.4817	0.4227	deloc

4T-C_{60} ε=1 singlet LC-BLYP(0.47) 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.9648	0.0001	0.0158	1.9755	0.0000	1.0000	0.0000	loc(A)
2	2.9842	0.0000	0.0062	1.9864	0.0000	1.0000	0.0000	loc(A)
3	2.9903	0.0000	0.0109	1.9838	0.0000	0.9707	0.0000	loc(A)
4	3.1212	0.0000	0.0109	1.9823	0.0000	1.0000	0.0000	loc(A)
5	3.1273	0.0000	0.0084	1.9852	0.0000	1.0000	0.0000	loc(A)
6	3.1331	0.0000	0.0060	1.9882	0.0000	1.0000	0.0000	loc(A)
7	3.2052	0.0000	0.0085	1.9828	0.0000	1.0000	0.0000	loc(A)
8	3.2095	0.0000	0.0155	1.9775	0.0000	1.0000	0.0000	loc(A)
9	3.2232	0.0000	0.0023	1.9909	0.0000	1.0000	0.0000	loc(A)
10	3.2262	0.0000	0.0066	1.9886	0.0000	1.0000	0.0000	loc(A)
11	3.6372	0.0001	0.0175	1.9778	0.0000	1.0000	0.0000	loc(A)
12	3.6409	0.0138	0.0062	1.9854	0.0000	1.0000	0.0000	loc(A)
13	3.6573	0.0002	0.0060	1.9869	0.0000	1.0000	0.0000	loc(A)
14	3.6628	0.0008	0.0455	1.9479	0.0000	0.9610	0.0390	loc(A)
15	3.6666	0.0045	0.0033	1.9898	0.0000	1.0000	0.0000	loc(A)
16	3.8188	0.6439	0.2643	0.3228	0.0000	0.0000	1.0000	loc(B)
17	3.8811	0.0028	0.0852	1.8927	0.0000	0.8746	0.0000	loc(A)
18	3.8942	0.0001	0.0618	1.8197	0.0000	0.7599	0.0328	loc(A)
19	3.9002	0.0192	-0.0046	1.8500	0.0000	0.7868	0.0000	loc(A)
20	4.0937	0.0021	0.8658	1.1129	0.0000	0.0730	0.8952	CTB->A
21	4.1489	0.0110	0.4908	1.4570	0.0000	0.3801	0.4762	deloc
22	4.1733	0.0002	0.0703	1.9167	0.0000	0.8829	0.0000	loc(A)
23	4.1913	0.0021	0.0590	1.7372	0.0000	0.7238	0.0392	loc(A)
24	4.1936	0.0008	0.0597	1.8020	0.0000	0.7055	0.0000	loc(A)
25	4.2110	0.0005	0.0956	1.8953	0.0000	0.7273	0.0000	loc(A)
26	4.2135	0.0006	0.1012	1.8274	0.0000	0.7794	0.0432	loc(A)
27	4.2190	0.0000	0.0359	1.8924	0.0000	0.8792	0.0000	loc(A)
28	4.2209	0.0001	0.0471	1.9248	0.0000	0.8964	0.0000	loc(A)
29	4.2270	0.0000	0.1552	1.8361	0.0000	0.5882	0.0548	loc(A)
30	4.2530	0.0231	0.6235	1.3454	0.0000	0.2957	0.6169	CTB->A
31	4.4379	0.0004	0.9457	1.0514	0.0000	0.0242	0.9758	CTB->A
32	4.7844	0.0012	0.1166	1.8733	0.0000	0.7594	0.0000	loc(A)

33	4.7963	0.0000	0.2079	1.7783	0.0000	0.4296	0.0000	loc(A)
34	4.8043	0.0002	0.2050	1.7866	0.0000	0.4915	0.0425	loc(A)
35	4.8166	0.0000	0.1153	1.8763	0.0000	0.7674	0.0000	loc(A)
36	4.8412	0.0398	0.1075	0.2158	0.0000	0.0301	0.9699	loc(B)
37	4.9724	0.4122	0.0431	1.8943	0.0000	0.8870	0.0000	loc(A)
38	4.9821	0.5658	-0.0112	1.8953	0.0000	0.9171	0.0000	loc(A)
39	4.9941	0.5363	0.0041	1.8399	0.0000	0.8510	0.0339	loc(A)
40	5.1587	0.0000	0.1621	1.8243	0.0000	0.7327	0.0288	loc(A)

4T- C_{60} ε=1 singlet LC-BLYP(0.29) 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.7493	0.0001	0.0267	1.9633	0.0000	1.0000	0.0000	loc(A)
2	2.7701	0.0000	0.0040	1.9878	0.0000	1.0000	0.0000	loc(A)
3	2.7778	0.0000	0.0055	1.9883	0.0000	1.0000	0.0000	loc(A)
4	2.8115	0.0000	0.0081	1.9854	0.0000	1.0000	0.0000	loc(A)
5	2.8161	0.0000	0.0116	1.9820	0.0000	1.0000	0.0000	loc(A)
6	2.8226	0.0000	0.0035	1.9908	0.0000	1.0000	0.0000	loc(A)
7	2.8553	0.0000	0.0112	1.9796	0.0000	1.0000	0.0000	loc(A)
8	2.8566	0.0000	0.0167	1.9760	0.0000	1.0000	0.0000	loc(A)
9	2.8711	0.0000	0.0006	1.9920	0.0000	1.0000	0.0000	loc(A)
10	2.8752	0.0000	0.0043	1.9901	0.0000	1.0000	0.0000	loc(A)
11	3.2007	0.0004	0.0476	1.9472	0.0000	0.9719	0.0281	loc(A)
12	3.2089	0.0016	0.0084	1.9827	0.0000	1.0000	0.0000	loc(A)
13	3.2207	0.0006	0.0059	1.9854	0.0000	1.0000	0.0000	loc(A)
14	3.2246	0.0009	0.0420	1.9521	0.0000	0.9602	0.0398	loc(A)
15	3.2315	0.0007	0.0029	1.9895	0.0000	1.0000	0.0000	loc(A)
16	3.4257	0.0005	0.9275	1.0611	0.0000	0.0468	0.9532	CTB->A
17	3.5303	0.0301	0.9041	1.0878	0.0000	0.0726	0.9274	CTB->A
18	3.5540	0.0050	0.0753	1.9071	0.0000	0.8722	0.0000	loc(A)
19	3.5706	0.0231	0.0738	1.8009	0.0000	0.7480	0.0374	loc(A)
20	3.5863	0.0001	0.1513	1.8051	0.0000	0.6758	0.0439	loc(A)
21	3.6231	0.6180	0.1973	0.2408	0.0000	0.0000	1.0000	loc(B)
22	3.7516	0.0201	0.9502	0.9933	0.0000	0.0000	1.0000	CTB->A
23	3.8064	0.0002	0.0719	1.9023	0.0000	0.9223	0.0000	loc(A)
24	3.8144	0.0001	0.0698	1.8130	0.0000	0.7468	0.0000	loc(A)
25	3.8242	0.0000	0.0672	1.8766	0.0000	0.7973	0.0000	loc(A)
26	3.8309	0.0001	0.1151	1.8569	0.0000	0.7043	0.0000	loc(A)
27	3.8351	0.0013	0.0140	1.9611	0.0000	0.9587	0.0000	loc(A)
28	3.9285	0.0000	0.0629	1.9260	0.0000	0.9422	0.0000	loc(A)
29	3.9435	0.0008	0.0663	1.8956	0.0000	0.7454	0.0000	loc(A)
30	3.9474	0.0000	0.0923	1.8588	0.0000	0.8291	0.0000	loc(A)
31	3.9497	0.0008	0.1248	1.8319	0.0000	0.6959	0.0000	loc(A)
32	4.3452	0.0004	0.1606	1.8281	0.0000	0.6338	0.0000	loc(A)
33	4.3556	0.0001	0.2765	1.7089	0.0000	0.4500	0.0000	loc(A)
34	4.3674	0.0000	0.2324	1.7591	0.0000	0.5582	0.0000	loc(A)
35	4.3798	0.0000	0.0569	1.9340	0.0000	0.9000	0.0000	loc(A)
36	4.5246	0.3502	0.0266	1.5823	0.0000	0.7367	0.1921	loc(A)
37	4.5302	0.2841	0.0483	1.9062	0.0000	0.8677	0.0000	loc(A)
38	4.5399	0.3811	0.0074	1.9428	0.0000	0.9699	0.0000	loc(A)
39	4.5633	0.0000	0.2675	1.7273	0.0000	0.4713	0.0385	loc(A)
40	4.5775	0.0002	0.3528	1.6391	0.0000	0.3171	0.0000	loc(A)

4T- C_{60} ε=1 singlet LC-BLYP(0.20) 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.4886	0.0001	0.0454	1.9436	0.0000	1.0000	0.0000	loc(A)
2	2.5066	0.0001	0.0736	1.9167	0.0000	0.9277	0.0723	loc(A)
3	2.5170	0.0000	0.0118	1.9790	0.0000	1.0000	0.0000	loc(A)
4	2.5204	0.0000	0.0432	1.9512	0.0000	0.9726	0.0274	loc(A)
5	2.5248	0.0001	0.0223	1.9704	0.0000	1.0000	0.0000	loc(A)
6	2.5266	0.0000	0.0071	1.9871	0.0000	1.0000	0.0000	loc(A)
7	2.5336	0.0000	0.0021	1.9936	0.0000	1.0000	0.0000	loc(A)

8	2.5344	0.0000	0.0016	1.9897	0.0000	1.0000	0.0000	loc(A)
9	2.5448	0.0000	0.0006	1.9910	0.0000	1.0000	0.0000	loc(A)
10	2.5489	0.0000	0.0031	1.9895	0.0000	1.0000	0.0000	loc(A)
11	2.7529	0.0028	0.5475	1.4442	0.0000	0.4512	0.5488	CTB->A
12	2.7895	0.0063	0.3668	1.6254	0.0000	0.6257	0.3743	loc(A)
13	2.7917	0.0006	0.0344	1.9563	0.0000	0.9758	0.0242	loc(A)
14	2.7983	0.0003	0.0491	1.9428	0.0000	0.9661	0.0339	loc(A)
15	2.8146	0.0003	0.0040	1.9877	0.0000	1.0000	0.0000	loc(A)
16	2.8233	0.0003	0.3223	1.6688	0.0000	0.6721	0.3279	loc(A)
17	2.8960	0.0190	0.6221	1.3691	0.0000	0.3647	0.6353	CTB->A
18	3.0518	0.0019	0.9160	1.0805	0.0000	0.0658	0.9342	CTB->A
19	3.3355	0.0036	0.0630	1.9125	0.0000	0.9303	0.0000	loc(A)
20	3.3519	0.0343	0.0414	1.8117	0.0000	0.8698	0.0553	loc(A)
21	3.3587	0.0000	0.0318	1.9263	0.0000	0.9683	0.0000	loc(A)
22	3.4087	0.6082	0.1757	0.2130	0.0000	0.0000	1.0000	loc(B)
23	3.4944	0.0008	0.0843	1.8920	0.0000	0.9169	0.0000	loc(A)
24	3.5016	0.0000	0.0930	1.8386	0.0000	0.7715	0.0000	loc(A)
25	3.5149	0.0000	0.0513	1.8876	0.0000	0.9179	0.0255	loc(A)
26	3.5207	0.0000	0.0374	1.9394	0.0000	0.9655	0.0000	loc(A)
27	3.5241	0.0015	0.0043	1.9724	0.0000	1.0000	0.0000	loc(A)
28	3.6191	0.0000	0.0572	1.9310	0.0000	0.9564	0.0000	loc(A)
29	3.6374	0.0002	0.0443	1.9277	0.0000	0.9576	0.0000	loc(A)
30	3.6407	0.0001	0.0314	1.9163	0.0000	0.9094	0.0000	loc(A)
31	3.6447	0.0016	0.0412	1.9165	0.0000	0.9758	0.0000	loc(A)
32	3.9021	0.0052	0.9149	0.9841	0.0000	0.0000	1.0000	CTB->A
33	3.9279	0.0006	0.1977	1.7963	0.0000	0.7946	0.1305	loc(A)
34	3.9414	0.0003	0.3012	1.6863	0.0000	0.5434	0.0813	loc(A)
35	3.9584	0.0000	0.1713	1.8203	0.0000	0.7894	0.0000	loc(A)
36	3.9749	0.0001	0.0412	1.9493	0.0000	1.0000	0.0000	loc(A)
37	4.0204	0.0003	0.2996	1.6943	0.0000	0.6572	0.1801	loc(A)
38	4.0403	0.0000	0.2194	1.7724	0.0000	0.6596	0.0000	loc(A)
39	4.0501	0.0002	0.2009	1.7909	0.0000	0.7783	0.0000	loc(A)
40	4.0571	0.0065	0.3533	1.6372	0.0000	0.6532	0.2925	loc(A)

4T- C_{60} ε=1 singlet CAM-B3LYP 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.5801	0.0001	0.0263	1.9645	0.0000	1.0000	0.0000	loc(A)
2	2.5992	0.0002	0.0434	1.9488	0.0000	0.9590	0.0410	loc(A)
3	2.6104	0.0000	0.0022	1.9914	0.0000	1.0000	0.0000	loc(A)
4	2.6434	0.0000	0.0454	1.9486	0.0000	0.9620	0.0380	loc(A)
5	2.6502	0.0000	0.0137	1.9799	0.0000	1.0000	0.0000	loc(A)
6	2.6565	0.0000	0.0268	1.9677	0.0000	0.9747	0.0253	loc(A)
7	2.6763	0.0001	0.0567	1.9367	0.0000	0.9589	0.0411	loc(A)
8	2.6811	0.0000	0.0096	1.9813	0.0000	1.0000	0.0000	loc(A)
9	2.6958	0.0000	-0.0001	1.9925	0.0000	1.0000	0.0000	loc(A)
10	2.7015	0.0000	0.0031	1.9907	0.0000	1.0000	0.0000	loc(A)
11	2.8890	0.0022	0.7369	1.2546	0.0000	0.2501	0.7499	CTB->A
12	2.9278	0.0128	0.6832	1.3086	0.0000	0.3021	0.6979	CTB->A
13	2.9571	0.0011	0.0885	1.9031	0.0000	0.9166	0.0834	loc(A)
14	2.9651	0.0005	0.0160	1.9772	0.0000	1.0000	0.0000	loc(A)
15	2.9835	0.0001	0.0609	1.9328	0.0000	0.9407	0.0593	loc(A)
16	2.9855	0.0005	0.0032	1.9892	0.0000	1.0000	0.0000	loc(A)
17	3.0272	0.0079	0.2993	1.6924	0.0000	0.6963	0.3037	loc(A)
18	3.0787	0.0007	0.8630	1.1339	0.0000	0.1198	0.8802	CTB->A
19	3.5036	0.6471	0.2546	0.2927	0.0000	0.0000	1.0000	loc(B)
20	3.5612	0.0045	0.0840	1.8888	0.0000	0.8779	0.0000	loc(A)
21	3.5843	0.0277	0.0052	1.8125	0.0000	0.9114	0.0353	loc(A)
22	3.5848	0.0000	0.0580	1.8816	0.0000	0.8040	0.0000	loc(A)
23	3.7172	0.0001	0.1091	1.8616	0.0000	0.8838	0.0243	loc(A)
24	3.7241	0.0000	0.0633	1.7653	0.0000	0.7548	0.0000	loc(A)
25	3.7384	0.0000	0.0612	1.8508	0.0000	0.7491	0.0000	loc(A)
26	3.7438	0.0000	0.0568	1.9056	0.0000	0.9317	0.0000	loc(A)
27	3.7486	0.0008	0.0002	1.9700	0.0000	1.0000	0.0000	loc(A)

28	3.7999	0.0001	0.0601	1.9232	0.0000	0.9454	0.0000	loc(A)
29	3.8173	0.0001	0.0747	1.8973	0.0000	0.9225	0.0000	loc(A)
30	3.8207	0.0001	0.0147	1.9168	0.0000	0.9337	0.0000	loc(A)
31	3.8238	0.0014	0.0584	1.8872	0.0000	0.8292	0.0000	loc(A)
32	4.0585	0.0033	0.9305	0.9833	0.0000	0.0000	1.0000	CTB->A
33	4.1189	0.0039	0.6940	1.3019	0.0000	0.2688	0.6947	CTB->A
34	4.1414	0.0025	0.8118	1.1806	0.0000	0.1031	0.7529	CTB->A
35	4.1863	0.0001	0.2909	1.7000	0.0000	0.6093	0.0604	loc(A)
36	4.1969	0.0014	0.4591	1.5334	0.0000	0.4367	0.2832	loc(A)
37	4.2062	0.0029	0.4006	1.5930	0.0000	0.4083	0.2895	loc(A)
38	4.2109	0.0003	0.1043	1.8877	0.0000	0.9386	0.0614	loc(A)
39	4.2979	0.0010	0.2952	1.6964	0.0000	0.4681	0.0463	loc(A)
40	4.3037	0.0134	0.2791	1.7069	0.0000	0.6434	0.0578	loc(A)

4T-C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6520	0.0001	0.0335	1.9579	0.0000	1.0000	0.0000	loc(A)
2	2.6722	0.0001	0.0254	1.9676	0.0000	0.9767	0.0233	loc(A)
3	2.6786	0.0000	0.0042	1.9886	0.0000	1.0000	0.0000	loc(A)
4	2.7218	0.0000	0.0159	1.9781	0.0000	1.0000	0.0000	loc(A)
5	2.7246	0.0000	0.0159	1.9778	0.0000	1.0000	0.0000	loc(A)
6	2.7351	0.0000	0.0054	1.9897	0.0000	1.0000	0.0000	loc(A)
7	2.7569	0.0000	0.0418	1.9514	0.0000	0.9757	0.0243	loc(A)
8	2.7610	0.0000	0.0073	1.9836	0.0000	1.0000	0.0000	loc(A)
9	2.7722	0.0000	0.0005	1.9927	0.0000	1.0000	0.0000	loc(A)
10	2.7769	0.0000	0.0017	1.9915	0.0000	1.0000	0.0000	loc(A)
11	3.0390	0.0012	0.1984	1.7957	0.0000	0.8192	0.1808	loc(A)
12	3.0610	0.0008	0.0108	1.9814	0.0000	1.0000	0.0000	loc(A)
13	3.0663	0.0043	0.1479	1.8448	0.0000	0.8518	0.1482	loc(A)
14	3.0765	0.0001	0.0465	1.9474	0.0000	0.9570	0.0430	loc(A)
15	3.0850	0.0012	0.0027	1.9891	0.0000	1.0000	0.0000	loc(A)
16	3.1289	0.0005	0.7436	1.2476	0.0000	0.2414	0.7586	CTB->A
17	3.2039	0.0239	0.7645	1.2259	0.0000	0.2188	0.7812	CTB->A
18	3.3783	0.0038	0.9321	1.0651	0.0000	0.0506	0.9494	CTB->A
19	3.5200	0.6532	0.2102	0.2462	0.0000	0.0000	1.0000	loc(B)
20	3.5604	0.0007	0.0631	1.9107	0.0000	0.9348	0.0000	loc(A)
21	3.5843	0.0412	0.0392	1.8039	0.0000	0.8275	0.0536	loc(A)
22	3.5862	0.0001	0.0649	1.8839	0.0000	0.7930	0.0000	loc(A)
23	3.7600	0.0001	0.0467	1.9253	0.0000	0.9411	0.0000	loc(A)
24	3.7662	0.0001	0.0737	1.7938	0.0000	0.7786	0.0000	loc(A)
25	3.7810	0.0000	0.0533	1.8800	0.0000	0.7524	0.0000	loc(A)
26	3.7834	0.0000	0.0717	1.8979	0.0000	0.8411	0.0000	loc(A)
27	3.7855	0.0006	0.0376	1.9352	0.0000	0.9071	0.0000	loc(A)
28	3.8378	0.0000	0.0371	1.9517	0.0000	0.9764	0.0000	loc(A)
29	3.8551	0.0003	0.0479	1.9157	0.0000	0.9195	0.0000	loc(A)
30	3.8596	0.0000	0.0511	1.8981	0.0000	0.8603	0.0000	loc(A)
31	3.8625	0.0010	0.0768	1.8757	0.0000	0.7446	0.0000	loc(A)
32	4.2382	0.0006	0.1724	1.8177	0.0000	0.6607	0.0601	loc(A)
33	4.2509	0.0006	0.2906	1.7020	0.0000	0.4871	0.0450	loc(A)
34	4.2705	0.0001	0.1311	1.8613	0.0000	0.7064	0.0000	loc(A)
35	4.2817	0.0006	0.0701	1.9218	0.0000	0.9196	0.0402	loc(A)
36	4.3071	0.0037	0.9138	0.9859	0.0000	0.0000	1.0000	CTB->A
37	4.3832	0.0058	0.3556	1.6391	0.0000	0.4899	0.1398	loc(A)
38	4.4135	0.0008	0.2497	1.7436	0.0000	0.4988	0.0000	loc(A)
39	4.4164	0.0679	0.4239	1.5591	0.0000	0.3700	0.2986	loc(A)
40	4.4241	0.0142	0.2555	1.7297	0.0000	0.5654	0.0425	loc(A)

4T-C_{60} ε=1 singlet ωB97X-D 6-311G(df,2p)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6121	0.0001	0.0492	1.9421	0.0000	1.0000	0.0000	loc(A)
2	2.6303	0.0003	0.0359	1.9560	0.0000	0.9651	0.0349	loc(A)

3	2.6393	0.0000	0.0040	1.9886	0.0000	1.0000	0.0000	loc(A)
4	2.6810	0.0000	0.0201	1.9731	0.0000	1.0000	0.0000	loc(A)
5	2.6830	0.0000	0.0248	1.9682	0.0000	1.0000	0.0000	loc(A)
6	2.6937	0.0000	0.0063	1.9882	0.0000	1.0000	0.0000	loc(A)
7	2.7103	0.0000	0.0718	1.9212	0.0000	0.9525	0.0475	loc(A)
8	2.7191	0.0000	0.0104	1.9807	0.0000	1.0000	0.0000	loc(A)
9	2.7281	0.0000	0.0005	1.9916	0.0000	1.0000	0.0000	loc(A)
10	2.7341	0.0000	0.0010	1.9923	0.0000	1.0000	0.0000	loc(A)
11	2.9378	0.0020	0.7462	1.2455	0.0000	0.2504	0.7496	CTB->A
12	2.9730	0.0163	0.6691	1.3217	0.0000	0.3184	0.6816	CTB->A
13	3.0061	0.0007	0.0388	1.9526	0.0000	0.9759	0.0241	loc(A)
14	3.0119	0.0003	0.0762	1.9168	0.0000	0.9481	0.0519	loc(A)
15	3.0310	0.0010	0.0050	1.9870	0.0000	1.0000	0.0000	loc(A)
16	3.0327	0.0004	0.0416	1.9523	0.0000	0.9590	0.0410	loc(A)
17	3.0767	0.0101	0.3511	1.6394	0.0000	0.6429	0.3571	loc(A)
18	3.2113	0.0000	0.9171	1.0794	0.0000	0.0687	0.9313	CTB->A
19	3.4734	0.6324	0.1372	0.1648	0.0000	0.0000	1.0000	loc(B)
20	3.5469	0.0020	0.0448	1.9364	0.0000	0.9481	0.0000	loc(A)
21	3.5707	0.0190	0.0347	1.8807	0.0000	0.9308	0.0254	loc(A)
22	3.5735	0.0001	0.0183	1.9488	0.0000	1.0000	0.0000	loc(A)
23	3.7406	0.0001	0.0319	1.9472	0.0000	1.0000	0.0000	loc(A)
24	3.7491	0.0000	0.0960	1.8575	0.0000	0.7697	0.0000	loc(A)
25	3.7647	0.0000	0.0262	1.9352	0.0000	0.9392	0.0000	loc(A)
26	3.7664	0.0000	0.0555	1.9197	0.0000	0.8463	0.0000	loc(A)
27	3.7693	0.0007	0.0128	1.9681	0.0000	1.0000	0.0000	loc(A)
28	3.8154	0.0000	0.0185	1.9673	0.0000	1.0000	0.0000	loc(A)
29	3.8323	0.0002	0.0110	1.9659	0.0000	1.0000	0.0000	loc(A)
30	3.8368	0.0000	0.0591	1.9112	0.0000	0.8916	0.0000	loc(A)
31	3.8395	0.0011	0.0518	1.9199	0.0000	0.9478	0.0265	loc(A)
32	4.1448	0.0080	0.9098	1.0127	0.0000	0.0000	1.0000	CTB->A
33	4.1886	0.0017	0.2310	1.7634	0.0000	0.7386	0.1647	loc(A)
34	4.2009	0.0016	0.3404	1.6513	0.0000	0.5381	0.2372	loc(A)
35	4.2280	0.0002	0.0935	1.8979	0.0000	0.8309	0.0000	loc(A)
36	4.2415	0.0002	0.0167	1.9741	0.0000	1.0000	0.0000	loc(A)
37	4.2912	0.0137	0.7793	1.2112	0.0000	0.1552	0.8180	CTB->A
38	4.3032	0.0122	0.6075	1.3859	0.0000	0.3485	0.6048	CTB->A
39	4.3714	0.0009	0.2118	1.7805	0.0000	0.6926	0.0450	loc(A)
40	4.3764	0.0001	0.2782	1.7141	0.0000	0.7435	0.2138	loc(A)

4T-C_{60} ε=1 singlet ωB97X-D/6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6522	0.0001	0.0295	1.9621	0.0000	1.0000	0.0000	loc(A)
2	2.6723	0.0001	0.0033	1.9895	0.0000	1.0000	0.0000	loc(A)
3	2.6808	0.0000	0.0042	1.9897	0.0000	1.0000	0.0000	loc(A)
4	2.7237	0.0000	0.0096	1.9846	0.0000	1.0000	0.0000	loc(A)
5	2.7287	0.0000	0.0157	1.9782	0.0000	1.0000	0.0000	loc(A)
6	2.7360	0.0000	0.0032	1.9919	0.0000	1.0000	0.0000	loc(A)
7	2.7571	0.0000	0.0418	1.9517	0.0000	0.9753	0.0247	loc(A)
8	2.7592	0.0000	0.0111	1.9805	0.0000	1.0000	0.0000	loc(A)
9	2.7742	0.0000	-0.0000	1.9930	0.0000	1.0000	0.0000	loc(A)
10	2.7785	0.0000	0.0026	1.9915	0.0000	1.0000	0.0000	loc(A)
11	3.0417	0.0018	0.2179	1.7765	0.0000	0.7959	0.2041	loc(A)
12	3.0618	0.0012	0.0104	1.9816	0.0000	1.0000	0.0000	loc(A)
13	3.0712	0.0030	0.0974	1.8956	0.0000	0.9034	0.0966	loc(A)
14	3.0733	0.0000	0.0491	1.9450	0.0000	0.9562	0.0438	loc(A)
15	3.0866	0.0006	0.0026	1.9901	0.0000	1.0000	0.0000	loc(A)
16	3.1366	0.0001	0.7613	1.2293	0.0000	0.2228	0.7772	CTB->A
17	3.2180	0.0241	0.8002	1.1919	0.0000	0.1834	0.8166	CTB->A
18	3.3863	0.0098	0.9503	1.0468	0.0000	0.0321	0.9679	CTB->A
19	3.5440	0.5603	0.1734	0.2850	0.0000	0.0394	0.9606	loc(B)
20	3.5637	0.0177	0.0624	1.8630	0.0000	0.8853	0.0317	loc(A)
21	3.5858	0.0000	0.0632	1.8971	0.0000	0.9328	0.0000	loc(A)
22	3.5882	0.1010	0.0370	1.6687	0.0000	0.8209	0.1360	loc(A)

23	3.7595	0.0000	0.0668	1.9101	0.0000	0.9399	0.0000	loc(A)
24	3.7672	0.0001	0.1031	1.8248	0.0000	0.7548	0.0345	loc(A)
25	3.7794	0.0001	0.0583	1.8899	0.0000	0.9377	0.0297	loc(A)
26	3.7858	0.0000	0.0432	1.9250	0.0000	0.9494	0.0000	loc(A)
27	3.7897	0.0007	0.0094	1.9695	0.0000	1.0000	0.0000	loc(A)
28	3.8397	0.0000	0.0565	1.9333	0.0000	0.9526	0.0000	loc(A)
29	3.8571	0.0003	0.0511	1.9262	0.0000	0.9701	0.0000	loc(A)
30	3.8601	0.0000	0.0435	1.9134	0.0000	0.8937	0.0000	loc(A)
31	3.8628	0.0011	0.0552	1.9075	0.0000	0.9752	0.0000	loc(A)
32	4.2414	0.0006	0.1466	1.8399	0.0000	0.8396	0.0747	loc(A)
33	4.2535	0.0005	0.2848	1.7013	0.0000	0.5671	0.0783	loc(A)
34	4.2702	0.0000	0.1446	1.8480	0.0000	0.8542	0.0000	loc(A)
35	4.2852	0.0001	0.0442	1.9476	0.0000	1.0000	0.0000	loc(A)
36	4.3192	0.0008	0.9308	0.9882	0.0000	0.0000	1.0000	CTB->A
37	4.3903	0.0015	0.2857	1.7095	0.0000	0.6885	0.1585	loc(A)
38	4.4131	0.0000	0.2199	1.7731	0.0000	0.6534	0.0000	loc(A)
39	4.4233	0.0059	0.2399	1.7531	0.0000	0.7442	0.0000	loc(A)
40	4.4325	0.0519	0.1573	1.8270	0.0000	0.8711	0.1289	loc(A)

6T- C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6520	0.0002	0.0851	1.9060	0.0000	0.9625	0.0375	loc(A)
2	2.6729	0.0002	0.0263	1.9659	0.0000	0.9774	0.0226	loc(A)
3	2.6774	0.0000	0.0052	1.9878	0.0000	1.0000	0.0000	loc(A)
4	2.7226	0.0000	0.0378	1.9559	0.0000	0.9773	0.0227	loc(A)
5	2.7259	0.0000	0.0252	1.9683	0.0000	1.0000	0.0000	loc(A)
6	2.7348	0.0000	0.0063	1.9884	0.0000	1.0000	0.0000	loc(A)
7	2.7555	0.0000	0.0553	1.9379	0.0000	0.9700	0.0300	loc(A)
8	2.7587	0.0000	0.0192	1.9717	0.0000	1.0000	0.0000	loc(A)
9	2.7737	0.0000	0.0005	1.9921	0.0000	1.0000	0.0000	loc(A)
10	2.7754	0.0000	0.0026	1.9907	0.0000	1.0000	0.0000	loc(A)
11	3.0004	0.0012	0.7172	1.2742	0.0000	0.2824	0.7176	CTB->A
12	3.0412	0.0115	0.5591	1.4322	0.0000	0.4339	0.5661	CTB->A
13	3.0592	0.0068	0.0443	1.9475	0.0000	0.9734	0.0266	loc(A)
14	3.0663	0.0003	0.1270	1.8664	0.0000	0.8953	0.1047	loc(A)
15	3.0833	0.0056	0.0039	1.9881	0.0000	1.0000	0.0000	loc(A)
16	3.0847	0.0005	0.0813	1.9124	0.0000	0.9212	0.0788	loc(A)
17	3.1371	0.0109	0.4846	1.5060	0.0000	0.5099	0.4901	loc(A)
18	3.2437	0.6722	0.6601	0.7332	0.0000	0.0256	0.9744	CTB->A
19	3.2725	0.7740	0.6447	0.6682	0.0000	0.0000	1.0000	CTB->A
20	3.5597	0.0004	0.1915	1.7754	0.0000	0.7051	0.0000	loc(A)
21	3.5797	0.0040	-0.0085	1.7595	0.0000	0.7561	0.0000	loc(A)
22	3.5835	0.0000	-0.0092	1.8209	0.0000	0.9082	0.0000	loc(A)
23	3.7566	0.0002	0.1863	1.7350	0.0000	0.7284	0.0252	loc(A)
24	3.7642	0.0000	-0.0440	1.6648	0.0000	0.7483	0.0000	loc(A)
25	3.7784	0.0001	-0.0546	1.7720	0.0000	0.9310	0.0000	loc(A)
26	3.7829	0.0000	0.0264	1.8696	0.0000	0.8938	0.0000	loc(A)
27	3.7862	0.0005	0.0503	1.9073	0.0000	0.8938	0.0000	loc(A)
28	3.8363	0.0000	0.1487	1.8372	0.0000	0.7996	0.0000	loc(A)
29	3.8530	0.0003	0.0394	1.8540	0.0000	0.8473	0.0000	loc(A)
30	3.8588	0.0002	0.0178	1.7785	0.0000	0.7676	0.0000	loc(A)
31	3.8603	0.0017	-0.0232	1.8234	0.0000	0.9682	0.0000	loc(A)
32	3.9334	0.0087	0.8499	1.1027	0.0000	0.0848	0.9152	CTB->A
33	3.9338	0.0110	0.1618	0.2242	0.0000	0.0000	1.0000	loc(B)
34	4.0580	0.0010	0.8880	1.1079	0.0000	0.0649	0.9351	CTB->A
35	4.0586	0.0012	0.8935	1.0972	0.0000	0.0531	0.9469	CTB->A
36	4.2508	0.0000	0.2578	1.7354	0.0000	0.6203	0.0000	loc(A)
37	4.2568	0.0001	0.2759	1.7080	0.0000	0.4727	0.0000	loc(A)
38	4.2698	0.0000	0.1421	1.8366	0.0000	0.8554	0.0000	loc(A)
39	4.2838	0.0001	0.1829	1.8062	0.0000	0.7085	0.0000	loc(A)
40	4.3974	0.7257	0.1754	0.6678	0.0000	0.2319	0.7681	deloc
41	4.4014	0.0001	0.3413	1.6531	0.0000	0.3697	0.0000	loc(A)
42	4.4119	0.0000	0.2340	1.7586	0.0000	0.5911	0.0000	loc(A)

43	4.4216	0.0197	0.2971	1.6951	0.0000	0.5028	0.0000	loc(A)
44	4.4330	0.0611	0.2982	1.6915	0.0000	0.4450	0.0000	loc(A)
45	4.4396	0.0019	0.1418	1.8503	0.0000	0.8364	0.0000	loc(A)
46	4.4436	0.1699	0.0185	1.7528	0.0000	0.7797	0.0000	loc(A)
47	4.4550	0.3461	-0.1644	1.8190	0.0000	1.0000	0.0000	loc(A)
48	4.4712	0.0228	-0.0416	1.3912	0.0000	0.7032	0.2683	deloc
49	4.5665	0.0060	0.2648	1.7033	0.0000	0.5859	0.0000	loc(A)
50	4.5702	0.0002	0.9068	1.0289	0.0000	0.0281	0.9334	CTB->A
51	4.5803	0.0000	0.2717	1.7055	0.0000	0.5978	0.1216	loc(A)
52	4.5994	0.0006	0.2468	1.7455	0.0000	0.5973	0.0000	loc(A)
53	4.6458	0.0005	0.9796	1.0044	0.0000	0.0000	1.0000	CTB->A
54	4.7066	0.0030	0.6103	0.6856	0.0000	0.0312	0.9688	CTB->A
55	4.7508	0.0011	-0.0544	1.2424	0.0000	0.5832	0.2446	deloc
56	4.7784	0.0006	-0.0193	1.5499	0.0000	0.6399	0.0548	loc(A)
57	4.7823	0.0012	0.1743	1.7983	0.0000	0.8231	0.0000	loc(A)
58	4.7883	0.0000	0.3296	1.4602	0.0000	0.5880	0.4120	deloc
59	4.8020	0.0001	0.2226	0.9867	0.0000	0.3834	0.6166	deloc
60	4.8055	0.0002	0.0721	1.7880	0.0000	0.8528	0.0314	loc(A)

6T- C_{60} ε=2 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6514	0.0003	0.0946	1.8966	0.0000	0.9554	0.0446	loc(A)
2	2.6720	0.0002	0.0266	1.9659	0.0000	0.9773	0.0227	loc(A)
3	2.6762	0.0000	0.0057	1.9872	0.0000	1.0000	0.0000	loc(A)
4	2.7215	0.0001	0.0431	1.9506	0.0000	0.9737	0.0263	loc(A)
5	2.7247	0.0000	0.0270	1.9664	0.0000	1.0000	0.0000	loc(A)
6	2.7337	0.0000	0.0070	1.9876	0.0000	1.0000	0.0000	loc(A)
7	2.7556	0.0000	0.0810	1.9121	0.0000	0.9447	0.0553	loc(A)
8	2.7590	0.0000	0.0208	1.9701	0.0000	1.0000	0.0000	loc(A)
9	2.7732	0.0000	0.0007	1.9921	0.0000	1.0000	0.0000	loc(A)
10	2.7751	0.0000	0.0027	1.9904	0.0000	1.0000	0.0000	loc(A)
11	3.0028	0.0017	0.6386	1.3533	0.0000	0.3649	0.6351	CTB->A
12	3.0390	0.0115	0.4814	1.5103	0.0000	0.5128	0.4872	loc(A)
13	3.0527	0.0108	0.0431	1.9489	0.0000	0.9768	0.0232	loc(A)
14	3.0595	0.0001	0.1500	1.8434	0.0000	0.8726	0.1274	loc(A)
15	3.0755	0.0097	0.0044	1.9874	0.0000	1.0000	0.0000	loc(A)
16	3.0787	0.0008	0.1370	1.8564	0.0000	0.8646	0.1354	loc(A)
17	3.1367	0.0160	0.5386	1.4517	0.0000	0.4547	0.5453	CTB->A
18	3.1913	1.5907	0.3314	0.3603	0.0000	0.0000	1.0000	loc(B)
19	3.2671	0.0647	0.9390	1.0173	0.0000	0.0301	0.9699	CTB->A
20	3.5558	0.0002	0.1915	1.7761	0.0000	0.7142	0.0000	loc(A)
21	3.5757	0.0028	0.0060	1.7604	0.0000	0.7524	0.0000	loc(A)
22	3.5797	0.0000	0.0028	1.8185	0.0000	0.9067	0.0000	loc(A)
23	3.7562	0.0001	0.1805	1.7750	0.0000	0.7430	0.0000	loc(A)
24	3.7630	0.0000	-0.0252	1.6648	0.0000	0.7426	0.0000	loc(A)
25	3.7776	0.0001	-0.0303	1.7784	0.0000	0.9225	0.0000	loc(A)
26	3.7820	0.0000	0.0391	1.8664	0.0000	0.8828	0.0000	loc(A)
27	3.7850	0.0005	0.0758	1.8841	0.0000	0.8684	0.0000	loc(A)
28	3.8337	0.0000	0.1440	1.8415	0.0000	0.8158	0.0000	loc(A)
29	3.8432	0.0037	0.1299	0.4780	0.0000	0.1251	0.8369	loc(B)
30	3.8515	0.0002	0.1008	1.5984	0.0000	0.6716	0.1506	loc(A)
31	3.8566	0.0001	0.0462	1.6476	0.0000	0.6879	0.0908	loc(A)
32	3.8571	0.0015	-0.0085	1.8205	0.0000	0.9673	0.0000	loc(A)
33	3.9456	0.0081	0.8465	1.1093	0.0000	0.0841	0.9159	CTB->A
34	4.0699	0.0016	0.8649	1.1309	0.0000	0.0704	0.9035	CTB->A
35	4.0706	0.0028	0.8848	1.1057	0.0000	0.0554	0.9446	CTB->A
36	4.2507	0.0001	0.2797	1.7135	0.0000	0.5717	0.0312	loc(A)
37	4.2557	0.0002	0.2888	1.6957	0.0000	0.4698	0.0000	loc(A)
38	4.2692	0.0000	0.1625	1.8178	0.0000	0.8314	0.0000	loc(A)
39	4.2833	0.0002	0.2057	1.7838	0.0000	0.6881	0.0000	loc(A)
40	4.3401	0.8243	0.1767	0.3341	0.0000	0.0498	0.9502	loc(B)

6T- C_{60} ε=3 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6514	0.0003	0.1066	1.8846	0.0000	0.9482	0.0518	loc(A)
2	2.6717	0.0002	0.0259	1.9666	0.0000	0.9780	0.0220	loc(A)
3	2.6757	0.0000	0.0065	1.9864	0.0000	1.0000	0.0000	loc(A)
4	2.7209	0.0001	0.0503	1.9435	0.0000	0.9686	0.0314	loc(A)
5	2.7243	0.0000	0.0494	1.9440	0.0000	0.9774	0.0226	loc(A)
6	2.7332	0.0000	0.0077	1.9869	0.0000	1.0000	0.0000	loc(A)
7	2.7558	0.0000	0.0867	1.9064	0.0000	0.9410	0.0590	loc(A)
8	2.7592	0.0000	0.0233	1.9675	0.0000	1.0000	0.0000	loc(A)
9	2.7729	0.0000	0.0008	1.9922	0.0000	1.0000	0.0000	loc(A)
10	2.7748	0.0000	0.0028	1.9903	0.0000	1.0000	0.0000	loc(A)
11	3.0071	0.0019	0.5593	1.4328	0.0000	0.4494	0.5506	CTB->A
12	3.0403	0.0098	0.3700	1.6224	0.0000	0.6262	0.3738	loc(A)
13	3.0492	0.0129	0.0232	1.9688	0.0000	1.0000	0.0000	loc(A)
14	3.0570	0.0000	0.1598	1.8336	0.0000	0.8617	0.1383	loc(A)
15	3.0713	0.0119	0.0051	1.9867	0.0000	1.0000	0.0000	loc(A)
16	3.0778	0.0012	0.2749	1.7178	0.0000	0.7242	0.2758	loc(A)
17	3.1412	0.0201	0.5964	1.3939	0.0000	0.3958	0.6042	CTB->A
18	3.1665	1.7183	0.2766	0.3079	0.0000	0.0000	1.0000	loc(B)
19	3.2768	0.0328	0.9597	1.0371	0.0000	0.0295	0.9705	CTB->A
20	3.5538	0.0002	0.2336	1.7248	0.0000	0.5457	0.0256	loc(A)
21	3.5735	0.0024	0.0568	1.7287	0.0000	0.6126	0.0000	loc(A)
22	3.5777	0.0000	0.0296	1.8001	0.0000	0.7605	0.0000	loc(A)
23	3.7563	0.0001	0.1710	1.7858	0.0000	0.6545	0.0000	loc(A)
24	3.7624	0.0000	0.0243	1.6286	0.0000	0.6466	0.0292	loc(A)
25	3.7774	0.0001	-0.0046	1.7945	0.0000	0.7996	0.0000	loc(A)
26	3.7816	0.0000	0.0901	1.8255	0.0000	0.7740	0.0000	loc(A)
27	3.7843	0.0005	0.1005	1.8610	0.0000	0.6705	0.0000	loc(A)
28	3.8078	0.0011	0.1254	0.2040	0.0000	0.0000	1.0000	loc(B)
29	3.8325	0.0000	0.1611	1.8244	0.0000	0.7040	0.0000	loc(A)
30	3.8487	0.0001	0.1464	1.7713	0.0000	0.6145	0.0000	loc(A)
31	3.8540	0.0001	0.0616	1.7880	0.0000	0.6729	0.0000	loc(A)
32	3.8556	0.0014	0.0059	1.8129	0.0000	0.8200	0.0000	loc(A)
33	3.9587	0.0077	0.8371	1.1221	0.0000	0.0883	0.9117	CTB->A
34	4.0832	0.0022	0.8454	1.1505	0.0000	0.0797	0.8896	CTB->A
35	4.0839	0.0048	0.8519	1.1386	0.0000	0.0840	0.9160	CTB->A
36	4.2509	0.0002	0.3241	1.6691	0.0000	0.2602	0.0239	loc(A)
37	4.2552	0.0004	0.3350	1.6504	0.0000	0.2519	0.0000	loc(A)
38	4.2687	0.0001	0.1988	1.7830	0.0000	0.6882	0.0000	loc(A)
39	4.2824	0.0003	0.2341	1.7556	0.0000	0.3833	0.0000	loc(A)
40	4.3108	0.8202	0.1246	0.3014	0.0000	0.0590	0.9410	loc(B)

6T- C_{60} ε=4 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6513	0.0003	0.1171	1.8741	0.0000	0.9420	0.0580	loc(A)
2	2.6716	0.0002	0.0254	1.9671	0.0000	0.9786	0.0214	loc(A)
3	2.6753	0.0000	0.0073	1.9856	0.0000	1.0000	0.0000	loc(A)
4	2.7206	0.0001	0.0580	1.9358	0.0000	0.9631	0.0369	loc(A)
5	2.7241	0.0001	0.0544	1.9390	0.0000	0.9742	0.0258	loc(A)
6	2.7329	0.0000	0.0084	1.9863	0.0000	1.0000	0.0000	loc(A)
7	2.7560	0.0000	0.0722	1.9210	0.0000	0.9583	0.0417	loc(A)
8	2.7593	0.0000	0.0257	1.9652	0.0000	1.0000	0.0000	loc(A)
9	2.7727	0.0000	0.0009	1.9921	0.0000	1.0000	0.0000	loc(A)
10	2.7747	0.0000	0.0030	1.9901	0.0000	1.0000	0.0000	loc(A)
11	3.0099	0.0019	0.5002	1.4922	0.0000	0.5133	0.4867	CTB->A
12	3.0409	0.0084	0.2960	1.6966	0.0000	0.7015	0.2985	loc(A)
13	3.0470	0.0141	0.0254	1.9666	0.0000	1.0000	0.0000	loc(A)
14	3.0558	0.0000	0.1376	1.8557	0.0000	0.8849	0.1151	loc(A)
15	3.0686	0.0132	0.0057	1.9861	0.0000	1.0000	0.0000	loc(A)
16	3.0792	0.0016	0.3962	1.5959	0.0000	0.6007	0.3993	loc(A)
17	3.1457	0.0232	0.6373	1.3529	0.0000	0.3540	0.6460	CTB->A

18	3.1528	1.7838	0.2534	0.2865	0.0000	0.0000	1.0000	loc(B)
19	3.2851	0.0239	0.9608	1.0359	0.0000	0.0283	0.9717	CTB->A
20	3.5525	0.0001	0.2165	1.7446	0.0000	0.5989	0.0276	loc(A)
21	3.5721	0.0023	0.0230	1.7683	0.0000	0.7108	0.0000	loc(A)
22	3.5764	0.0000	0.0296	1.8161	0.0000	0.8057	0.0000	loc(A)
23	3.7565	0.0000	0.1751	1.7835	0.0000	0.6531	0.0000	loc(A)
24	3.7621	0.0000	0.0459	1.6357	0.0000	0.6617	0.0351	loc(A)
25	3.7771	0.0001	0.0189	1.7979	0.0000	0.7898	0.0000	loc(A)
26	3.7810	0.0000	0.0571	1.8011	0.0000	0.8427	0.0321	loc(A)
27	3.7839	0.0005	0.0999	1.8617	0.0000	0.6939	0.0000	loc(A)
28	3.7872	0.0001	0.1005	0.2355	0.0000	0.0251	0.9749	loc(B)
29	3.8319	0.0000	0.1616	1.8236	0.0000	0.7149	0.0000	loc(A)
30	3.8477	0.0001	0.0994	1.8546	0.0000	0.7869	0.0000	loc(A)
31	3.8529	0.0001	0.0631	1.7954	0.0000	0.6740	0.0000	loc(A)
32	3.8546	0.0014	0.0317	1.8058	0.0000	0.8065	0.0000	loc(A)
33	3.9688	0.0073	0.8094	1.1529	0.0000	0.1152	0.8848	CTB->A
34	4.0934	0.0027	0.8280	1.1679	0.0000	0.0885	0.8773	CTB->A
35	4.0941	0.0068	0.8361	1.1543	0.0000	0.0935	0.9065	CTB->A
36	4.2512	0.0003	0.2653	1.7280	0.0000	0.4089	0.0268	loc(A)
37	4.2549	0.0010	0.3113	1.6746	0.0000	0.3401	0.0000	loc(A)
38	4.2683	0.0003	0.2197	1.7633	0.0000	0.7056	0.0383	loc(A)
39	4.2815	0.0006	0.2486	1.7413	0.0000	0.3809	0.0000	loc(A)
40	4.2933	0.8106	0.1037	0.2798	0.0000	0.0562	0.9438	loc(B)

6T- C_{60} ε=6 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6513	0.0004	0.1520	1.8392	0.0000	0.9102	0.0898	loc(A)
2	2.6714	0.0002	0.0046	1.9880	0.0000	1.0000	0.0000	loc(A)
3	2.6748	0.0000	0.0087	1.9842	0.0000	1.0000	0.0000	loc(A)
4	2.7201	0.0001	0.0686	1.9252	0.0000	0.9537	0.0463	loc(A)
5	2.7239	0.0001	0.0596	1.9338	0.0000	0.9704	0.0296	loc(A)
6	2.7326	0.0000	0.0095	1.9852	0.0000	1.0000	0.0000	loc(A)
7	2.7563	0.0000	0.0823	1.9109	0.0000	0.9510	0.0490	loc(A)
8	2.7595	0.0000	0.0490	1.9418	0.0000	0.9779	0.0221	loc(A)
9	2.7724	0.0000	0.0009	1.9921	0.0000	1.0000	0.0000	loc(A)
10	2.7745	0.0000	0.0033	1.9898	0.0000	1.0000	0.0000	loc(A)
11	3.0128	0.0018	0.4166	1.5765	0.0000	0.6048	0.3952	loc(A)
12	3.0410	0.0067	0.2181	1.7745	0.0000	0.7808	0.2192	loc(A)
13	3.0443	0.0151	0.0482	1.9438	0.0000	0.9782	0.0218	loc(A)
14	3.0544	0.0000	0.1151	1.8784	0.0000	0.9058	0.0942	loc(A)
15	3.0655	0.0143	0.0067	1.9850	0.0000	1.0000	0.0000	loc(A)
16	3.0838	0.0018	0.5506	1.4407	0.0000	0.4432	0.5568	CTB->A
17	3.1381	1.8577	0.2228	0.2588	0.0000	0.0000	1.0000	loc(B)
18	3.1532	0.0270	0.6878	1.3023	0.0000	0.3025	0.6975	CTB->A
19	3.2972	0.0175	0.9624	1.0344	0.0000	0.0266	0.9734	CTB->A
20	3.5510	0.0001	0.2023	1.7606	0.0000	0.5898	0.0333	loc(A)
21	3.5704	0.0021	0.0312	1.7815	0.0000	0.6511	0.0000	loc(A)
22	3.5748	0.0000	0.0363	1.8221	0.0000	0.8089	0.0000	loc(A)
23	3.7566	0.0000	0.1820	1.7786	0.0000	0.5089	0.0000	loc(A)
24	3.7609	0.0000	0.0834	1.3085	0.0000	0.5066	0.2698	deloc
25	3.7642	0.0002	0.0542	0.5264	0.0000	0.1809	0.7779	deloc
26	3.7771	0.0001	0.0310	1.7896	0.0000	0.7753	0.0000	loc(A)
27	3.7812	0.0000	0.0677	1.8982	0.0000	0.7760	0.0000	loc(A)
28	3.7832	0.0005	0.1198	1.8442	0.0000	0.6798	0.0000	loc(A)
29	3.8310	0.0000	0.1574	1.8276	0.0000	0.6520	0.0000	loc(A)
30	3.8466	0.0002	0.0851	1.8731	0.0000	0.7397	0.0000	loc(A)
31	3.8515	0.0001	0.0682	1.8002	0.0000	0.6350	0.0000	loc(A)
32	3.8535	0.0014	0.0545	1.7989	0.0000	0.7306	0.0000	loc(A)
33	3.9830	0.0069	0.7885	1.1770	0.0000	0.1294	0.8706	CTB->A
34	4.1076	0.0036	0.7997	1.1960	0.0000	0.1033	0.8572	CTB->A
35	4.1083	0.0111	0.8100	1.1804	0.0000	0.1099	0.8901	CTB->A
36	4.2516	0.0006	0.2539	1.7394	0.0000	0.4036	0.0332	loc(A)
37	4.2544	0.0054	0.3147	1.6720	0.0000	0.2005	0.0000	loc(A)

38	4.2678	0.0005	0.2227	1.7622	0.0000	0.5590	0.0287	loc(A)
39	4.2735	0.7892	0.0768	0.2226	0.0000	0.0362	0.9638	loc(B)
40	4.2810	0.0018	0.2565	1.7338	0.0000	0.2547	0.0000	loc(A)

6T- C_{60} ε=8 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6513	0.0004	0.1669	1.8243	0.0000	0.8997	0.1003	loc(A)
2	2.6713	0.0002	0.0047	1.9879	0.0000	1.0000	0.0000	loc(A)
3	2.6744	0.0000	0.0097	1.9832	0.0000	1.0000	0.0000	loc(A)
4	2.7198	0.0001	0.0764	1.9174	0.0000	0.9477	0.0523	loc(A)
5	2.7238	0.0001	0.0645	1.9289	0.0000	0.9669	0.0331	loc(A)
6	2.7323	0.0000	0.0104	1.9843	0.0000	1.0000	0.0000	loc(A)
7	2.7564	0.0000	0.0903	1.9029	0.0000	0.9450	0.0550	loc(A)
8	2.7595	0.0000	0.0541	1.9367	0.0000	0.9756	0.0244	loc(A)
9	2.7723	0.0000	0.0009	1.9921	0.0000	1.0000	0.0000	loc(A)
10	2.7743	0.0000	0.0035	1.9895	0.0000	1.0000	0.0000	loc(A)
11	3.0142	0.0016	0.3793	1.6140	0.0000	0.6471	0.3529	loc(A)
12	3.0408	0.0058	0.1845	1.8082	0.0000	0.8151	0.1849	loc(A)
13	3.0427	0.0154	0.0531	1.9389	0.0000	0.9756	0.0244	loc(A)
14	3.0535	0.0000	0.0951	1.8984	0.0000	0.9248	0.0752	loc(A)
15	3.0636	0.0146	0.0076	1.9842	0.0000	1.0000	0.0000	loc(A)
16	3.0883	0.0019	0.6349	1.3562	0.0000	0.3572	0.6428	CTB->A
17	3.1303	1.8989	0.2037	0.2420	0.0000	0.0000	1.0000	loc(B)
18	3.1589	0.0294	0.7171	1.2730	0.0000	0.2726	0.7274	CTB->A
19	3.3054	0.0148	0.9633	1.0334	0.0000	0.0255	0.9745	CTB->A
20	3.5502	0.0001	0.1980	1.7667	0.0000	0.5787	0.0369	loc(A)
21	3.5694	0.0020	0.0373	1.7872	0.0000	0.6519	0.0000	loc(A)
22	3.5739	0.0000	0.0419	1.8242	0.0000	0.8118	0.0000	loc(A)
23	3.7509	0.0008	0.0524	0.2325	0.0000	0.0407	0.9593	loc(B)
24	3.7567	0.0000	0.1870	1.7747	0.0000	0.5135	0.0000	loc(A)
25	3.7616	0.0001	0.0901	1.6429	0.0000	0.6402	0.0628	loc(A)
26	3.7770	0.0001	0.0412	1.7919	0.0000	0.7749	0.0000	loc(A)
27	3.7809	0.0000	0.0708	1.8976	0.0000	0.7750	0.0000	loc(A)
28	3.7827	0.0006	0.1262	1.8388	0.0000	0.6711	0.0000	loc(A)
29	3.8306	0.0000	0.1488	1.8361	0.0000	0.6428	0.0000	loc(A)
30	3.8460	0.0002	0.0792	1.8814	0.0000	0.7372	0.0000	loc(A)
31	3.8507	0.0001	0.0745	1.8022	0.0000	0.6293	0.0000	loc(A)
32	3.8529	0.0014	0.0692	1.7951	0.0000	0.7161	0.0000	loc(A)
33	3.9926	0.0067	0.7714	1.1961	0.0000	0.1414	0.8586	CTB->A
34	4.1169	0.0044	0.7778	1.2179	0.0000	0.1152	0.8412	CTB->A
35	4.1177	0.0151	0.7893	1.2010	0.0000	0.1232	0.8768	CTB->A
36	4.2519	0.0010	0.2567	1.7365	0.0000	0.4033	0.0373	loc(A)
37	4.2539	0.0303	0.3128	1.6742	0.0000	0.2090	0.0000	loc(A)
38	4.2626	0.7485	0.0571	0.2179	0.0000	0.0408	0.9592	loc(B)
39	4.2676	0.0007	0.2220	1.7636	0.0000	0.5631	0.0279	loc(A)
40	4.2807	0.0010	0.2422	1.7483	0.0000	0.2638	0.0000	loc(A)

6T- C_{60} ε=16 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6512	0.0004	0.2047	1.7865	0.0000	0.8711	0.1289	loc(A)
2	2.6711	0.0002	0.0053	1.9873	0.0000	1.0000	0.0000	loc(A)
3	2.6738	0.0000	0.0126	1.9803	0.0000	1.0000	0.0000	loc(A)
4	2.7192	0.0001	0.0957	1.8981	0.0000	0.9314	0.0686	loc(A)
5	2.7235	0.0001	0.0774	1.9160	0.0000	0.9573	0.0427	loc(A)
6	2.7319	0.0000	0.0130	1.9817	0.0000	1.0000	0.0000	loc(A)
7	2.7566	0.0000	0.1105	1.8827	0.0000	0.9286	0.0714	loc(A)
8	2.7595	0.0000	0.0679	1.9229	0.0000	0.9694	0.0306	loc(A)
9	2.7719	0.0000	0.0012	1.9918	0.0000	1.0000	0.0000	loc(A)
10	2.7740	0.0000	0.0044	1.9887	0.0000	1.0000	0.0000	loc(A)
11	3.0160	0.0011	0.3301	1.6636	0.0000	0.7059	0.2941	loc(A)
12	3.0398	0.0153	0.0664	1.9255	0.0000	0.9684	0.0316	loc(A)

13	3.0403	0.0045	0.1441	1.8484	0.0000	0.8566	0.1434	loc(A)
14	3.0515	0.0000	0.0693	1.9241	0.0000	0.9509	0.0491	loc(A)
15	3.0604	0.0143	0.0097	1.9821	0.0000	1.0000	0.0000	loc(A)
16	3.1005	0.0017	0.7662	1.2243	0.0000	0.2230	0.7770	CTB->A
17	3.1181	1.9705	0.1674	0.2115	0.0000	0.0000	1.0000	loc(B)
18	3.1720	0.0335	0.7676	1.2224	0.0000	0.2209	0.7791	CTB->A
19	3.3230	0.0112	0.9651	1.0317	0.0000	0.0235	0.9765	CTB->A
20	3.5485	0.0002	0.1911	1.7752	0.0000	0.7236	0.0498	loc(A)
21	3.5674	0.0018	0.0494	1.7929	0.0000	0.6728	0.0000	loc(A)
22	3.5721	0.0000	0.0427	1.8373	0.0000	0.8473	0.0000	loc(A)
23	3.7313	0.0033	0.0110	0.2238	0.0000	0.0440	0.9560	loc(B)
24	3.7567	0.0000	0.2174	1.7462	0.0000	0.5134	0.0302	loc(A)
25	3.7609	0.0001	0.1645	1.6488	0.0000	0.6981	0.0505	loc(A)
26	3.7766	0.0001	0.0565	1.7979	0.0000	0.7739	0.0000	loc(A)
27	3.7803	0.0000	0.0798	1.8922	0.0000	0.7931	0.0000	loc(A)
28	3.7818	0.0006	0.1234	1.8437	0.0000	0.7217	0.0000	loc(A)
29	3.8296	0.0000	0.1614	1.8230	0.0000	0.7437	0.0235	loc(A)
30	3.8448	0.0002	0.0644	1.8997	0.0000	0.8376	0.0000	loc(A)
31	3.8492	0.0001	0.1082	1.7836	0.0000	0.6224	0.0000	loc(A)
32	3.8516	0.0014	0.0761	1.8032	0.0000	0.7626	0.0000	loc(A)
33	4.0125	0.0061	0.7262	1.2448	0.0000	0.1747	0.8253	CTB->A
34	4.1361	0.0065	0.7235	1.2721	0.0000	0.1473	0.7997	CTB->A
35	4.1370	0.0289	0.7364	1.2539	0.0000	0.1590	0.8410	CTB->A
36	4.2445	0.7047	-0.0032	0.2024	0.0000	0.0559	0.9441	loc(B)
37	4.2526	0.0020	0.2608	1.7316	0.0000	0.4480	0.0505	loc(A)
38	4.2542	0.0339	0.3783	1.6093	0.0000	0.2137	0.0000	loc(A)
39	4.2671	0.0014	0.2209	1.7656	0.0000	0.6649	0.0320	loc(A)
40	4.2801	0.0030	0.2260	1.7649	0.0000	0.4249	0.0000	loc(A)

6T- C_{60} ε=1 triplet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	1.7517	0.0000	0.0655	1.9261	0.0000	0.9720	0.0280	loc(A)
2	1.7644	0.0000	0.0074	1.9846	0.0000	1.0000	0.0000	loc(A)
3	1.7686	0.0000	0.0059	1.9874	0.0000	1.0000	0.0000	loc(A)
4	1.9197	0.0000	0.3368	0.3556	0.0000	0.0000	1.0238	loc(B)
5	2.3263	0.0000	0.1528	0.2147	0.0000	0.0000	1.0000	loc(B)
6	2.4398	0.0000	0.0261	1.9665	0.0000	1.0000	0.0000	loc(A)
7	2.4457	0.0000	0.0168	1.9758	0.0000	1.0000	0.0000	loc(A)
8	2.4519	0.0000	0.0067	1.9868	0.0000	1.0000	0.0000	loc(A)
9	2.5596	0.0000	0.0958	1.8997	0.0000	0.9463	0.0537	loc(A)
10	2.5661	0.0000	0.0253	1.9668	0.0000	1.0000	0.0000	loc(A)
11	2.5781	0.0000	0.0070	1.9881	0.0000	1.0000	0.0000	loc(A)
12	2.5802	0.0000	0.0026	1.9883	0.0000	1.0000	0.0000	loc(A)
13	2.5833	0.0000	0.1045	1.8851	0.0000	0.8607	0.0000	loc(A)
14	2.5867	0.0000	0.0723	1.8223	0.0000	0.7584	0.0000	loc(A)
15	2.5902	0.0000	0.0422	1.9214	0.0000	0.9446	0.0000	loc(A)
16	2.5954	0.0000	0.0350	1.8519	0.0000	0.9152	0.0000	loc(A)
17	2.5986	0.0000	0.0341	1.8268	0.0000	0.7815	0.0000	loc(A)
18	2.6655	0.0000	0.0201	1.9709	0.0000	1.0000	0.0000	loc(A)
19	2.6681	0.0000	0.0149	1.9772	0.0000	1.0000	0.0000	loc(A)
20	2.6791	0.0000	0.0016	1.9916	0.0000	1.0000	0.0000	loc(A)
21	2.6819	0.0000	0.0022	1.9913	0.0000	1.0000	0.0000	loc(A)
22	2.6840	0.0000	0.2241	0.4375	0.0000	0.0819	0.9181	loc(B)
23	2.9990	0.0000	0.9854	1.0047	0.0000	0.0000	1.0000	CTB->A
24	3.0720	0.0000	0.9603	1.0294	0.0000	0.0254	0.9746	CTB->A
25	3.1290	0.0000	0.2468	1.7396	0.0000	0.6560	0.1092	loc(A)
26	3.1497	0.0000	0.0845	1.9008	0.0000	0.9080	0.0000	loc(A)
27	3.1655	0.0000	-0.0065	1.7581	0.0000	0.8754	0.0291	loc(A)
28	3.1695	0.0000	-0.0588	1.7111	0.0000	0.7702	0.0000	loc(A)
29	3.1711	0.0000	0.0476	1.8533	0.0000	0.9196	0.0522	loc(A)
30	3.1748	0.0000	-0.0863	1.7840	0.0000	0.8812	0.0000	loc(A)
31	3.2475	0.0000	0.1573	0.2936	0.0000	0.0000	0.9132	loc(B)
32	3.2647	0.0000	0.9568	1.0394	0.0000	0.0323	0.9677	CTB->A

33	3.4004	0.0000	0.1740	1.7821	0.0000	0.7724	0.0000	loc(A)
34	3.4063	0.0000	0.0361	1.7293	0.0000	0.7256	0.0000	loc(A)
35	3.4124	0.0000	-0.0122	1.7668	0.0000	0.8870	0.0000	loc(A)
36	3.4178	0.0000	0.0707	1.9166	0.0000	0.9204	0.0000	loc(A)
37	3.4212	0.0000	0.0581	1.8998	0.0000	0.8730	0.0000	loc(A)
38	3.6168	0.0000	0.0228	0.2268	0.0000	0.0360	0.8846	loc(B)
39	3.8553	0.0000	0.2567	1.7360	0.0000	0.5777	0.0000	loc(A)
40	3.8658	0.0000	0.2343	1.7563	0.0000	0.5670	0.0000	loc(A)
41	3.8776	0.0000	0.3303	1.6362	0.0000	0.4748	0.0700	loc(A)
42	3.9023	0.0000	0.0569	0.1963	0.0000	0.0000	0.9261	loc(B)
43	3.9238	0.0000	0.8747	1.0808	0.0000	0.0401	0.9325	CTB->A
44	4.0504	0.0000	0.8735	1.1224	0.0000	0.0519	0.8749	CTB->A
45	4.0561	0.0000	0.8862	1.1045	0.0000	0.0461	0.9301	CTB->A
46	4.0822	0.0000	-0.0547	0.7231	0.0000	0.0460	0.0461	deloc
47	4.1262	0.0000	0.0186	1.9112	0.0000	1.0000	0.0000	loc(A)
48	4.1290	0.0000	-0.0711	1.9105	0.0000	1.0000	0.0000	loc(A)
49	4.1296	0.0000	0.0212	1.9506	0.0000	1.0000	0.0000	loc(A)
50	4.1361	0.0000	-0.0063	1.8570	0.0000	0.8591	0.0000	loc(A)
51	4.1394	0.0000	0.2889	1.7044	0.0000	0.6214	0.0840	loc(A)
52	4.1400	0.0000	0.2804	1.7027	0.0000	0.4735	0.0316	loc(A)
53	4.1507	0.0000	0.1454	1.8348	0.0000	0.8527	0.0000	loc(A)
54	4.1626	0.0000	0.1887	1.8000	0.0000	0.7034	0.0000	loc(A)
55	4.2378	0.0000	-0.2328	0.8972	0.0000	0.0771	0.0000	deloc
56	4.2533	0.0000	0.0361	0.3518	0.0000	0.0000	0.6230	loc(B)
57	4.2540	0.0000	0.0748	0.3526	0.0000	0.0000	0.6887	loc(B)
58	4.2782	0.0000	0.2765	1.6920	0.0000	0.4728	0.0000	loc(A)
59	4.2844	0.0000	0.2118	1.7620	0.0000	0.6240	0.0000	loc(A)
60	4.2932	0.0000	0.3079	1.6832	0.0000	0.4568	0.0000	loc(A)
61	4.3014	0.0000	0.3076	1.6828	0.0000	0.4126	0.0000	loc(A)
62	4.3021	0.0000	0.1111	1.8606	0.0000	0.8593	0.0000	loc(A)
63	4.4016	0.0000	0.1520	0.2073	0.0000	0.0000	0.9386	loc(B)
64	4.4031	0.0000	0.1446	0.1966	0.0000	0.0000	0.9452	loc(B)
65	4.5683	0.0000	0.9342	0.9623	0.0000	0.0000	1.0000	CTB->A
66	4.6076	0.0000	0.9442	1.0400	0.0000	0.0359	0.9641	CTB->A
67	4.6288	0.0000	0.0672	1.8746	0.0000	0.9019	0.0417	loc(A)
68	4.6295	0.0000	-0.0203	1.9246	0.0000	1.0000	0.0000	loc(A)
69	4.6435	0.0000	0.2246	1.7307	0.0000	0.7670	0.2330	loc(A)
70	4.6495	0.0000	-0.1084	1.6097	0.0000	0.8332	0.0000	loc(A)

S3HT- C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6576	0.0000	0.0225	1.9558	0.0000	1.0000	0.0000	loc(A)
2	2.6581	0.0001	0.1328	1.8436	0.0000	0.9222	0.0778	loc(A)
3	2.6673	0.0000	0.0137	1.9636	0.0000	1.0000	0.0000	loc(A)
4	2.7067	0.0000	0.0345	1.9415	0.0000	1.0000	0.0000	loc(A)
5	2.7189	0.0000	0.0741	1.9026	0.0000	0.9583	0.0417	loc(A)
6	2.7231	0.0000	0.0258	1.9504	0.0000	1.0000	0.0000	loc(A)
7	2.7485	0.0004	0.0781	1.8989	0.0000	0.9632	0.0368	loc(A)
8	2.7571	0.0000	0.0566	1.9197	0.0000	0.9686	0.0314	loc(A)
9	2.7698	0.0000	0.0105	1.9672	0.0000	1.0000	0.0000	loc(A)
10	2.7725	0.0000	0.0019	1.9775	0.0000	1.0000	0.0000	loc(A)
11	2.8909	0.0001	0.9511	1.0267	0.0000	0.0231	0.9769	CTB->A
12	2.9157	0.0321	0.8983	1.0800	0.0000	0.0910	0.9090	CTB->A
13	3.0419	0.0002	0.0251	1.9508	0.0000	1.0000	0.0000	loc(A)
14	3.0474	0.0003	0.1043	1.8725	0.0000	0.9123	0.0877	loc(A)
15	3.0722	0.0002	0.0369	1.9416	0.0000	0.9683	0.0317	loc(A)
16	3.0748	0.0001	0.0257	1.9508	0.0000	1.0000	0.0000	loc(A)
17	3.0784	0.0007	0.1846	1.7936	0.0000	0.8559	0.1441	loc(A)
18	3.1171	0.0059	0.9205	1.0545	0.0000	0.0561	0.9439	CTB->A
19	3.5026	1.4395	0.0018	0.0227	0.0000	0.0000	1.0000	loc(B)
20	3.5565	0.0120	0.1057	1.8705	0.0000	0.9211	0.0541	loc(A)
21	3.5642	0.0116	0.1197	1.8590	0.0000	0.8208	0.0238	loc(A)
22	3.5694	0.0002	0.0847	1.8946	0.0000	0.9703	0.0297	loc(A)

23	3.7548	0.0000	0.1945	1.7846	0.0000	0.8344	0.1656	loc(A)
24	3.7595	0.0000	0.1199	1.8560	0.0000	0.9303	0.0697	loc(A)
25	3.7650	0.0012	0.0611	1.9159	0.0000	0.9527	0.0000	loc(A)
26	3.7682	0.0002	0.0903	1.8904	0.0000	0.8847	0.0240	loc(A)
27	3.7761	0.0000	0.0533	1.9259	0.0000	1.0000	0.0000	loc(A)
28	3.8182	0.0002	0.2100	1.7662	0.0000	0.8001	0.1999	loc(A)
29	3.8406	0.0003	0.0669	1.9111	0.0000	0.9422	0.0249	loc(A)
30	3.8449	0.0002	0.1078	1.8703	0.0000	0.8416	0.0000	loc(A)
31	3.8469	0.0002	0.0557	1.9233	0.0000	1.0000	0.0000	loc(A)
32	3.8843	0.0007	0.7973	1.1808	0.0000	0.1943	0.8057	CTB->A
33	3.9324	0.0012	0.9799	0.9983	0.0000	0.0000	1.0000	CTB->A
34	3.9587	0.0173	0.9734	1.0014	0.0000	0.0000	1.0000	CTB->A
35	4.0575	0.3155	0.0404	0.0646	0.0000	0.0000	1.0000	loc(B)
36	4.2241	0.0005	0.2427	1.7333	0.0000	0.7481	0.1619	loc(A)
37	4.2346	0.0024	0.1327	1.8427	0.0000	0.9194	0.0806	loc(A)
38	4.2611	0.0006	0.1523	1.8235	0.0000	0.7368	0.0000	loc(A)
39	4.2665	0.0001	0.0749	1.9008	0.0000	0.9677	0.0000	loc(A)
40	4.3458	0.0072	0.8498	1.1283	0.0000	0.0685	0.9315	CTB->A
41	4.3610	0.0190	0.5163	1.4597	0.0000	0.4387	0.4817	CTB->A
42	4.3733	0.0094	0.5845	1.3928	0.0000	0.3554	0.5715	CTB->A
43	4.3806	0.0117	0.4710	1.5054	0.0000	0.3453	0.3626	loc(A)
44	4.3879	0.5971	0.0882	0.8140	0.0000	0.3548	0.6452	deloc
45	4.4028	0.0291	0.2560	1.7214	0.0000	0.7158	0.1664	loc(A)
46	4.4108	0.0509	0.0599	1.9163	0.0000	1.0000	0.0000	loc(A)
47	4.4207	0.2509	0.0698	1.9096	0.0000	0.9663	0.0337	loc(A)
48	4.4252	0.0018	0.0435	1.9343	0.0000	0.9557	0.0000	loc(A)
49	4.4327	0.2680	0.1444	1.8316	0.0000	0.8713	0.1287	loc(A)
50	4.4565	0.0122	0.0702	1.1024	0.0000	0.5248	0.4752	deloc
51	4.4873	0.0120	0.7259	1.2506	0.0000	0.2119	0.7881	CTB->A
52	4.5197	0.0211	0.8964	0.9536	0.0000	0.0000	1.0000	CTB->A
53	4.5431	0.0017	0.3960	1.5830	0.0000	0.5842	0.3635	loc(A)
54	4.5481	0.0003	0.1850	1.7930	0.0000	0.7952	0.0836	loc(A)
55	4.5712	0.0053	0.8488	1.1281	0.0000	0.1149	0.8851	CTB->A
56	4.5888	0.0003	0.1099	1.8673	0.0000	0.9408	0.0592	loc(A)
57	4.5947	0.0000	0.9539	1.0207	0.0000	0.0000	1.0000	CTB->A
58	4.6040	0.0004	0.7810	1.1987	0.0000	0.1977	0.8023	CTB->A
59	4.6191	0.0024	0.9525	1.0254	0.0000	0.0000	1.0000	CTB->A
60	4.6816	0.0014	0.6624	1.3139	0.0000	0.2225	0.6403	CTB->A
61	4.7282	0.0101	0.6527	1.3269	0.0000	0.2800	0.7200	CTB->A
62	4.7794	0.0003	0.1342	1.8439	0.0000	0.8908	0.0560	loc(A)
63	4.7835	0.0009	0.0681	1.9128	0.0000	0.9745	0.0255	loc(A)
64	4.7857	0.0000	0.0677	1.9100	0.0000	0.9662	0.0338	loc(A)
65	4.7887	0.0003	0.0891	1.8898	0.0000	0.9586	0.0414	loc(A)
66	4.8091	0.0002	0.0361	1.9408	0.0000	1.0000	0.0000	loc(A)
67	4.8252	0.0001	0.0740	1.9028	0.0000	0.9637	0.0363	loc(A)
68	4.8330	0.0016	0.2923	1.6836	0.0000	0.6961	0.2380	loc(A)
69	4.8357	0.0001	0.0400	1.9382	0.0000	1.0000	0.0000	loc(A)
70	4.8432	0.0058	0.1445	1.8331	0.0000	0.7883	0.0335	loc(A)

S3HT-PCBM ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.5455	0.0024	-0.0002	1.9751	0.0000	1.0000	0.0000	loc(A)
2	2.5711	0.0000	0.0003	1.9756	0.0000	1.0000	0.0000	loc(A)
3	2.6495	0.0000	-0.0046	1.9792	0.0000	1.0000	0.0000	loc(A)
4	2.6707	0.0000	-0.0003	1.9752	0.0000	1.0000	0.0000	loc(A)
5	2.8045	0.0002	0.0003	1.9757	0.0000	1.0000	0.0000	loc(A)
6	2.8406	0.0002	0.0051	1.9698	0.0000	1.0000	0.0000	loc(A)
7	2.9245	0.0000	-0.0024	1.9762	0.0000	1.0000	0.0000	loc(A)
8	2.9393	0.0007	0.0363	1.9390	0.0000	1.0000	0.0000	loc(A)
9	2.9536	0.0000	0.0064	1.9688	0.0000	1.0000	0.0000	loc(A)
10	2.9757	0.0043	0.9811	0.9948	0.0000	0.0000	1.0000	CTB->A
11	3.0930	0.0024	0.0555	1.9165	0.0000	0.9438	0.0562	loc(A)
12	3.1069	0.0187	0.5396	1.4326	0.0000	0.4477	0.5523	CTB->A

13	3.1474	0.0055	0.9806	0.9942	0.0000	0.0000	1.0000	CTB->A
14	3.1560	0.0037	0.0623	1.9110	0.0000	0.9369	0.0631	loc(A)
15	3.1652	0.0142	0.2336	1.7396	0.0000	0.7671	0.2329	loc(A)
16	3.1937	0.0073	0.1108	1.8626	0.0000	0.9109	0.0891	loc(A)
17	3.2719	0.0076	0.0341	1.9382	0.0000	1.0000	0.0000	loc(A)
18	3.2987	0.0004	0.0030	1.9691	0.0000	1.0000	0.0000	loc(A)
19	3.5041	1.4434	0.0068	0.0207	0.0000	0.0000	1.0000	loc(B)
20	3.5105	0.0402	0.1917	1.7856	0.0000	0.6514	0.0304	loc(A)
21	3.5684	0.0002	0.2869	1.6884	0.0000	0.4822	0.0500	loc(A)
22	3.5973	0.0025	0.0908	1.8885	0.0000	0.8128	0.0000	loc(A)
23	3.7930	0.0066	0.0152	1.9637	0.0000	0.9683	0.0000	loc(A)
24	3.8042	0.0069	0.0160	1.9635	0.0000	0.9649	0.0000	loc(A)
25	3.8179	0.0004	0.0921	1.8825	0.0000	0.8969	0.0000	loc(A)
26	3.8661	0.0068	0.0656	1.9140	0.0000	0.8378	0.0000	loc(A)
27	3.8821	0.0001	0.0698	1.9081	0.0000	0.8846	0.0000	loc(A)
28	3.9415	0.0228	0.0774	1.8999	0.0000	0.7714	0.0000	loc(A)
29	3.9716	0.0028	0.9748	1.0015	0.0000	0.0000	1.0000	CTB->A
30	3.9814	0.0010	0.0572	1.9219	0.0000	0.9348	0.0000	loc(A)
31	4.0206	0.0465	0.8661	0.8827	0.0000	0.0000	1.0000	CTB->A
32	4.0619	0.3083	0.1262	0.1417	0.0000	0.0000	1.0000	loc(B)
33	4.1384	0.1054	0.2855	1.6933	0.0000	0.5037	0.0722	loc(A)
34	4.1509	0.0391	0.1611	1.8168	0.0000	0.7863	0.0280	loc(A)
35	4.1809	0.0031	0.9722	1.0003	0.0000	0.0000	1.0000	CTB->A
36	4.2244	0.0025	0.3067	1.6652	0.0000	0.3379	0.0506	loc(A)
37	4.2743	0.0143	0.1539	1.8227	0.0000	0.7176	0.0000	loc(A)
38	4.2762	0.0178	0.0793	1.8968	0.0000	0.8254	0.0000	loc(A)
39	4.3065	0.0017	0.0814	1.8950	0.0000	0.9248	0.0000	loc(A)
40	4.3564	0.0042	0.0589	1.9178	0.0000	0.9617	0.0383	loc(A)
41	4.3588	0.0132	0.0358	1.9344	0.0000	0.9701	0.0000	loc(A)
42	4.4207	0.3946	0.0180	0.0346	0.0000	0.0000	1.0000	loc(B)
43	4.4609	0.3823	0.0601	1.9198	0.0000	0.9253	0.0317	loc(A)
44	4.4696	0.1899	0.0894	1.8879	0.0000	0.9291	0.0709	loc(A)
45	4.4746	0.0316	0.9762	0.9994	0.0000	0.0000	1.0000	CTB->A
46	4.4941	0.0050	0.0141	1.9661	0.0000	1.0000	0.0000	loc(A)
47	4.5156	0.0369	0.1567	1.8208	0.0000	0.8736	0.0711	loc(A)
48	4.5441	0.0028	0.5143	1.4610	0.0000	0.4250	0.4763	CTB->A
49	4.5540	0.0117	0.8228	1.1530	0.0000	0.1464	0.8052	CTB->A
50	4.5667	0.0064	0.9849	0.9992	0.0000	0.0000	1.0000	CTB->A
51	4.5920	0.0004	0.0239	1.9497	0.0000	0.9620	0.0000	loc(A)
52	4.6338	0.0875	0.2279	1.7491	0.0000	0.7352	0.1263	loc(A)
53	4.6581	0.0124	0.8694	1.1062	0.0000	0.1005	0.8995	CTB->A
54	4.6785	0.0002	0.9733	0.9989	0.0000	0.0000	1.0000	CTB->A
55	4.6958	0.0048	0.0626	1.9135	0.0000	0.7911	0.0000	loc(A)
56	4.7108	0.0027	0.2113	1.7628	0.0000	0.6985	0.0420	loc(A)
57	4.7340	0.0025	0.4940	1.4799	0.0000	0.4204	0.3900	deloc
58	4.7388	0.0029	0.3647	1.6091	0.0000	0.6214	0.3126	loc(A)
59	4.7587	0.0294	0.5628	1.4140	0.0000	0.4152	0.5848	CTB->A
60	4.7844	0.0187	0.1309	1.8476	0.0000	0.7762	0.0702	loc(A)
61	4.7939	0.0028	0.2870	1.6904	0.0000	0.6289	0.1950	loc(A)
62	4.8090	0.0204	0.5228	1.4536	0.0000	0.2662	0.3203	CTB->A
63	4.8263	0.0528	0.0882	1.8911	0.0000	0.8905	0.0766	loc(A)
64	4.8292	0.0310	0.3242	1.6544	0.0000	0.6310	0.3006	loc(A)
65	4.8703	0.0239	0.1240	1.8509	0.0000	0.8676	0.1034	loc(A)
66	4.8777	0.0002	0.1364	1.8418	0.0000	0.8061	0.0912	loc(A)
67	4.8839	0.0151	0.0669	1.9048	0.0000	0.9120	0.0000	loc(A)
68	4.9026	0.0029	0.4389	1.5386	0.0000	0.4090	0.3107	loc(A)
69	4.9324	0.0009	0.0518	1.9279	0.0000	0.9005	0.0000	loc(A)
70	4.9436	0.0023	0.0092	0.0375	0.0000	0.0000	1.0000	loc(B)

8T-C_{60} ε =1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6542	0.0002	0.0338	1.9578	0.0000	0.9458	0.0000	loc(A)
2	2.6719	0.0001	0.1902	1.8021	0.0000	0.5158	0.0000	loc(A)

3	2.6800	0.0000	0.0350	1.9587	0.0000	0.9415	0.0000	loc(A)
4	2.7236	0.0001	0.1912	1.8027	0.0000	0.5608	0.0000	loc(A)
5	2.7279	0.0000	0.0263	1.9672	0.0000	0.9560	0.0000	loc(A)
6	2.7352	0.0000	0.0735	1.9213	0.0000	0.8248	0.0000	loc(A)
7	2.7561	0.0000	0.1963	1.7971	0.0000	0.5462	0.0000	loc(A)
8	2.7604	0.0000	0.0052	1.9863	0.0000	1.0000	0.0000	loc(A)
9	2.7727	0.0000	0.0861	1.9068	0.0000	0.7760	0.0000	loc(A)
10	2.7771	0.0000	0.0079	1.9859	0.0000	1.0000	0.0000	loc(A)
11	2.9866	0.0006	0.7869	1.2037	0.0000	0.1507	0.7408	CTB->A
12	3.0292	0.0129	0.6774	1.3140	0.0000	0.1785	0.6190	CTB->A
13	3.0591	0.0788	0.0706	1.8646	0.0000	0.8412	0.0652	loc(A)
14	3.0650	0.0003	0.0935	1.9003	0.0000	0.8769	0.0258	loc(A)
15	3.0825	0.1167	0.0057	1.9093	0.0000	0.9579	0.0421	loc(A)
16	3.0831	0.0002	0.0932	1.9011	0.0000	0.8483	0.0395	loc(A)
17	3.1211	2.1155	0.0744	0.2594	0.0000	0.0763	0.8898	loc(B)
18	3.1246	0.0069	0.6137	1.3772	0.0000	0.1346	0.3515	CTB->A
19	3.2243	0.0360	0.9606	1.0362	0.0000	0.0000	0.9032	CTB->A
20	3.5610	0.0004	0.1713	1.7988	0.0000	0.5815	0.0000	loc(A)
21	3.5802	0.0037	0.0976	1.8487	0.0000	0.7595	0.0000	loc(A)
22	3.5831	0.0002	0.1409	1.7608	0.0000	0.6249	0.0268	loc(A)
23	3.6071	0.0016	0.0717	0.0808	0.0000	0.0000	1.0000	loc(B)
24	3.7483	0.0042	0.4058	1.5710	0.0000	0.5184	0.3224	loc(A)
25	3.7673	0.0000	0.1445	1.7209	0.0000	0.6170	0.0000	loc(A)
26	3.7798	0.0000	0.0538	1.8910	0.0000	0.9368	0.0000	loc(A)
27	3.7841	0.0000	0.1725	1.7870	0.0000	0.5836	0.0000	loc(A)
28	3.7867	0.0006	0.0630	1.9055	0.0000	0.8305	0.0000	loc(A)
29	3.8022	0.0139	0.7410	1.2398	0.0000	0.2576	0.7424	CTB->A
30	3.8423	0.0039	0.2103	1.7689	0.0000	0.6479	0.0836	loc(A)
31	3.8545	0.0001	0.1799	1.7816	0.0000	0.5778	0.0000	loc(A)
32	3.8585	0.0000	0.1090	1.8427	0.0000	0.7742	0.0000	loc(A)
33	3.8625	0.0015	0.1356	1.8177	0.0000	0.6478	0.0000	loc(A)
34	3.9029	0.0004	0.9940	1.0017	0.0000	0.0000	1.0000	CTB->A
35	3.9110	0.0004	0.9921	0.9996	0.0000	0.0000	1.0000	CTB->A
36	3.9953	0.6283	-0.0960	0.1645	0.0000	0.0000	0.7221	loc(B)
37	4.2489	0.0000	0.2305	1.7569	0.0000	0.5412	0.0000	loc(A)
38	4.2584	0.0000	0.3231	1.6585	0.0000	0.4686	0.0000	loc(A)
39	4.2711	0.0001	0.2123	1.7796	0.0000	0.7349	0.0452	loc(A)
40	4.2827	0.0000	0.1506	1.8396	0.0000	0.6167	0.0000	loc(A)
41	4.3675	0.0117	0.6883	1.2987	0.0000	0.0000	0.3441	CTB->A
42	4.4054	0.0000	0.3150	1.6794	0.0000	0.4640	0.0413	loc(A)
43	4.4126	0.0609	0.5149	1.4692	0.0000	0.1047	0.1425	CTB->A
44	4.4221	0.0011	0.3237	1.6683	0.0000	0.2764	0.0000	loc(A)
45	4.4251	0.1012	0.5049	1.4744	0.0000	0.2734	0.2336	CTB->A
46	4.4320	0.0334	0.2352	1.7523	0.0000	0.5268	0.0000	loc(A)
47	4.4396	0.0150	0.2310	1.7614	0.0000	0.6185	0.0421	loc(A)
48	4.4438	0.2039	0.1365	1.8024	0.0000	0.6006	0.0000	loc(A)
49	4.4558	0.2540	0.0160	1.9100	0.0000	0.8684	0.0000	loc(A)
50	4.4796	0.1654	0.2673	1.6213	0.0000	0.4964	0.1068	loc(A)

10T-C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6541	0.0007	0.0287	1.9633	0.0000	1.0000	0.0000	loc(A)
2	2.6713	0.0003	0.0051	1.9881	0.0000	1.0000	0.0000	loc(A)
3	2.6784	0.0000	0.0058	1.9870	0.0000	1.0000	0.0000	loc(A)
4	2.7234	0.0001	0.0156	1.9774	0.0000	1.0000	0.0000	loc(A)
5	2.7266	0.0001	0.0167	1.9764	0.0000	1.0000	0.0000	loc(A)
6	2.7341	0.0001	0.0070	1.9858	0.0000	1.0000	0.0000	loc(A)
7	2.7561	0.0007	0.0191	1.9735	0.0000	1.0000	0.0000	loc(A)
8	2.7617	0.0001	0.0116	1.9800	0.0000	1.0000	0.0000	loc(A)
9	2.7718	0.0000	0.0034	1.9898	0.0000	1.0000	0.0000	loc(A)
10	2.7760	0.0000	0.0060	1.9866	0.0000	1.0000	0.0000	loc(A)
11	2.9984	0.3365	0.6358	1.1642	0.0000	0.2638	0.7362	CTB->A
12	3.0285	0.1559	0.4949	1.4225	0.0000	0.4639	0.5361	deloc

13	3.0611	0.3405	0.0218	1.8047	0.0000	0.9120	0.0880	loc(A)
14	3.0671	0.0186	0.0447	1.9479	0.0000	0.9655	0.0345	loc(A)
15	3.0824	0.6364	0.0146	1.6523	0.0000	0.8264	0.1736	loc(A)
16	3.0872	0.2143	0.0339	1.8774	0.0000	0.9298	0.0702	loc(A)
17	3.0997	1.4091	0.2762	0.8678	0.0000	0.2938	0.7062	deloc
18	3.1410	0.0089	0.4350	1.5546	0.0000	0.5655	0.4345	loc(A)
19	3.2573	0.0045	0.9882	1.0049	0.0000	0.0000	1.0000	CTB->A
20	3.4503	0.0647	0.0894	0.1008	0.0000	0.0000	1.0000	loc(B)
21	3.5616	0.0003	0.0999	1.8378	0.0000	0.7131	0.0338	loc(A)
22	3.5788	0.0067	0.0836	1.8499	0.0000	0.8150	0.0000	loc(A)
23	3.5851	0.0009	0.0307	1.8837	0.0000	0.8386	0.0000	loc(A)
24	3.7397	0.5170	0.1719	0.2563	0.0000	0.0337	0.9663	loc(B)
25	3.7587	0.1429	0.1116	1.3624	0.0000	0.6011	0.2819	deloc
26	3.7683	0.0001	0.1322	1.7978	0.0000	0.6614	0.0310	loc(A)
27	3.7800	0.0017	0.0143	1.9063	0.0000	1.0000	0.0000	loc(A)
28	3.7831	0.0006	0.0471	1.8938	0.0000	0.8454	0.0000	loc(A)
29	3.7859	0.0033	0.0518	1.8836	0.0000	0.7620	0.0000	loc(A)
30	3.8115	0.0162	0.8292	1.0988	0.0000	0.1344	0.8656	CTB->A
31	3.8414	0.0007	0.1594	1.7854	0.0000	0.6547	0.0997	loc(A)
32	3.8536	0.0001	0.0433	1.8875	0.0000	0.8233	0.0000	loc(A)
33	3.8584	0.0002	0.0597	1.8692	0.0000	0.8651	0.0000	loc(A)
34	3.8624	0.0003	0.0590	1.8631	0.0000	0.8410	0.0000	loc(A)
35	3.8979	0.0007	0.9922	0.9997	0.0000	0.0000	1.0000	CTB->A
36	3.9073	0.0007	0.9934	1.0009	0.0000	0.0000	1.0000	CTB->A
37	4.1466	0.0603	0.0244	0.0491	0.0000	0.0000	1.0000	loc(B)
38	4.2472	0.0001	0.3287	1.6642	0.0000	0.3471	0.0433	loc(A)
39	4.2546	0.0001	0.3001	1.6925	0.0000	0.5086	0.0000	loc(A)
40	4.2717	0.0000	0.2499	1.7429	0.0000	0.5201	0.0420	loc(A)
41	4.2786	0.0002	0.9511	1.0392	0.0000	0.0000	0.9618	CTB->A
42	4.2828	0.0001	0.2602	1.7323	0.0000	0.4234	0.1179	loc(A)
43	4.3301	0.0228	0.9734	1.0111	0.0000	0.0000	1.0000	CTB->A
44	4.3858	0.0027	0.9668	1.0267	0.0000	0.0000	0.9662	CTB->A
45	4.4035	0.0007	0.3480	1.6453	0.0000	0.3810	0.0961	loc(A)
46	4.4144	0.0018	0.3609	1.6318	0.0000	0.3414	0.0751	loc(A)
47	4.4283	0.0077	0.4277	1.5633	0.0000	0.1678	0.0754	loc(A)
48	4.4312	0.0397	0.1164	0.6116	0.0000	0.1775	0.7352	deloc
49	4.4354	0.0207	0.3398	1.5554	0.0000	0.3238	0.1228	loc(A)
50	4.4412	0.0759	0.1186	1.8427	0.0000	0.7436	0.0000	loc(A)

12T-C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6651	0.0001	0.1442	1.8485	0.0000	0.8973	0.0000	loc(A)
2	2.6728	0.0000	0.0782	1.9162	0.0000	0.9750	0.0000	loc(A)
3	2.6779	0.0000	0.0373	1.9561	0.0000	1.0000	0.0000	loc(A)
4	2.7284	0.0002	0.1321	1.8620	0.0000	0.9380	0.0000	loc(A)
5	2.7303	0.0000	0.0498	1.9444	0.0000	0.9700	0.0000	loc(A)
6	2.7349	0.0000	0.0392	1.9549	0.0000	1.0000	0.0000	loc(A)
7	2.7638	0.0001	0.1158	1.8768	0.0000	0.9303	0.0000	loc(A)
8	2.7681	0.0001	0.0996	1.8938	0.0000	0.9329	0.0000	loc(A)
9	2.7730	0.0000	0.0100	1.9838	0.0000	1.0000	0.0000	loc(A)
10	2.7786	0.0001	0.0905	1.9034	0.0000	0.9647	0.0000	loc(A)
11	3.0395	0.1431	0.4623	1.5305	0.0000	0.5689	0.3747	loc(A)
12	3.0514	0.7713	0.1678	1.5098	0.0000	0.7136	0.2864	loc(A)
13	3.0714	0.9174	0.1048	1.5430	0.0000	0.7426	0.2329	loc(A)
14	3.0733	1.5681	0.0901	1.3156	0.0000	0.6222	0.3245	deloc
15	3.0800	0.5952	0.0891	1.7369	0.0000	0.8441	0.1215	loc(A)
16	3.0870	0.1095	0.0740	1.9190	0.0000	0.9718	0.0000	loc(A)
17	3.1062	0.0046	0.5927	1.3998	0.0000	0.4252	0.5748	CTB->A
18	3.1508	0.0121	0.8059	1.1728	0.0000	0.2010	0.7990	CTB->A
19	3.2806	0.0542	0.9937	1.0012	0.0000	0.0000	1.0000	CTB->A
20	3.3248	0.0753	0.3234	0.3270	0.0000	0.0000	1.0000	loc(B)
21	3.5701	0.0014	0.1073	1.6130	0.0000	0.6112	0.0000	loc(A)
22	3.5770	0.0946	-0.0157	1.5680	0.0000	0.7461	0.1154	loc(A)

23	3.5832	0.0070	-0.0647	1.7035	0.0000	0.8979	0.0000	loc(A)
24	3.6033	0.4301	0.1457	0.2799	0.0000	0.0629	0.9371	loc(B)
25	3.7592	0.0000	0.0569	1.5983	0.0000	0.6955	0.0000	loc(A)
26	3.7733	0.0000	0.2450	1.5939	0.0000	0.6074	0.2016	loc(A)
27	3.7786	0.0001	0.1423	1.6311	0.0000	0.6054	0.0900	loc(A)
28	3.7876	0.0001	0.0264	1.6919	0.0000	0.7631	0.0674	loc(A)
29	3.7891	0.0002	0.1025	1.6866	0.0000	0.7845	0.1358	loc(A)
30	3.7958	0.0002	0.5463	1.3669	0.0000	0.4133	0.5126	CTB->A
31	3.8459	0.0000	0.1059	1.6144	0.0000	0.7255	0.1079	loc(A)
32	3.8516	0.0001	0.2499	1.5110	0.0000	0.5028	0.2454	loc(A)
33	3.8590	0.0001	0.0120	1.6629	0.0000	0.8462	0.0673	loc(A)
34	3.8612	0.0005	-0.0560	1.8085	0.0000	0.9375	0.0000	loc(A)
35	3.8695	0.0026	0.8507	1.1121	0.0000	0.0877	0.7731	CTB->A
36	3.8842	0.0002	0.9694	1.0248	0.0000	0.0000	0.8728	CTB->A
37	3.9547	0.0886	0.1192	0.2009	0.0000	0.0000	0.8223	loc(B)
38	4.1727	0.0204	0.0768	0.1457	0.0000	0.0000	0.8634	loc(B)
39	4.2037	0.0001	0.9872	1.0044	0.0000	0.0000	1.0000	CTB->A
40	4.2401	0.0049	0.8567	1.1377	0.0000	0.1361	0.8261	CTB->A
41	4.2477	0.0007	0.4225	1.5707	0.0000	0.1333	0.0455	loc(A)
42	4.2580	0.0083	0.7539	1.2401	0.0000	0.1830	0.6808	CTB->A
43	4.2737	0.0001	0.2509	1.7426	0.0000	0.5079	0.0000	loc(A)
44	4.2812	0.0000	0.3721	1.6169	0.0000	0.5285	0.2821	loc(A)
45	4.2984	0.0002	0.8003	1.1943	0.0000	0.1405	0.7744	CTB->A
46	4.4126	0.0027	0.4423	1.5511	0.0000	0.1649	0.0783	loc(A)
47	4.4171	0.0028	0.3491	1.6448	0.0000	0.3207	0.0000	loc(A)
48	4.4230	0.0032	0.3358	1.6575	0.0000	0.2416	0.0000	loc(A)
49	4.4324	0.0700	0.2957	1.6620	0.0000	0.4274	0.0000	loc(A)
50	4.4377	0.0259	0.2888	1.6694	0.0000	0.5606	0.0447	loc(A)
51	4.4466	0.1572	0.1007	1.6782	0.0000	0.7057	0.0498	loc(A)
52	4.4545	0.2436	-0.0988	1.6867	0.0000	0.9578	0.0000	loc(A)
53	4.4581	0.2768	-0.1937	1.7446	0.0000	1.0000	0.0000	loc(A)
54	4.4822	0.1252	0.0015	0.3750	0.0000	0.1547	0.6951	loc(B)
55	4.5515	0.0010	0.3144	1.6462	0.0000	0.4062	0.0000	loc(A)
56	4.5887	0.0001	0.6179	1.2993	0.0000	0.1916	0.4415	CTB->A
57	4.5975	0.0007	0.5764	1.3288	0.0000	0.2390	0.4472	CTB->A
58	4.6033	0.0005	0.2641	1.7295	0.0000	0.4844	0.0397	loc(A)
59	4.6327	0.0001	0.2356	0.2921	0.0000	0.0000	0.8869	loc(B)
60	4.6615	0.0003	0.8413	1.0063	0.0000	0.0299	0.7168	CTB->A

14T-C_{60} ε=1 singlet ωB97X-D 6-31G(d)

St	E(eV)	Osc	ΔP_A	ΣP_A	cR	cA	cB	Class
1	2.6625	0.0002	0.1248	1.8680	0.0000	1.0000	0.0000	loc(A)
2	2.6729	0.0000	0.0888	1.9044	0.0000	0.9319	0.0000	loc(A)
3	2.6788	0.0000	0.0781	1.9160	0.0000	0.9541	0.0000	loc(A)
4	2.7274	0.0002	0.1751	1.8181	0.0000	0.8809	0.0000	loc(A)
5	2.7311	0.0000	0.0515	1.9420	0.0000	1.0000	0.0000	loc(A)
6	2.7353	0.0000	0.0545	1.9391	0.0000	0.9734	0.0000	loc(A)
7	2.7621	0.0003	0.1433	1.8500	0.0000	0.9466	0.0000	loc(A)
8	2.7665	0.0001	0.0772	1.9161	0.0000	1.0000	0.0000	loc(A)
9	2.7743	0.0000	0.0170	1.9769	0.0000	1.0000	0.0000	loc(A)
10	2.7787	0.0000	0.0632	1.9306	0.0000	0.9462	0.0000	loc(A)
11	3.0274	3.2765	0.2165	0.4387	0.0000	0.1176	0.8824	loc(B)
12	3.0392	0.7430	0.2987	1.4181	0.0000	0.6155	0.3572	deloc
13	3.0577	1.0392	0.2333	1.4158	0.0000	0.6464	0.3536	deloc
14	3.0729	0.0005	0.0506	1.9431	0.0000	1.0000	0.0000	loc(A)
15	3.0775	0.0295	0.0677	1.9261	0.0000	0.9735	0.0000	loc(A)
16	3.0865	0.0029	0.0459	1.9475	0.0000	0.9749	0.0000	loc(A)
17	3.1055	0.0331	0.6052	1.3873	0.0000	0.3823	0.5172	CTB->A
18	3.1568	0.0058	0.8692	1.1242	0.0000	0.0857	0.7372	CTB->A
19	3.2341	0.1058	0.0277	0.0318	0.0000	0.0000	1.0000	loc(B)
20	3.2844	0.0471	0.9818	1.0118	0.0000	0.0000	0.9598	CTB->A
21	3.4728	0.4772	0.0155	0.0394	0.0000	0.0000	0.9697	loc(B)
22	3.5696	0.0002	0.2391	1.7186	0.0000	0.6551	0.0000	loc(A)

23	3.5803	0.0006	0.0472	1.9076	0.0000	0.9681	0.0000	loc(A)
24	3.5845	0.0002	0.1650	1.7914	0.0000	0.7158	0.0000	loc(A)
25	3.7579	0.0005	0.2387	1.7290	0.0000	0.6624	0.0372	loc(A)
26	3.7739	0.0193	0.1667	1.2142	0.0000	0.4531	0.3517	deloc
27	3.7760	0.0470	0.0289	0.3662	0.0000	0.1860	0.8140	loc(B)
28	3.7789	0.0000	0.1526	1.8069	0.0000	0.7608	0.0403	loc(A)
29	3.7876	0.0001	0.1014	1.8572	0.0000	0.8427	0.0000	loc(A)
30	3.7905	0.0007	0.0809	1.8785	0.0000	0.9195	0.0000	loc(A)
31	3.8018	0.0007	0.8437	1.1418	0.0000	0.1506	0.8494	CTB->A
32	3.8467	0.0001	0.1524	1.8070	0.0000	0.7810	0.0000	loc(A)
33	3.8547	0.0002	0.2184	1.7523	0.0000	0.7338	0.0992	loc(A)
34	3.8597	0.0002	0.1586	1.8099	0.0000	0.7360	0.0327	loc(A)
35	3.8609	0.0001	0.0512	1.8975	0.0000	0.9613	0.0000	loc(A)
36	3.8777	0.0001	0.9946	0.9991	0.0000	0.0000	1.0000	CTB->A
37	3.8940	0.0002	0.9948	0.9994	0.0000	0.0000	1.0000	CTB->A
38	3.9688	0.0327	-0.0122	0.0583	0.0000	0.0000	0.8894	loc(B)
39	4.1769	0.0002	0.9442	1.0481	0.0000	0.0000	0.8321	CTB->A
40	4.2173	0.0154	0.9495	1.0447	0.0000	0.0000	0.8473	CTB->A
41	4.2374	0.0020	0.8407	1.1530	0.0000	0.0483	0.7067	CTB->A
42	4.2482	0.0048	0.3350	1.6584	0.0000	0.4105	0.0000	loc(A)
43	4.2571	0.0065	0.1111	0.1703	0.0000	0.0000	0.9116	loc(B)
44	4.2675	0.0002	0.5678	1.4255	0.0000	0.2962	0.3864	CTB->A
45	4.2735	0.0001	0.2369	1.7546	0.0000	0.4611	0.0000	loc(A)
46	4.2873	0.0001	0.2014	1.7920	0.0000	0.7251	0.0354	loc(A)
47	4.4110	0.0047	0.4986	1.4948	0.0000	0.1467	0.0644	deloc
48	4.4165	0.0016	0.3456	1.6478	0.0000	0.4779	0.1504	loc(A)
49	4.4225	0.0072	0.3706	1.6229	0.0000	0.4826	0.0618	loc(A)
50	4.4317	0.2802	0.1745	1.2874	0.0000	0.4383	0.2691	deloc
51	4.4359	0.0149	0.3170	1.6724	0.0000	0.4861	0.0000	loc(A)
52	4.4396	0.1695	0.2370	1.3083	0.0000	0.3280	0.2342	deloc
53	4.4504	0.2348	0.0948	1.8534	0.0000	0.8861	0.0000	loc(A)
54	4.4585	0.2834	0.0869	1.8564	0.0000	0.9019	0.0000	loc(A)
55	4.4719	0.0318	0.0145	0.9367	0.0000	0.4637	0.4873	deloc
56	4.5133	0.0005	0.9882	0.9954	0.0000	0.0000	1.0000	CTB->A
57	4.5514	0.0041	0.3317	1.6561	0.0000	0.5580	0.0882	loc(A)
58	4.5731	0.0008	0.9628	1.0284	0.0000	0.0306	0.9694	CTB->A
59	4.5931	0.0007	0.9310	1.0632	0.0000	0.0439	0.9161	CTB->A
60	4.5954	0.0004	0.3022	1.6906	0.0000	0.4542	0.0679	loc(A)

XI. Cartesian coordinates of the ground state species (in Angstrom)

Optimization at the wB97X-D/6-31G(d) level

C_{60}

60

C	0.000000	1.236302	3.327536
C	-1.175793	0.382038	3.327536
C	-0.726680	-1.000189	3.327536
C	0.726680	-1.000189	3.327536
C	1.175793	0.382038	3.327536
C	2.304741	0.748856	2.593901
C	3.031421	-0.251334	1.829825
C	2.600201	-1.578491	1.829825
C	1.424408	-1.960529	2.593901
C	0.697728	-2.960719	1.829825
C	-0.697728	-2.960719	1.829825
C	-1.424408	-1.960529	2.593901
C	-2.600201	-1.578491	1.829825
C	-3.031421	-0.251334	1.829825
C	-2.304741	0.748856	2.593901
C	-2.304741	1.985158	1.829825

C	-3.031421	1.749045	0.593523
C	-3.480533	0.366817	0.593523
C	-3.480533	-0.366817	-0.593523
C	-3.031421	-1.749045	-0.593523
C	-2.600201	-2.342568	0.593523
C	-1.424408	-3.196831	0.593523
C	-0.726680	-3.423537	-0.593523
C	0.726680	-3.423537	-0.593523
C	1.424408	-3.196831	0.593523
C	2.600201	-2.342568	0.593523
C	3.031421	-1.749045	-0.593523
C	3.480533	-0.366817	-0.593523
C	3.480533	0.366817	0.593523
C	3.031421	1.749045	0.593523
C	2.600201	2.342568	-0.593523
C	2.600201	1.578491	-1.829825
C	3.031421	0.251334	-1.829825
C	2.304741	-0.748856	-2.593901
C	2.304741	-1.985158	-1.829825
C	1.175793	-2.805386	-1.829825
C	0.000000	-2.423348	-2.593901
C	-1.175793	-2.805386	-1.829825
C	-2.304741	-1.985158	-1.829825
C	-2.304741	-0.748856	-2.593901
C	-3.031421	0.251334	-1.829825
C	-2.600201	1.578491	-1.829825
C	-2.600201	2.342568	-0.593523
C	-1.424408	3.196831	-0.593523
C	-0.697728	2.960719	-1.829825
C	-1.424408	1.960529	-2.593901
C	-0.726680	1.000189	-3.327536
C	-1.175793	-0.382038	-3.327536
C	0.000000	-1.236302	-3.327536
C	1.175793	-0.382038	-3.327536
C	0.726680	1.000189	-3.327536
C	1.424408	1.960529	-2.593901
C	0.697728	2.960719	-1.829825
C	1.424408	3.196831	-0.593523
C	0.726680	3.423537	0.593523
C	-0.726680	3.423537	0.593523
C	-1.175793	2.805386	1.829825
C	0.000000	2.423348	2.593901
C	1.175793	2.805386	1.829825
C	2.304741	1.985158	1.829825

6T

44

C	0.176074	0.704581	-0.600140
C	-0.176074	-0.704581	-0.600140
S	-1.021705	1.916487	-0.251395
S	1.021705	-1.916487	-0.251395
C	0.125014	3.204569	-0.476614
C	-0.125014	-3.204569	-0.476614
C	1.366522	2.701002	-0.768849
C	-1.366522	-2.701002	-0.768849
C	1.395560	1.284581	-0.838732
C	-1.395560	-1.284581	-0.838732
C	-0.284595	4.591286	-0.337367
C	0.284595	-4.591286	-0.337367
S	0.864099	5.812842	0.125073
S	-0.864099	-5.812842	0.125073
C	-0.336635	7.067036	0.031289

C	0.336635	-7.067036	0.031289
C	-1.557760	6.543388	-0.305273
C	1.557760	-6.543388	-0.305273
C	-1.528465	5.140368	-0.514137
C	1.528465	-5.140368	-0.514137
H	2.282127	0.713173	-1.090212
H	-2.282127	-0.713173	-1.090212
H	2.228142	3.330475	-0.961308
H	-2.228142	-3.330475	-0.961308
H	-2.392353	4.559514	-0.817698
H	2.392353	-4.559514	-0.817698
H	-2.446203	7.152020	-0.430680
H	2.446203	-7.152020	-0.430680
C	0.017069	8.451161	0.306431
C	1.225344	9.075614	0.134054
S	-1.157985	9.558520	0.951797
C	1.204360	10.448364	0.510734
H	2.095968	8.573342	-0.272775
C	-0.017069	10.850765	0.962268
H	2.061231	11.107627	0.439158
H	-0.312913	11.833068	1.303925
C	-0.017069	-8.451161	0.306431
C	-1.225344	-9.075614	0.134054
S	1.157985	-9.558520	0.951797
C	-1.204360	-10.448364	0.510734
H	-2.095968	-8.573342	-0.272775
C	0.017069	-10.850765	0.962268
H	-2.061231	-11.107627	0.439158
H	0.312913	-11.833068	1.303925

2T-C_{60}

76

C	0.589558	-0.364435	-4.715315
C	0.589655	-1.742797	-4.267001
C	-0.589601	-2.331858	-3.838881
C	-0.589781	-3.184159	-2.666256
C	0.588669	-3.408834	-1.972360
C	1.822365	-2.793042	-2.420494
C	1.822522	-1.978374	-3.541957
C	0.588935	-0.363356	2.209062
C	0.588900	-1.742007	1.768442
C	1.822717	-1.978592	1.045321
C	2.584492	-2.411839	-1.248125
C	1.822717	-2.794069	-0.075253
C	0.588935	-3.409764	-0.522837
C	-0.590041	-3.184091	0.170849
C	-0.590710	-2.332709	1.344028
C	-1.822704	-2.948714	-0.554774
C	-1.822557	-2.948592	-1.941016
C	-0.589558	0.364435	-4.715315
C	-1.822436	-0.251931	-4.267043
C	-1.823019	-1.569855	-3.838739
C	-2.585016	-1.951578	-2.665872
C	-3.313758	-0.997645	-1.972726
C	-3.313070	0.381143	-2.420685
C	-2.585067	0.745715	-3.542322
C	-0.588935	0.363356	2.209062
C	-1.822524	-0.252215	1.768387
C	-2.586005	0.745362	1.046170
C	-3.313290	1.233039	-1.248124
C	-3.314492	0.380932	-0.075131
C	-3.315092	-0.997884	-0.522752

C	-2.585105	-1.951548	0.170214
C	-1.824574	-1.570866	1.343665
C	1.822436	0.251931	-4.267043
C	1.823019	1.569855	-3.838739
C	2.585016	1.951578	-2.665872
C	3.313758	0.997645	-1.972726
C	3.313070	-0.381143	-2.420685
C	2.585067	-0.745715	-3.542322
C	1.822524	0.252215	1.768387
C	2.586005	-0.745362	1.046170
C	3.313290	-1.233039	-1.248124
C	3.314492	-0.380932	-0.075131
C	3.315092	0.997884	-0.522752
C	2.585105	1.951548	0.170214
C	1.824574	1.570866	1.343665
C	1.822704	2.948714	-0.554774
C	1.822557	2.948592	-1.941016
C	-0.589655	1.742797	-4.267001
C	0.589601	2.331858	-3.838881
C	0.589781	3.184159	-2.666256
C	-0.588669	3.408834	-1.972360
C	-1.822365	2.793042	-2.420494
C	-1.822522	1.978374	-3.541957
C	-0.588900	1.742007	1.768442
C	-1.822717	1.978592	1.045321
C	-2.584492	2.411839	-1.248125
C	-1.822717	2.794069	-0.075253
C	-0.588935	3.409764	-0.522837
C	0.590041	3.184091	0.170849
C	0.590710	2.332709	1.344028
C	0.726105	-0.029121	5.319020
C	-0.726105	0.029121	5.319020
S	1.676909	1.426828	5.295674
S	-1.676909	-1.426828	5.295674
C	3.143415	0.535417	5.137525
C	-3.143415	-0.535417	5.137525
C	2.917041	-0.807834	5.112218
C	-2.917041	0.807834	5.112218
C	1.535106	-1.131904	5.214456
C	-1.535106	1.131904	5.214456
H	4.088501	1.057237	5.080998
H	-4.088501	-1.057237	5.080998
H	1.154303	-2.146880	5.183677
H	-1.154303	2.146880	5.183677
H	3.705031	-1.544757	5.014369
H	-3.705031	1.544757	5.014369

4T-C_{60}

90

C	-0.589384	0.364333	-5.402432
C	-0.589233	1.743054	-4.954742
C	0.589872	2.332284	-4.526365
C	0.589626	3.184353	-3.353720
C	-0.589484	3.409108	-2.660512
C	-1.823070	2.792858	-3.108933
C	-1.822584	1.978425	-4.230409
C	-0.588766	0.364005	1.518630
C	-0.588766	1.742748	1.079693
C	-1.823349	1.979195	0.357572
C	-2.585946	2.412527	-1.936435
C	-1.823606	2.794061	-0.763223
C	-0.589625	3.409917	-1.211394

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C     0.590077     3.184593    -0.518667
C     0.591189     2.332880     0.654127
C     1.823375     2.949129    -1.243465
C     1.823020     2.949055    -2.629495
C     0.589384    -0.364333    -5.402432
C     1.822641     0.252193    -4.955130
C     1.822980     1.570225    -4.526384
C     2.585429     1.951161    -3.353756
C     3.314281     0.997135    -2.660885
C     3.313715    -0.381667    -3.109178
C     2.584889    -0.745726    -4.230781
C     0.588766    -0.364005     1.518630
C     1.822599     0.251425     1.078579
C     2.586616    -0.745904     0.357862
C     3.314608    -1.233601    -1.936401
C     3.315666    -0.381502    -0.763061
C     3.316064     0.997329    -1.211123
C     2.586366     1.951483    -0.518960
C     1.824380     1.570547     0.653459
C    -1.822641    -0.252193    -4.955130
C    -1.822980    -1.570225    -4.526384
C    -2.585429    -1.951161    -3.353756
C    -3.314281    -0.997135    -2.660885
C    -3.313715     0.381667    -3.109178
C    -2.584889     0.745726    -4.230781
C    -1.822599    -0.251425     1.078579
C    -2.586616     0.745904     0.357862
C    -3.314608     1.233601    -1.936401
C    -3.315666     0.381502    -0.763061
C    -3.316064    -0.997329    -1.211123
C    -2.586366    -1.951483    -0.518960
C    -1.824380    -1.570547     0.653459
C    -1.823375    -2.949129    -1.243465
C    -1.823020    -2.949055    -2.629495
C     0.589233    -1.743054    -4.954742
C    -0.589872    -2.332284    -4.526365
C    -0.589626    -3.184353    -3.353720
C     0.589484    -3.409108    -2.660512
C     1.823070    -2.792858    -3.108933
C     1.822584    -1.978425    -4.230409
C     0.588766    -1.742748     1.079693
C     1.823349    -1.979195     0.357572
C     2.585946    -2.412527    -1.936435
C     1.823606    -2.794061    -0.763223
C     0.589625    -3.409917    -1.211394
C    -0.590077    -3.184593    -0.518667
C    -0.591189    -2.332880     0.654127
C    -0.725529    -0.008157     4.645037
C     0.725529     0.008157     4.645037
S    -1.587264    -1.497134     4.389942
S     1.587264     1.497134     4.389942
C    -3.103327    -0.665155     4.220309
C     3.103327     0.665155     4.220309
C    -2.939494     0.683733     4.399334
C     2.939494    -0.683733     4.399334
C    -1.591962     1.055466     4.640347
C     1.591962    -1.055466     4.640347
C    -4.313787    -1.400813     3.890867
C     4.313787     1.400813     3.890867
S    -5.866609    -0.889123     4.479705
S     5.866609     0.889123     4.479705
C    -6.664585    -2.165726     3.641395
C     6.664585     2.165726     3.641395
C    -5.784070    -2.951104     2.958259
C     5.784070     2.951104     2.958259
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C    -4.437133    -2.513160     3.098713
C     4.437133     2.513160     3.098713
H    -1.268633     2.083699     4.761246
H     1.268633    -2.083699     4.761246
H    -3.755577     1.392674     4.319093
H     3.755577    -1.392674     4.319093
H    -3.591282    -2.979752     2.606362
H     3.591282     2.979752     2.606362
H    -6.081739    -3.806434     2.363587
H     6.081739     3.806434     2.363587
H    -7.739446    -2.266018     3.702944
H     7.739446     2.266018     3.702944
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6T-C_{60}

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 104

C    -0.589238     0.364462     5.843945
C    -1.823112    -0.250899     5.396209
C    -1.823498    -1.569212     4.967770
C    -2.585600    -1.949870     3.795378
C    -3.313399    -0.995114     3.102251
C    -3.313562     0.384211     3.551076
C    -2.584311     0.748098     4.672293
C    -0.588643     0.363791    -1.076004
C    -1.822774    -0.251668    -0.637278
C    -2.585681     0.748160     0.084355
C    -3.314491     1.236857     2.378496
C    -3.314802     0.383980     1.205171
C    -3.313972    -0.995465     1.653791
C    -2.585262    -1.950515     0.961213
C    -1.823171    -1.570590    -0.210945
C    -1.823450    -2.949270     1.685511
C    -1.823686    -2.948751     3.071494
C     0.589238    -0.364462     5.843945
C     0.588280    -1.743372     5.397134
C    -0.590853    -2.332227     4.967813
C    -0.589928    -3.185144     3.795525
C     0.589524    -3.412108     3.103260
C     1.822488    -2.795651     3.551736
C     1.821911    -1.980530     4.673460
C     0.588643    -0.363791    -1.076004
C     0.589524    -1.742887    -0.635591
C     1.823560    -1.982039     0.083292
C     2.585422    -2.415676     2.378544
C     1.823443    -2.797410     1.204781
C     0.590458    -3.413920     1.652992
C    -0.589524    -3.186147     0.961509
C    -0.590026    -2.333542    -0.210014
C    -0.588280     1.743372     5.397134
C     0.590853     2.332227     4.967813
C     0.589928     3.185144     3.795525
C    -0.589524     3.412108     3.103260
C    -1.822488     2.795651     3.551736
C    -1.821911     1.980530     4.673460
C    -0.589524     1.742887    -0.635591
C    -1.823560     1.982039     0.083292
C    -2.585422     2.415676     2.378544
C    -1.823443     2.797410     1.204781
C    -0.590458     3.413920     1.652992
C     0.589524     3.186147     0.961509
C     0.590026     2.333542    -0.210014
C     1.823450     2.949270     1.685511
C     1.823686     2.948751     3.071494
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C	1.823112	0.250899	5.396209
C	1.823498	1.569212	4.967770
C	2.585600	1.949870	3.795378
C	3.313399	0.995114	3.102251
C	3.313562	-0.384211	3.551076
C	2.584311	-0.748098	4.672293
C	1.822774	0.251668	-0.637278
C	2.585681	-0.748160	0.084355
C	3.314491	-1.236857	2.378496
C	3.314802	-0.383980	1.205171
C	3.313972	0.995465	1.653791
C	2.585262	1.950515	0.961213
C	1.823171	1.570590	-0.210945
C	-0.374170	0.621879	-4.220051
C	0.374170	-0.621879	-4.220051
S	0.441638	2.137434	-3.965331
S	-0.441638	-2.137434	-3.965331
C	-1.061646	2.982293	-3.746302
C	1.061646	-2.982293	-3.746302
C	-2.125085	2.134462	-3.920732
C	2.125085	-2.134462	-3.920732
C	-1.735134	0.797789	-4.189498
C	1.735134	-0.797789	-4.189498
C	-1.071378	4.385919	-3.374620
C	1.071378	-4.385919	-3.374620
S	-2.350754	5.440478	-3.892718
S	2.350754	-5.440478	-3.892718
C	-1.695550	6.777743	-2.995623
C	1.695550	-6.777743	-2.995623
C	-0.532181	6.415815	-2.366788
C	0.532181	-6.415815	-2.366788
C	-0.178068	5.058449	-2.580660
C	0.178068	-5.058449	-2.580660
H	-2.442118	-0.017570	-4.300313
H	2.442118	0.017570	-4.300313
H	-3.155734	2.448988	-3.803484
H	3.155734	-2.448988	-3.803484
H	0.680418	4.577160	-2.125697
H	-0.680418	-4.577160	-2.125697
H	0.035944	7.092767	-1.738881
H	-0.035944	-7.092767	-1.738881
C	-2.369790	8.066967	-2.992552
C	-3.704754	8.334999	-3.151130
S	-1.472342	9.540093	-2.770155
C	-4.008718	9.723617	-3.083535
H	-4.450460	7.559521	-3.287033
C	-2.904308	10.493966	-2.871525
H	-5.009352	10.127510	-3.181381
H	-2.849367	11.568888	-2.768859
C	2.369790	-8.066967	-2.992552
C	3.704754	-8.334999	-3.151130
S	1.472342	-9.540093	-2.770155
C	4.008718	-9.723617	-3.083535
H	4.450460	-7.559521	-3.287033
C	2.904308	-10.493966	-2.871525
H	5.009352	-10.127510	-3.181381
H	2.849367	-11.568888	-2.768859

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C	0.589631	0.364057	6.155918
C	0.590015	1.742736	5.708083

C	-0.588793	2.332495	5.279661
C	-0.588416	3.184579	4.106840
C	0.590733	3.408853	3.413659
C	1.823985	2.792298	3.861900
C	1.823284	1.977850	4.983472
C	0.588793	0.363886	-0.765457
C	0.589631	1.742836	-0.327116
C	1.824191	1.978997	0.395198
C	2.586775	2.411466	2.689473
C	1.824701	2.793458	1.516308
C	0.590891	3.409658	1.964255
C	-0.588833	3.185214	1.271415
C	-0.590054	2.333378	0.098411
C	-1.822106	2.950204	1.996432
C	-1.821865	2.949760	3.382561
C	-0.589631	-0.364057	6.155918
C	-1.822671	0.252627	5.707947
C	-1.822118	1.570668	5.279650
C	-2.584430	1.952186	4.107066
C	-3.313744	0.998578	3.413951
C	-3.314314	-0.380282	3.862217
C	-2.585306	-0.744876	4.983385
C	-0.588793	-0.363886	-0.765457
C	-1.822561	0.251568	-0.324591
C	-2.587299	-0.745389	0.395194
C	-3.315882	-1.232481	2.689626
C	-3.314754	-0.380033	1.516611
C	-3.314463	0.998737	1.964381
C	-2.584990	1.952749	1.271852
C	-1.823277	1.570915	0.099696
C	1.822671	-0.252627	5.707947
C	1.822118	-1.570668	5.279650
C	2.584430	-1.952186	4.107066
C	3.313744	-0.998578	3.413951
C	3.314314	0.380282	3.862217
C	2.585306	0.744876	4.983385
C	1.822561	-0.251568	-0.324591
C	2.587299	0.745389	0.395194
C	3.315882	1.232481	2.689626
C	3.314754	0.380033	1.516611
C	3.314463	-0.998737	1.964381
C	2.584990	-1.952749	1.271852
C	1.823277	-1.570915	0.099696
C	1.822106	-2.950204	1.996432
C	1.821865	-2.949760	3.382561
C	-0.590015	-1.742736	5.708083
C	0.588793	-2.332495	5.279661
C	0.588416	-3.184579	4.106840
C	-0.590733	-3.408853	3.413659
C	-1.823985	-2.792298	3.861900
C	-1.823284	-1.977850	4.983472
C	-0.589631	-1.742836	-0.327116
C	-1.824191	-1.978997	0.395198
C	-2.586775	-2.411466	2.689473
C	-1.824701	-2.793458	1.516308
C	-0.590891	-3.409658	1.964255
C	0.588833	-3.185214	1.271415
C	0.590054	-2.333378	0.098411
C	0.723904	0.046560	-3.927715
C	-0.723904	-0.046560	-3.927715
S	1.693805	-1.372107	-3.657211
S	-1.693805	1.372107	-3.657211
C	3.137306	-0.424370	-3.462310
C	-3.137306	0.424370	-3.462310
C	2.873078	0.907703	-3.652359

C	-2.873078	-0.907703	-3.652359
C	1.505893	1.173761	-3.916634
C	-1.505893	-1.173761	-3.916634
C	4.390906	-1.053030	-3.086945
C	-4.390906	1.053030	-3.086945
S	5.913872	-0.371354	-3.573793
S	-5.913872	0.371354	-3.573793
C	6.805019	-1.570056	-2.683643
C	-6.805019	1.570056	-2.683643
C	5.952095	-2.460794	-2.083268
C	-5.952095	2.460794	-2.083268
C	4.583548	-2.166958	-2.310312
C	-4.583548	2.166958	-2.310312
H	1.105985	2.173461	-4.045784
H	-1.105985	-2.173461	-4.045784
H	3.629334	1.678044	-3.554106
H	-3.629334	-1.678044	-3.554106
H	3.765567	-2.730137	-1.876009
H	-3.765567	2.730137	-1.876009
H	6.296369	-3.281606	-1.464155
H	-6.296369	3.281606	-1.464155
C	8.256968	-1.540152	-2.654276
C	9.094772	-0.466512	-2.812387
S	9.170306	-2.997613	-2.397462
C	10.467967	-0.805052	-2.701529
H	8.735054	0.544121	-2.970445
C	10.680220	-2.137498	-2.459065
H	11.273034	-0.081887	-2.767876
C	11.939678	-2.840731	-2.271884
C	-8.256968	1.540152	-2.654276
C	-9.094772	0.466512	-2.812387
S	-9.170306	2.997613	-2.397462
C	-10.467967	0.805052	-2.701529
H	-8.735054	-0.544121	-2.970445
C	-10.680220	2.137498	-2.459065
H	-11.273034	0.081887	-2.767876
C	-11.939678	2.840731	-2.271884
S	-13.408950	2.241559	-2.984176
C	-14.327182	3.538981	-2.316769
C	-13.544622	4.394623	-1.600556
C	-12.178506	3.995827	-1.572917
H	-11.402932	4.531758	-1.036997
H	-13.926616	5.276684	-1.100680
H	-15.392166	3.597151	-2.494234
S	13.408950	-2.241559	-2.984176
C	14.327182	-3.538981	-2.316769
C	13.544622	-4.394623	-1.600556
C	12.178506	-3.995827	-1.572917
H	11.402932	-4.531758	-1.036997
H	13.926616	-5.276684	-1.100680
H	15.392166	-3.597151	-2.494234

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C	-1.142748	6.098098	0.423161
C	-0.769734	5.728097	1.774175
C	0.554624	5.452799	2.076457
C	0.884454	4.333817	2.937143
C	-0.124817	3.539075	3.457418
C	-1.510400	3.826973	3.141475
C	-1.825284	4.896884	2.318521
C	-0.376255	-0.775722	0.621835

C	-0.101941	-0.266249	1.948071
C	-1.318823	0.339751	2.452524
C	-2.207141	2.565236	2.989129
C	-1.251434	1.497409	3.210971
C	0.035489	2.099322	3.500260
C	1.198429	1.517041	3.019668
C	1.129241	0.305578	2.226518
C	2.253964	2.348281	2.475331
C	2.100267	3.725248	2.434782
C	-0.174896	6.177064	-0.565759
C	1.210313	5.889561	-0.249519
C	1.566657	5.535478	1.042152
C	2.522167	4.467819	1.263431
C	3.078702	3.800555	0.183627
C	2.705636	4.170697	-1.167447
C	1.792172	5.191528	-1.378897
C	0.591121	-0.703147	-0.365853
C	1.878971	-0.107247	-0.076102
C	2.301868	0.632834	-1.247299
C	2.635974	2.959313	-1.960410
C	2.966297	1.840242	-1.099712
C	3.240430	2.360317	0.225264
C	2.836879	1.650513	1.345770
C	2.142235	0.387679	1.192016
C	-2.429108	5.495804	0.132891
C	-2.690896	4.998325	-1.133813
C	-3.387140	3.736092	-1.287830
C	-3.790697	3.026059	-0.167636
C	-3.516383	3.546387	1.157575
C	-2.850813	4.753278	1.304276
C	-1.759919	-0.492964	0.307724
C	-2.344827	0.197117	1.437635
C	-3.187968	2.427849	2.018919
C	-3.259651	1.215993	1.226070
C	-3.632665	1.585837	-0.125546
C	-3.074713	0.920186	-1.205874
C	-2.118018	-0.144936	-0.984057
C	-2.652337	1.662164	-2.377358
C	-2.804967	3.039152	-2.417478
C	-0.448843	5.657005	-1.890827
C	-1.678553	5.081106	-2.168026
C	-1.748750	3.869926	-2.961354
C	-0.586356	3.287204	-3.441348
C	0.699839	3.889337	-3.151071
C	0.766915	5.047846	-2.393172
C	0.218616	-0.340527	-1.716517
C	1.275006	0.489327	-2.261765
C	1.655273	2.821864	-2.930226
C	0.959335	1.559203	-3.084237
C	-0.426270	1.847131	-3.400118
C	-1.436044	1.052932	-2.879563
C	-1.106625	-0.065853	-2.018740
C	-0.444092	-3.904094	0.521673
C	0.959925	-3.878250	0.156533
S	-1.668914	-3.804371	-0.709535
S	2.164826	-3.424205	1.326213
C	-2.920120	-3.541621	0.467393
C	3.401419	-3.331729	0.109095
C	-2.408280	-3.591038	1.738866
C	2.900853	-3.676113	-1.119652
C	-1.006059	-3.798824	1.768778
C	1.517420	-3.984482	-1.092510
C	-4.270506	-3.223497	0.043382
C	4.749405	-2.912392	0.452836
S	-5.631202	-3.492838	1.091100

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S     6.124947    -3.582625    -0.371339
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C     7.229322    -2.601591     0.545346
C    -6.064346    -2.382680    -1.183021
C     6.549895    -1.807071     1.433361
C    -4.671146    -2.638398    -1.131169
C     5.142829    -1.981079     1.378785
H    -0.424824    -3.815128     2.684172
H     0.944783    -4.237579    -1.978059
H    -3.010074    -3.426657     2.625433
H     3.499701    -3.668440    -2.023311
H    -3.977992    -2.357585    -1.916107
H     4.439792    -1.420603     1.985001
H    -6.554561    -1.893513    -2.017231
H     7.046633    -1.124923     2.114143
C    -8.141935    -2.639626     0.263773
C    -8.746534    -2.567305     1.492505
S    -9.324015    -2.540696    -1.008026
C   -10.157054    -2.436894     1.417343
H    -8.194288    -2.593162     2.425297
C   -10.631010    -2.404537     0.131085
H   -10.804085    -2.381477     2.285604
C   -12.001699    -2.270183    -0.332278
C     8.660867    -2.697059     0.314782
C     9.379198    -3.766450    -0.154788
S     9.706890    -1.342336     0.622544
C    10.771210    -3.511326    -0.244554
H     8.925067    -4.721017    -0.396062
C    11.117318    -2.246204     0.156342
H    11.498933    -4.248976    -0.563402
C    12.438295    -1.644635     0.213847
S   -13.186648    -1.437739     0.630876
C   -14.438644    -1.737101    -0.537339
C   -13.939143    -2.414302    -1.619394
C   -12.557713    -2.716266    -1.503435
H   -11.999068    -3.274523    -2.246463
H   -14.552862    -2.714952    -2.461139
C   -15.796836    -1.271034    -0.302989
S    13.713316    -2.218033    -0.820363
C    14.855538    -1.098304    -0.139973
C    14.254270    -0.309089     0.805789
C    12.883788    -0.618208     1.006416
H    12.255697    -0.120897     1.737125
H    14.788318     0.450153     1.366077
C    16.237633    -1.088739    -0.593974
S   -16.840320    -0.873877    -1.636129
C   -18.132336    -0.459233    -0.573378
C   -17.775484    -0.601723     0.734347
C   -16.439306    -1.067652     0.890883
H   -15.975719    -1.265365     1.850955
H   -18.442704    -0.390768     1.561544
H   -19.080570    -0.130444    -0.975620
S    17.191153     0.363843    -0.525388
C    18.567719    -0.442928    -1.178392
C    18.303598    -1.752158    -1.449907
C    16.970975    -2.123373    -1.115193
H    16.573445    -3.125234    -1.234031
H    19.034427    -2.436081    -1.864687
H    19.493688     0.095581    -1.325509
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C	-0.934033	6.205500	0.784097
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C	-0.843483	3.244043	3.614451
C	-2.079413	3.634005	2.964417
C	-2.137590	4.811765	2.236052
C	-0.323685	-0.666411	0.274852
C	-0.431942	-0.338052	1.679725
C	-1.735949	0.255507	1.899956
C	-2.717068	2.435272	2.457469
C	-1.874309	1.304100	2.794193
C	-0.716093	1.804450	3.509325
C	0.529464	1.232435	3.300466
C	0.674792	0.134534	2.365174
C	1.704183	2.073858	3.187992
C	1.581952	3.450847	3.289242
C	0.274933	6.361157	0.124484
C	1.510974	5.971418	0.774016
C	1.483506	5.442895	2.054904
C	2.325988	4.312124	2.390966
C	3.158930	3.759057	1.430978
C	3.187808	4.311615	0.091215
C	2.382043	5.392902	-0.229761
C	0.883667	-0.521609	-0.385231
C	2.041470	-0.024518	0.329469
C	2.786360	0.834413	-0.567348
C	3.332894	3.213260	-0.843736
C	3.394868	1.981242	-0.081280
C	3.287530	2.318953	1.324112
C	2.575362	1.495534	2.182744
C	1.938654	0.297618	1.674183
C	-2.091207	5.705241	0.068787
C	-1.989049	5.382665	-1.275182
C	-2.625948	4.183653	-1.783410
C	-3.337457	3.359741	-0.925209
C	-3.444772	3.697356	0.480777
C	-2.835447	4.843905	0.966187
C	-1.559598	-0.282166	-0.372980
C	-2.434697	0.288158	0.629989
C	-3.385291	2.466076	1.243437
C	-3.241906	1.367121	0.308045
C	-3.212127	1.919622	-1.032144
C	-2.378359	1.367463	-1.992835
C	-1.535041	0.237712	-1.656596
C	-1.633405	2.228758	-2.890327
C	-1.754885	3.605739	-2.787914
C	0.382068	6.023692	-1.281063
C	-0.724511	5.545431	-1.964805
C	-0.579789	4.447121	-2.899807
C	0.665102	3.874548	-3.108497
C	1.822393	4.374856	-2.393153
C	1.684228	5.425274	-1.499663
C	0.912162	0.026337	-1.726052
C	2.087679	0.866775	-1.838171
C	2.665055	3.244191	-2.057636
C	2.028633	2.044677	-2.566137
C	0.792910	2.434743	-3.215692
C	-0.331082	1.630173	-3.108622
C	-0.269939	0.398837	-2.346933
C	-0.671999	-3.790871	0.748769
C	0.735234	-3.852892	0.397293
S	-1.886669	-3.672547	-0.490375
S	1.944771	-3.387824	1.557322
C	-3.122499	-3.293330	0.670911

C	3.201272	-3.428620	0.358668
C	-2.619225	-3.325781	1.945441
C	2.701530	-3.824572	-0.855049
C	-1.230699	-3.609689	1.988784
C	1.304076	-4.064662	-0.832715
C	-4.458649	-2.929260	0.233009
C	4.559184	-3.038124	0.698462
S	-5.856550	-3.350670	1.172945
S	5.922494	-3.787884	-0.075607
C	-6.917752	-2.505303	0.085186
C	7.045961	-2.793748	0.803560
C	-6.210857	-1.964155	-0.958929
C	6.381521	-1.937315	1.643764
C	-4.815386	-2.202936	-0.874328
C	4.970888	-2.073972	1.582445
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H	0.732342	-4.346464	-1.710134
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H	3.312049	-3.899750	-1.747731
H	-4.089541	-1.814347	-1.580402
H	4.279495	-1.465671	2.154915
H	-6.674428	-1.380968	-1.746727
H	6.891820	-1.237248	2.295701
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C	-9.008362	-2.575683	1.535572
S	-9.474054	-2.221059	-0.963287
C	-10.417962	-2.487660	1.408166
H	-8.498414	-2.713671	2.482423
C	-10.835792	-2.292508	0.116525
H	-11.103877	-2.577201	2.243148
C	-12.190414	-2.155374	-0.388864
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S	9.542690	-1.575131	0.786128
C	10.576336	-3.828048	0.119956
H	8.711598	-5.017796	0.063177
C	10.940830	-2.537511	0.408982
H	11.293411	-4.601914	-0.130022
C	12.270067	-1.952519	0.415515
S	-13.485228	-1.668040	0.665261
C	-14.657874	-1.793597	-0.612625
C	-14.054450	-2.156734	-1.788979
C	-12.656960	-2.362547	-1.661823
H	-12.021038	-2.686039	-2.478457
H	-14.602187	-2.305727	-2.712705
C	-16.061687	-1.519558	-0.355762
S	13.555778	-2.676037	-0.505810
C	14.701309	-1.487536	0.040618
C	14.093888	-0.570308	0.859034
C	12.716282	-0.834182	1.072055
H	12.082524	-0.233689	1.715088
H	14.627049	0.252387	1.322093
C	16.088790	-1.552279	-0.385087
S	-17.093142	-0.914320	-1.618297
C	-18.469198	-0.864658	-0.556939
C	-18.127799	-1.295065	0.698804
C	-16.763690	-1.668989	0.812470
H	-16.317034	-2.050212	1.723942
H	-18.833909	-1.330276	1.520767
C	-19.763475	-0.410220	-1.042991
S	17.056214	-0.110773	-0.485237
C	18.456264	-1.009968	-0.989427
C	18.160442	-2.343829	-1.101255
C	16.818266	-2.651258	-0.759566
H	16.411950	-3.656559	-0.757284

H	18.893715	-3.087991	-1.390795
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C	-22.198335	-0.040487	-1.393070
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C	2.534440	4.445629	2.415577
C	3.321867	3.842452	1.447374
C	3.319186	4.351691	0.090134
C	2.528783	5.441790	-0.239130
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C	2.029141	0.421035	1.841876
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C	-3.167758	1.573901	0.610407
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H	-16.326914	-1.434383	1.838572
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C	-19.846957	-0.663413	-1.195941
S	17.105863	-0.446837	-0.049615
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C	18.148950	-2.710885	-0.661499
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H	16.357117	-3.970371	-0.346938
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C	-21.566264	0.000997	-2.621815
C	-20.168016	-0.118984	-2.412650
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H	-22.006885	0.436917	-3.511327
C	-23.760709	-0.479074	-1.418129
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H	19.710644	1.025679	0.453583
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C	23.388876	-0.248197	-2.205944
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C     0.589907    -2.333795    -1.313599
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S     0.643165    -2.090991     3.043806
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C    -0.707918    -3.119333     2.653307
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C    -4.969191    -2.652807     0.173471
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C    -6.417162    -2.168474    -1.876771
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S3HT-PCBM

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