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Supporting Information

Reducing the Excessive Exoergicity Through Helically Locked Tether-Driven Approach for the High-Efficiency Singlet Fission Chromophores

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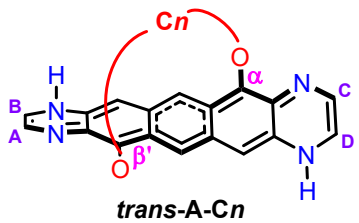
1. Tables

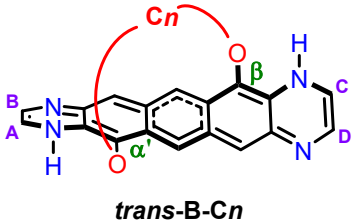
Table S1. The optimized range-separating parameter μ values (in $Bohr^{-1}$) of ***trans*-A-C*n***, ***trans*-B-C*n***, and ***cis*-C*n*** using LRC-BLYP/6-311+G* method.

	trans*-A-C*n						***trans*-B-C*n***						***cis*-C*n***					
n	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6
μ	0.186	0.181	0.183	0.185	0.187	0.188	0.187	0.190	0.190	0.190	0.190	0.189	0.184	0.186	0.188	0.190	0.191	0.190

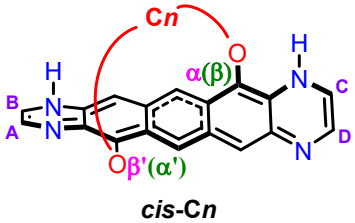
Table S2. Calculated total energies (kcal mol^{-1}) required for twisting the tetraazaacenes cores, dihedral angle (τ) of A-B-C-D positions.



trans*-A-C*n



trans*-B-C*n



cis*-C*n

	τ (◦)	n = 1	n = 2	n = 3	n = 4	n = 5	n = 6
	-108.00	-690749	-715282	--	--	--	--
	-90.00	-690756	-715302	-740014	--	--	--
	-72.00	-690608	-715321	-740031	-764736	-789421	-814125
	-54.00	-690626	-715337	-740047	-764750	-789434	-814136
	-36.00	-690642	-715352	-740060	-764761	-789446	-814146
	-18.00	-690657	-715365	-740072	-764769	-789456	-814153
trans*-A-C*n	0.00	-690670	-715376	-740082	-764778	-789464	-814159
	18.00	-690681	-715385	-740090	-764785	-789470	-814160
	36.00	690689	-715392	-740096	-764790	-789474	-814163
	54.00	-690696	-715398	-740100	-764793	-789475	-814164
	72.00	-690701	-715401	-740103	-764793	-789476	-814165
	90.00	-690704	-715403	-740103	--	--	--
	108.00	-690706	-715403	--	--	--	--
	-108.00	-690834	-715270	--	--	--	--
	-90.00	-690840	-715288	-740000	--	--	--
	-72.00	-690844	-715305	-740017	-764712	-789420	-814122
	-54.00	-690846	-715321	-740032	-764728	-789436	-814137
	-36.00	-690847	-715336	-740047	-764744	-789450	-814149
	-18.00	-690660	-715350	-740061	-764758	-789463	-814149
trans*-B-C*n	0.00	-690671	-715363	-740074	-764770	-789473	-814156
	18.00	-690680	-715376	-740086	-764780	-789480	-814159
	36.00	-690688	-715386	-740094	-764787	-789486	-814159
	54.00	-690693	-715395	-740101	-764792	-789487	-814160

	72.00	-690697	-715401	-740105	-764794	-789489	-814162
	90.00	-690698	-715405	-740106	--	--	--
	108.00	-690698	-715406	--	--	--	--
cis*-C*n	-108.00	-690756	-715276	--	--	--	--
	-90.00	-690763	-715295	-740008	--	--	--
	-72.00	-690769	-715313	-740024	-764736	-789429	-814121
	-54.00	-690773	-715329	-740039	-764750	-789442	-814133
	-36.00	-690776	-715343	-740053	-764761	-789454	-814144
	-18.00	-690646	-715356	-740065	-764769	-789464	-814153
	0.00	-690659	-715368	-740076	-764778	-789473	-814160
	18.00	-690670	-715378	-740085	-764785	-789477	-814164
	36.00	-690680	-715387	-740093	-764790	-789481	-814165
	54.00	-690688	-715394	-740098	-764793	-789482	-814167
	72.00	-690693	-715399	-740101	-764793	-789484	-814168
	90.00	-690697	-715401	-740101	--	--	--
	108.00	-690700	-715402	--	--	--	--

Table S3. Calculated relative energy barriers (kcal mol^{-1}) required to twist back and forth, the dihedral angle (τ), and the diradical parameter (y_0) for tethered **TP$_e$(*trans*-1H)** and **TP$_e$(*cis*-1H)**.

	trans*-A-C*n			***trans*-B-C*n***			***cis*-C*n***		
	energy barriers	τ	y_0	energy barriers	τ	y_0	energy barrier	τ	y_0
n = 1	148	125.3	0.29	38	125.5	0.03	54	123.16	0.65
n = 2	121	100.0	0.47	136	107.9	0.29	125	102.8	0.71
n = 3	89	85.9	0.53	106	90.6	0.65	93	92.1	0.76
n = 4	57	74.2	0.64	82	79.4	0.71	66	76.4	0.82
n = 5	55	65.0	0.67	69	62.3	0.74	55	59.9	0.83
n = 6	40	46.2	0.70	39	57.9	0.76	47	49.1	0.84

Table S4. Calculated vertical excitation energies (eV) (NEVPT2/Def2-TZVP (6e,6o)) of ***trans*-A-C*n*** (***n* = 3 ~ 6**) with different torsion angles from 54° to 0°.

	twist angle	54°	36°	18°	0°
***n*=3**	$E(S_1)$	2.63	2.72	2.43	3.47
	$E(T_1)$	1.05	1.09	1.14	1.63
	$2E(T_1)$	2.09	2.17	2.28	3.25
	$E(T_2)$	2.60	2.64	2.04	3.06
	ΔE_1	0.53	0.55	0.16	0.21
***n*=4**	$E(S_1)$	1.94	1.87	2.11	2.76
	$E(T_1)$	0.73	0.74	0.85	1.08
	$2E(T_1)$	1.46	1.48	1.69	2.16
	$E(T_2)$	1.89	1.74	1.94	2.99
	ΔE_1	0.48	0.39	0.42	0.60

***n*=5**	$E(S_1)$	1.88	2.00	1.93	2.13
	$E(T_1)$	0.69	0.77	0.74	0.87
	$2E(T_1)$	1.37	1.54	1.48	1.74
	$E(T_2)$	1.85	1.89	1.83	1.93
	ΔE_1	0.51	0.46	0.44	0.39
***n*=6**	$E(S_1)$	2.03	1.81	1.87	2.04
	$E(T_1)$	0.57	0.57	0.63	0.58
	$2E(T_1)$	1.13	1.14	1.26	1.16
	$E(T_2)$	2.16	1.82	1.82	2.11
	ΔE_1	0.90	0.67	0.61	0.88

Table S5. Calculated vertical excitation energies (eV) (NEVPT2/Def2-TZVP (6e,6o)) of ***trans*-B-C*n*** (***n* = 3 ~ 6**) with different torsion angles from +54° to 0°.

	twist angle	54°	36°	18°	0°
***n*=3**	$E(S_1)$	1.48	1.13	1.41	1.05
	$E(T_1)$	0.53	0.40	0.40	0.42
	$2E(T_1)$	1.05	0.80	0.80	0.85
	$E(T_2)$	1.46	1.16	1.45	1.11
	ΔE_1	0.43	0.33	0.61	0.20
***n*=4**	$E(S_1)$	1.58	1.48	1.28	1.15
	$E(T_1)$	0.56	0.51	0.46	0.41
	$2E(T_1)$	1.11	1.02	0.92	0.81
	$E(T_2)$	1.55	1.46	1.28	1.19
	ΔE_1	0.46	0.46	0.36	0.34
***n*=5**	$E(S_1)$	1.52	1.48	1.56	1.37
	$E(T_1)$	0.48	0.45	0.52	0.42
	$2E(T_1)$	0.97	0.91	1.05	0.84
	$E(T_2)$	1.49	1.46	1.52	1.37
	ΔE_1	0.55	0.57	0.51	0.52
***n*=6**	$E(S_1)$	1.90	1.62	1.54	1.51
	$E(T_1)$	0.47	0.50	0.47	0.44
	$2E(T_1)$	0.94	1.00	0.94	0.88
	$E(T_2)$	1.91	1.62	1.54	1.51
	ΔE_1	0.96	0.62	0.60	0.63

Table S6. Calculated vertical excitation energies (eV) (NEVPT2/Def2-TZVP (6e,6o)) of ***cis*-C*n*** (***n* = 3 ~ 6**) with different torsion angles from +54° to 0°.

	twist angle	54°	36°	18°	0°
***n*=3**	$E(S_1)$	1.46	1.98	2.14	2.43

	$E(T_1)$	0.41	0.23	0.60	0.52
	$2E(T_1)$	0.83	0.46	1.21	1.04
	$E(T_2)$	1.64	2.03	2.53	2.52
	ΔE_1	0.63	1.52	0.93	1.39
***n*=4**	$E(S_1)$	1.29	1.28	2.15	1.34
	$E(T_1)$	0.28	0.28	0.16	0.37
	$2E(T_1)$	0.56	0.57	0.32	0.74
	$E(T_2)$	1.46	1.44	2.28	1.46
	ΔE_1	0.74	0.71	1.83	0.59
***n*=5**	$E(S_1)$	1.34	1.40	1.30	1.57
	$E(T_1)$	0.23	0.24	0.19	0.34
	$2E(T_1)$	0.47	0.48	0.38	0.69
	$E(T_2)$	1.57	1.64	1.52	2.26
	ΔE_1	0.87	0.92	0.92	0.88
***n*=6**	$E(S_1)$	1.37	1.27	1.30	1.23
	$E(T_1)$	0.22	0.19	0.17	0.19
	$2E(T_1)$	0.44	0.39	0.35	0.38
	$E(T_2)$	1.59	1.48	1.58	1.43
	ΔE_1	0.93	0.89	0.95	0.85

Table S7. Vertical excitation energies (eV) of ***trans*-A-C*n*** are calculated using the NEVPT2/Def2-TZVP method, and the active spaces are selected for 6 electrons and 6π orbitals (6e,6o), 8 electrons and 8π orbitals (8e,8o) and 10 electrons and 10π orbitals (10e,10o), respectively.

	***trans*-A-C1**			***trans*-A-C2**			***trans*-A-C3**			***trans*-A-C4**			***trans*-A-C5**			***trans*-A-C6**		
	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o
$E(S_1)$	2.68	5.04	3.06	3.76	3.32	3.09	2.17	2.50	2.29	2.16	2.31	1.95	1.79	1.79	2.59	2.03	1.98	1.67
$E(T_1)$	1.93	2.53	2.10	1.96	1.78	1.64	0.94	0.99	0.95	0.49	0.47	0.66	0.52	0.51	0.64	0.32	0.35	0.39
$2E(T_1)$	3.86	5.05	4.19	3.92	3.56	3.28	1.89	1.98	1.90	0.98	0.94	1.31	1.04	1.03	1.28	0.64	0.70	0.78
$E(T_2)$	2.81	2.58	2.70	2.37	2.49	2.44	2.10	2.42	2.06	2.19	2.39	1.92	1.88	1.88	2.72	2.07	2.05	1.74

Table S8. Vertical excitation energies (eV) of ***trans*-B-C*n*** are calculated using the NEVPT2/Def2-TZVP method, and the active spaces are selected for 6 electrons and 6π orbitals (6e,6o), 8 electrons and 8π orbitals (8e,8o) and 10 electrons and 10π orbitals (10e,10o), respectively.

	***trans*-B-C1**			***trans*-B-C2**			***trans*-B-C3**			***trans*-B-C4**			***trans*-B-C5**			***trans*-B-C6**		
	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o
$E(S_1)$	2.11	2.01	1.96	2.51	2.48	2.00	1.71	2.31	2.52	2.26	1.74	1.91	1.70	2.01	1.65	1.63	2.08	1.89
$E(T_1)$	1.55	1.06	1.51	1.25	1.28	1.31	0.72	0.62	0.57	0.44	0.59	0.45	0.41	0.50	0.46	0.44	0.52	0.31
$2E(T_1)$	3.11	2.11	3.01	2.51	2.56	2.63	1.45	1.24	1.13	0.87	1.18	0.89	0.82	1.01	0.92	0.88	1.04	0.62
$E(T_2)$	2.11	2.07	2.06	2.21	2.27	1.98	1.62	2.37	2.54	2.33	1.73	1.94	1.76	2.05	1.68	1.67	1.90	1.94

Table S9. Vertical excitation energies (eV) of ***cis*-C*n*** are calculated using the NEVPT2/Def2-TZVP method, and the active spaces are selected for 6 electrons and 6π orbitals (6e,6o), 8 electrons and 8π orbitals (8e,8o) and 10 electrons and 10π orbitals (10e,10o), respectively.

	***cis*-C1**			***cis*-C2**			***cis*-C3**			***cis*-C4**			***cis*-C5**			***cis*-C6**		
	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o	6e,6o	8e,8o	10e,10o
$E(S_1)$	1.94	1.48	1.86	1.33	1.41	1.18	1.39	1.68	1.40	1.43	1.58	1.52	1.45	1.47	1.44	2.27	2.37	1.71
$E(T_1)$	0.54	0.64	0.49	0.61	0.54	0.57	0.30	0.33	0.35	0.19	0.21	0.18	0.15	0.14	0.14	0.11	0.12	0.26
$2E(T_1)$	1.07	1.29	0.99	1.22	1.09	1.15	0.59	0.66	0.70	0.38	0.41	0.36	0.30	0.29	0.27	0.23	0.23	0.52
$E(T_2)$	2.11	1.68	2.04	2.00	1.96	1.88	1.67	2.00	2.29	1.69	1.84	1.84	1.71	1.72	1.64	2.33	2.42	1.82

Table S10. The dihedral angle (τ), ΔE_1 (eV), and ΔE_2 (eV) of ***trans*-A-C*n*** are calculated using the NEVPT2/Def2-TZVP (6e,6o) method.

	***trans*-A-C1**	***trans*-A-C2**	***trans*-A-C3**	***trans*-A-C4**	***trans*-A-C5**	***trans*-A-C6**
τ	125.34	99.97	85.86	74.19	65.01	46.21
ΔE_1	-1.18	-0.16	0.29	1.18	0.75	1.39
ΔE_2	-1.05	-1.55	0.22	1.21	0.84	1.43

Table S11. The dihedral angle (τ), ΔE_1 (eV), and ΔE_2 (eV) of ***trans*-B-C*n*** are calculated using the NEVPT2/Def2-TZVP (6e,6o) method.

	***trans*-B-C1**	***trans*-B-C2**	***trans*-B-C3**	***trans*-B-C4**	***trans*-B-C5**	***trans*-B-C6**
τ	125.52	107.86	90.62	79.38	62.28	57.88
ΔE_1	-0.99	0.01	0.27	1.38	0.88	0.75
ΔE_2	-0.99	-0.29	0.18	1.45	0.94	0.79

Table S12. The dihedral angle (τ), ΔE_1 (eV), and ΔE_2 (eV) of ***cis*-C*n*** are calculated using the NEVPT2/Def2-TZVP (6e,6o) method.

	***cis*-C1**	***cis*-C2**	***cis*-C3**	***cis*-C4**	***cis*-C5**	***cis*-C6**
τ	122.08	102.84	92.13	76.41	59.88	49.14
ΔE_1	0.86	0.11	0.79	1.05	1.15	2.05
ΔE_2	1.03	0.78	1.07	1.31	1.41	2.11

Table S13. The dihedral angle (τ) of the T_1 state and the MECP structure of ***trans*-A-C*n***. The energy difference between the T_1 state and the MECP structure. The energy of MECP structure of ***trans*-A-C*n***. The maximum and minimum potential energy surface scan energy of ***trans*-A-C*n***.

n	**τ(T_1 state)**	**τ(MECP)**	**τ(MECP-T_1)**	**ΔE(MECP-T_1)/eV**	**MECP energies/Kcal mol^{-1}**	**torsion energies / Kcal mol^{-1}**	
						Max	**Min**
2	97.36	97.86	0.50	0.11	-1140.05	-1139.91	-1140.07
3	83.90	85.03	1.13	0.11	-1179.41	-1179.29	-1179.43
4	72.49	72.78	0.29	0.04	-1218.76	-1218.66	-1218.78
5	63.48	63.84	0.36	0.02	-1258.10	-1258.00	-1258.11
6	44.91	45.07	0.16	0.01	-1297.45	-1297.37	-1297.45

Table S14. The dihedral angle (τ) of the T_1 state and the MECP structure of ***trans*-B-C*n***. The energy difference between the T_1 state and the MECP structure. The energy of MECP structure of ***trans*-B-C*n***. The maximum and minimum potential energy surface scan energy of ***trans*-B-C*n***.

n	**τ(T_1 state)**	**τ(MECP)**	**τ(MECP-T_1)**	**ΔE(MECP-T_1)/eV**	**MECP energies/Kcal mol^{-1}**	**torsion energies / Kcal mol^{-1}**	
						Max	**Min**
2	102.68	103.27	0.59	0.13	-1140.05	-1139.88	-1140.07
3	85.20	85.87	0.66	0.10	-1179.42	-1179.27	-1179.43
4	75.30	75.75	0.45	0.07	-1218.76	-1218.62	-1218.78

5	59.26	59.52	0.26	0.03	-1258.12	-1257.99	-1258.13
6	54.93	55.18	0.26	0.02	-1297.44	-1297.36	-1297.45

Table S15. The dihedral angle (***τ***) of the T_1 state and the MECP structure of ***cis*-C*n***. The energy difference between the T_1 state and the MECP structure. The energy of MECP structure of ***cis*-C*n***. The maximum and minimum potential energy surface scan energy of ***cis*-C*n***.

n	***τ*(T$_1$ state)**	***τ*(MECP)**	***τ*(T$_1$-MECP)**	ΔE(MECP-T$_1$)/eV	MECP energies/Kcal mol^{-1}	torsion energies / Kcal mol^{-1}	
						Max	Min
2	99.08	98.74	0.34	0.86	-1140.05	-1139.90	-1140.06
3	88.64	88.30	0.34	0.57	-1179.41	-1179.28	-1179.43
4	73.61	73.56	0.05	0.01	-1218.77	-1218.65	-1218.78
5	58.59	58.07	0.52	0.00	-1258.12	-1258.01	-1258.12
6	47.67	47.68	-0.01	0.00	-1297.46	-1297.36	-1297.46

2. Figures

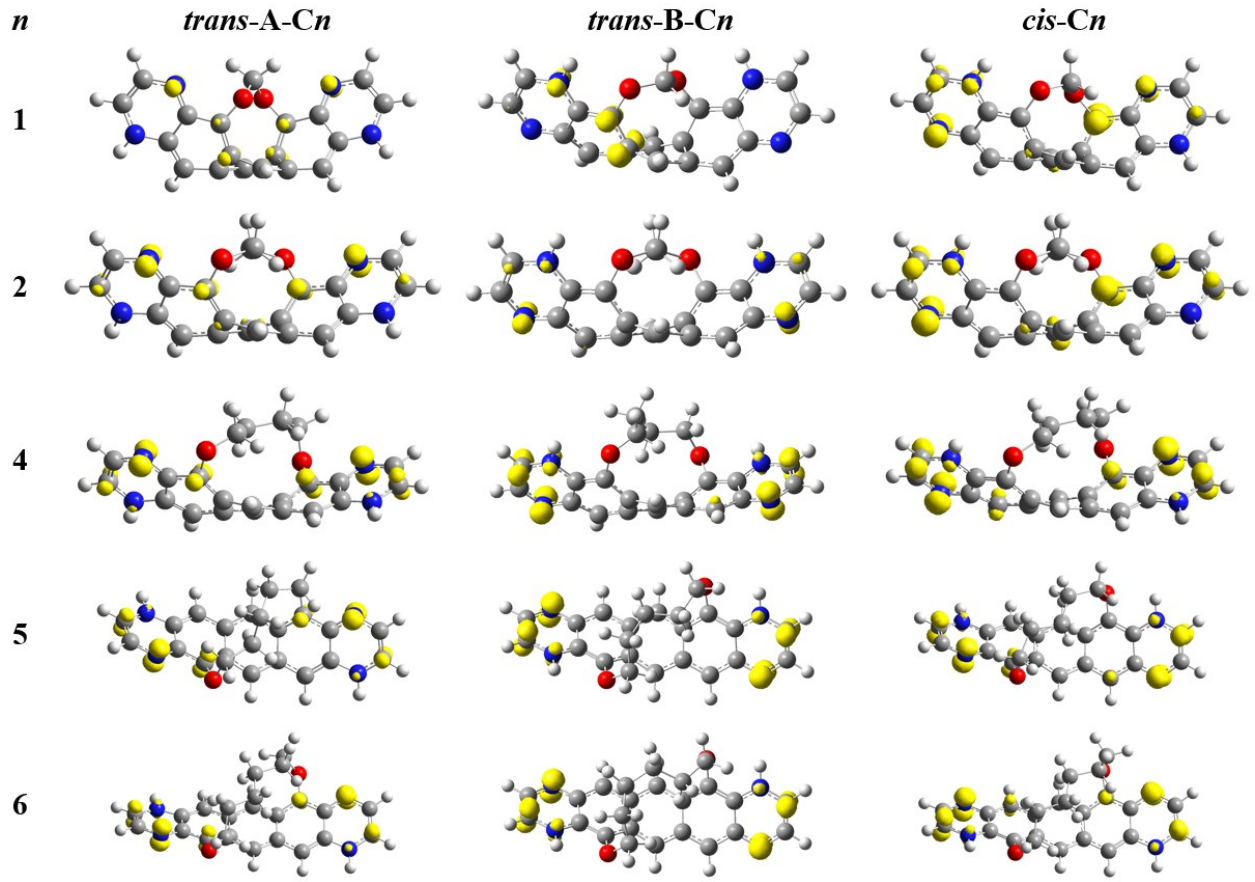


Figure S1. The odd electron densities for ***trans*-A-C*n***, ***trans*-B-C*n*** and ***cis*-C*n***.

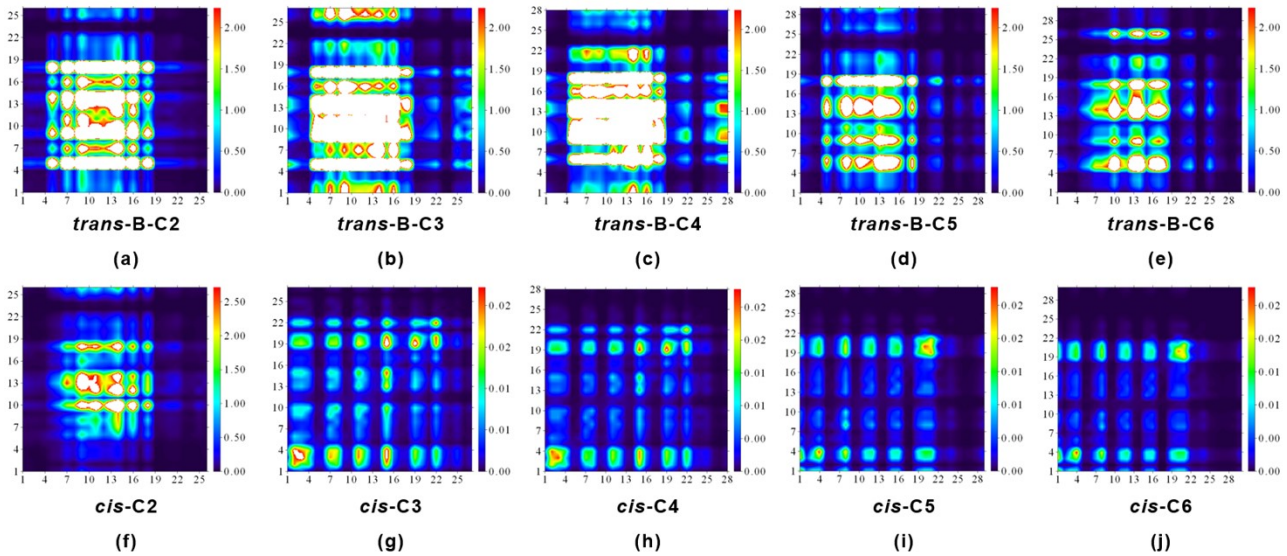


Figure S2. The TDM for $S_0 \rightarrow T_1$ transition of ***trans*-B-C*n*** and ***cis*-C*n*** (***n*** = 2~6).

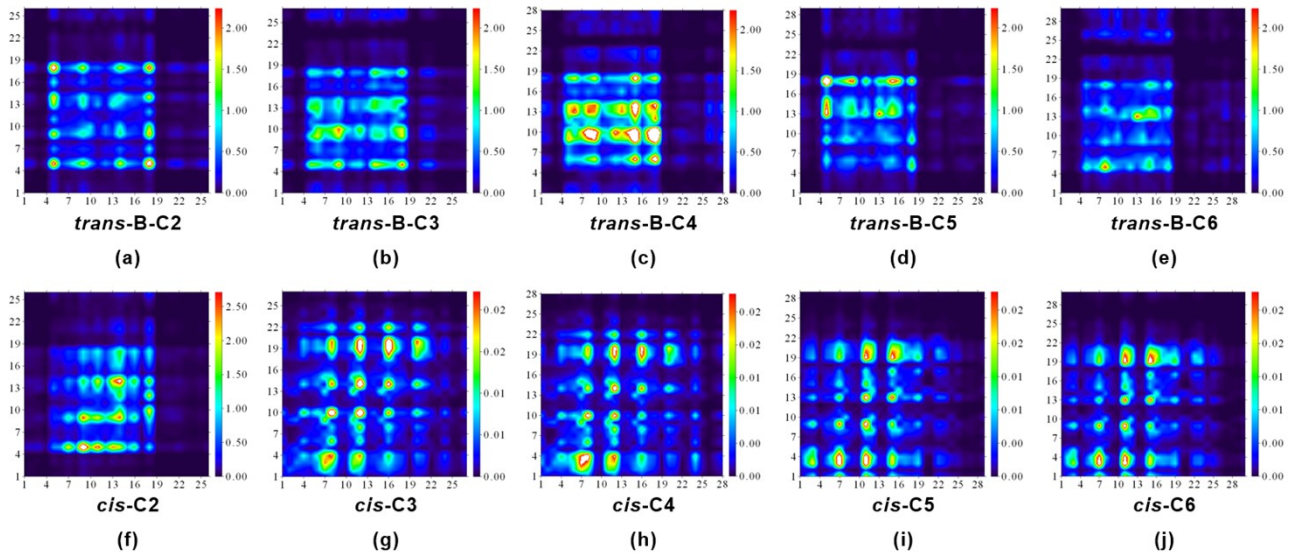


Figure S3. The TDM for $S_0 \rightarrow T_2$ transition of ***trans*-B-C*n*** and ***cis*-C*n*** (***n*** = 2~6).

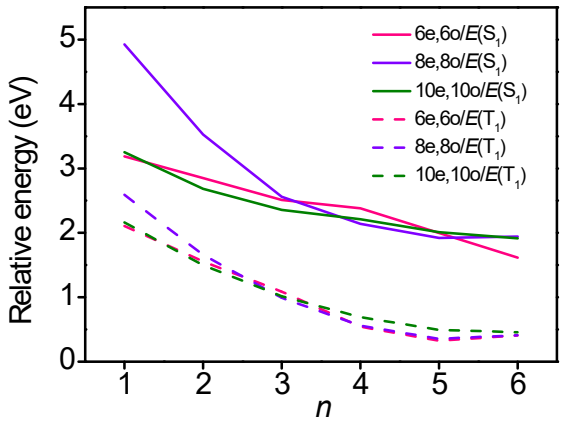


Figure S4. Relative vertical excitation energies (eV) of ***trans*-A-C*n*** during increasing ***n***. The active spaces for NEVPT2/Def2-TZVP method are selected for 6 electrons and 6π orbitals (6e,6o), 8 electrons and 8π orbitals (8e,8o) and 10 electrons and 10π orbitals (10e,10o), respectively.

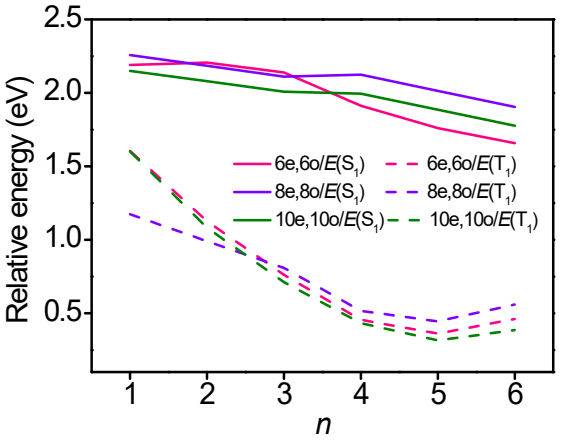


Figure S5. Relative vertical excitation energies (eV) of ***trans*-B-C*n*** during increasing ***n***. The active spaces for NEVPT2/Def2-TZVP method are selected for 6 electrons and 6π orbitals (6e,6o), 8 electrons and 8π orbitals (8e,8o) and 10 electrons and 10π orbitals (10e,10o), respectively.

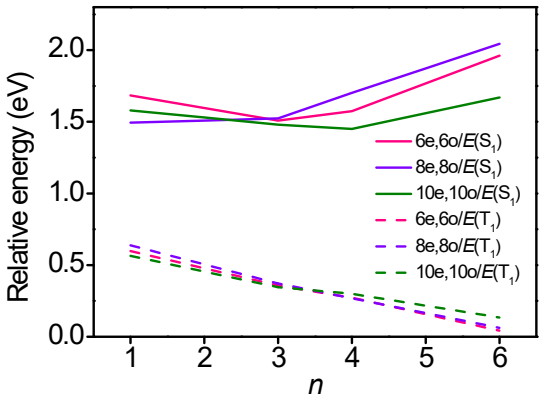


Figure S6. Relative vertical excitation energies (eV) of ***cis*-C*n*** during increasing ***n***. The active spaces for NEVPT2/Def2-TZVP method are selected for 6 electrons and 6π orbitals (6e,6o), 8 electrons and 8π orbitals (8e,8o) and 10 electrons and 10π orbitals (10e,10o), respectively.

3. Summary of geometries

***trans*-A-C1**

The lowest vibrational frequency: 61.35 cm^{-1}

C	-5.33385000	-0.28676500	0.76381700
C	-3.46642500	-0.47996400	-0.75133900
C	-2.73738300	0.35658400	0.23227900
C	-4.54179200	0.34053200	1.67109100
C	-2.80326400	-1.10541600	-1.76002300
C	-1.40147200	0.79960400	-0.14833600
C	-0.97193600	0.58375800	-1.43352400
C	-1.38436900	-0.78734300	-1.83252600
C	-0.31594000	-1.61374500	-1.68117100
H	-0.40972000	-2.69405200	-1.66780300
C	0.92926900	-0.97328400	-1.22469100
C	1.35173000	0.26117500	-1.93701300
C	0.28261800	1.09726900	-2.00941200
H	-3.24943400	-1.90212300	-2.34657600
H	-6.37590100	-0.52191600	0.93699000
H	-4.92456700	0.62257400	2.64368700
H	0.37851700	2.14882500	-2.25645600
C	2.76973700	0.59084900	-1.91831500
C	3.41290000	0.23136900	-0.77576000
C	1.33424200	-0.86832000	0.08199100
C	2.66402700	-0.34296000	0.36821300
H	3.22838800	1.22142600	-2.67320300
C	5.25100800	0.41806400	0.77550700
C	4.44088700	0.02828700	1.79322600
H	6.29004200	0.69113300	0.90583500
H	4.80495400	-0.00758100	2.81214500
N	-3.23822600	0.68183400	1.39489300
N	-4.81618400	-0.64533100	-0.45456900
N	4.75718500	0.46761000	-0.50301900
N	3.14232700	-0.37388400	1.58420500

H	5.34240000	0.81463700	-1.24776300
H	-5.38837600	-1.16385900	-1.10363500
O	-0.50837600	1.23000500	0.81643800
O	0.42283700	-1.05348500	1.10589400
C	-0.05003300	0.17950700	1.70284100
H	0.75404900	0.65340100	2.26092600
H	-0.86570700	-0.14747500	2.34347700

***trans*-A-C2**

The lowest vibrational frequency: 48.44 cm^{-1}

C	-5.27713400	-2.36213000	-1.25535100
C	-3.32596300	-0.98483700	-1.58909800
C	-3.46615900	-0.63438600	-0.16194500
C	-5.25875900	-2.06647500	0.07275200
C	-2.20132200	-0.64646800	-2.29196100
C	-2.52884700	0.34220200	0.34383400
C	-1.76229600	1.07159000	-0.54938500
C	-1.25915200	0.22151900	-1.63886700
C	0.10723200	0.09023200	-1.57837800
H	0.61282500	-0.73241100	-2.07333900
C	0.83121200	0.87992800	-0.60915300
C	0.34706600	2.24233300	-0.34113900
C	-1.02304600	2.27443200	-0.24255500
H	-1.95501000	-1.12561700	-3.23480900
H	-5.99839900	-3.02077300	-1.72027600
H	-5.98466100	-2.50774800	0.74519900
H	-1.52872100	3.09126500	0.26187500
C	1.29263800	3.19129900	0.18148900
C	2.38678500	2.68630500	0.83050100
C	1.55492900	0.38330000	0.46160100
C	2.48801700	1.24796700	1.14701300
H	1.06791500	4.25366000	0.18983600
C	4.29733000	2.95344100	2.27750600
C	4.24120100	1.63159300	2.59561400
H	5.01947500	3.64611100	2.68847100
H	4.93475900	1.20755700	3.31188100
N	-4.35270900	-1.20402400	0.62533500
N	-4.33115000	-1.80154400	-2.07718800
N	3.39047800	3.46349600	1.38188500
N	3.33629600	0.77405000	2.03374500
H	3.38523000	4.45470600	1.19192800
H	-4.29790300	-2.06948600	-3.04969200
O	-2.28091400	0.37788100	1.69518200

O	1.26477400	-0.84083700	1.01450700
C	-0.87944800	0.14634800	2.06995400
H	-0.32049700	1.07095500	1.93260800
H	-0.94972000	-0.04967800	3.13888000
C	-0.15129000	-1.04461400	1.34994800
H	-0.69016300	-1.32633400	0.44638900
H	-0.11621900	-1.91303100	2.00614400

***trans*-A-C3**

The lowest vibrational frequency: 42.78 cm^{-1}

C	-5.93493800	-0.36581400	-0.36718400
C	-3.67349900	-0.03280900	-1.13372200
C	-3.40550700	0.48317600	0.22212000
C	-5.56717600	0.02731900	0.88490900
C	-2.65581300	-0.28668500	-2.01313000
C	-2.07157300	0.96880100	0.45572500
C	-1.20767900	1.15947400	-0.61629800
C	-1.33212100	0.13686200	-1.65319200
C	-0.15754900	-0.54528300	-1.88645700
H	-0.17229700	-1.51507600	-2.37123200
C	1.04114300	-0.11847400	-1.22351100
C	1.19458500	1.30119800	-0.92127400
C	0.01369200	1.90411500	-0.54476100
H	-2.81415500	-0.89805600	-2.89683500
H	-6.93431200	-0.68143900	-0.63505800
H	-6.28739700	0.02500400	1.69460100
H	0.02836500	2.83443600	0.01388500
C	2.51709800	1.80289600	-0.67851500
C	3.49792700	0.90787200	-0.34850300
C	1.87957100	-0.95306500	-0.49957800
C	3.18592500	-0.51011400	-0.09985000
H	2.69262100	2.87375600	-0.62960900
C	5.69369000	0.39559300	0.50620000
C	5.28037600	-0.86827700	0.80347900
H	6.68697600	0.77322300	0.70777100
H	5.95440800	-1.56613100	1.28630300
N	-4.30573300	0.45015900	1.18542800
N	-4.99581000	-0.36916000	-1.36576100
N	4.80964900	1.26149900	-0.08748500
N	4.03085300	-1.32754400	0.50496300
H	5.08850400	2.21697300	-0.25489300
H	-5.24572600	-0.71633400	-2.28006900
O	-1.60478300	1.04044100	1.74225400

O	1.37939900	-2.14523000	-0.02844100
C	-0.40252900	0.22845700	1.98765500
H	0.45883200	0.73548700	1.55273400
H	-0.30263300	0.26841100	3.07293800
C	-0.49017900	-1.24328300	1.50127000
H	-1.02985400	-1.29991900	0.55641400
H	-1.09906200	-1.80038400	2.22095600
C	0.84867200	-2.02193800	1.32868000
H	0.69261200	-3.06056900	1.61928400
H	1.64086500	-1.61731400	1.96717600

***trans*-A-C4**

The lowest vibrational frequency: 40.47 cm^{-1}

C	-6.33202100	-0.46200200	0.13294300
C	-3.97715400	-0.64945200	-0.34764600
C	-3.90829300	0.79127600	-0.07850900
C	-6.15145100	0.85081100	0.47164900
C	-2.84232300	-1.40136400	-0.51171100
C	-2.64028300	1.40480500	-0.24574000
C	-1.56018000	0.69424900	-0.78597500
C	-1.57507800	-0.74205600	-0.57751500
C	-0.36379300	-1.28529500	-0.17547200
H	-0.33387700	-2.27452300	0.26975400
C	0.80248500	-0.47638100	-0.13205900
C	0.86339200	0.69876500	-0.98610900
C	-0.35824800	1.30881300	-1.22557800
H	-2.88599500	-2.48702700	-0.49588200
H	-7.28293300	-0.97507100	0.17601700
H	-6.99120000	1.43895500	0.82510800
H	-0.39365100	2.33031100	-1.58716400
C	2.14760900	1.27338400	-1.24178900
C	3.20533400	0.90504200	-0.45186800
C	1.72838900	-0.49655500	0.92158900
C	3.01514600	0.09437000	0.75879500
H	2.25246600	2.05608800	-1.98791000
C	5.47050100	1.21378100	0.31094200
C	5.17074300	0.53095100	1.45781200
H	6.43978900	1.64234400	0.09515900
H	5.92413200	0.40547100	2.22754000
N	-4.95654300	1.48531600	0.37969100
N	-5.24855900	-1.19250600	-0.28731800
N	4.49378400	1.37717200	-0.63580700
N	3.95663300	-0.02378100	1.69408900
H	4.68520500	1.93245300	-1.45666300
H	-5.35723800	-2.17756000	-0.47798500
O	-2.36870600	2.64692000	0.26848300

O	1.34869300	-0.91016600	2.16719400
C	-2.27917600	2.69192500	1.73038600
H	-1.65765200	3.56870000	1.92368100
H	-3.28783700	2.89170900	2.10118700
C	-1.73624000	1.44957700	2.47665800
H	-2.33495000	0.58160000	2.18480100
H	-1.98815200	1.62480300	3.53000600
C	-0.22863000	1.10940900	2.35437700
H	0.09879400	1.35127900	1.34669800
H	0.35665100	1.74976400	3.02250700
C	0.07527000	-0.37844100	2.66439700
H	0.14919900	-0.54908000	3.73935200
H	-0.73249000	-1.00373700	2.27906200

***trans*-A-C5**

The lowest vibrational frequency: 32.70 cm^{-1}

C	-6.75524400	0.77332500	-0.31524500
C	-4.41454000	0.27888700	-0.60407000
C	-4.16862200	1.65906100	-0.16772300
C	-6.42459200	2.00343200	0.18957700
C	-3.39119000	-0.62156300	-0.74297000
C	-2.81768400	2.08460000	-0.15665100
C	-1.79735700	1.26264500	-0.67298100
C	-2.03993900	-0.16753100	-0.62303400
C	-0.97427100	-0.94237400	-0.18499800
H	-1.14238500	-1.96545300	0.13187400
C	0.29704800	-0.35551400	0.04353100
C	0.60530200	0.90782600	-0.60173400
C	-0.48014000	1.72385500	-0.89167200
H	-3.59519500	-1.68347600	-0.85075400
H	-7.76937400	0.41127600	-0.41508100
H	-7.20517500	2.67239600	0.53543000
H	-0.32171300	2.77723500	-1.09364100
C	1.96446100	1.33989500	-0.64700900
C	2.90499100	0.69077700	0.10813600
C	1.18748400	-0.80046700	1.03420400
C	2.53426800	-0.35474800	1.06245600
H	2.22462100	2.22836700	-1.21619800
C	5.13395900	0.50606900	1.00850600
C	4.68082500	-0.41197300	1.91857700
H	6.15808500	0.84820000	0.94950200
H	5.36562400	-0.83377900	2.64632200
N	-5.15224700	2.45493500	0.27435900
N	-5.75125400	-0.06571900	-0.72284200
N	4.24638600	1.03718100	0.10907700
N	3.39964600	-0.84370200	1.96426100
H	4.55638600	1.74788700	-0.53678000
H	-5.97809100	-0.99909500	-1.03266200
O	-2.43410900	3.20000900	0.55190200

O	0.70973000	-1.61625300	2.02640100
C	-2.24075000	2.88561900	1.97455700
H	-2.01231500	3.85297500	2.42403500
H	-3.20417000	2.54615200	2.36925000
C	-1.14099300	1.83777200	2.24684600
H	-1.24913500	1.06043700	1.50176900
H	-0.15896000	2.28598200	2.07402200
C	-1.18927600	1.11728300	3.61455100
H	-2.18479000	1.24501400	4.05834300
H	-0.49520500	1.57992900	4.32607400
C	-0.93295500	-0.41552200	3.55665000
H	-1.25551400	-0.82507400	4.52109100
H	-1.59846800	-0.86570700	2.81354500
C	0.50457800	-0.95135500	3.30719500
H	0.73487800	-1.72945400	4.03539200
H	1.25698400	-0.16805100	3.42315800

***trans*-A-C6**

The lowest vibrational frequency: 34.20 cm^{-1}

C	-6.56501600	-0.65283000	-0.40621600
C	-4.15882800	-0.65157100	-0.25795300
C	-4.25223400	0.80678500	-0.22819900
C	-6.56033100	0.71521400	-0.30281700
C	-2.96897000	-1.30732400	-0.07642300
C	-3.03323200	1.52368000	-0.16536200
C	-1.79297500	0.85893500	-0.23857200
C	-1.75587100	-0.56746100	0.02396300
C	-0.55770700	-1.10550800	0.47935400
H	-0.52386800	-2.13475800	0.81933300
C	0.60893700	-0.31800700	0.58387500
C	0.64312100	0.96568200	-0.09095000
C	-0.57374100	1.54138000	-0.43775700
H	-2.94476200	-2.38898200	0.02992800
H	-7.46011900	-1.25256200	-0.49834200
H	-7.50046200	1.25686700	-0.29772400
H	-0.60075700	2.55807700	-0.81422400
C	1.90049700	1.61703200	-0.24513600
C	3.01513600	1.11071600	0.37129900
C	1.69327200	-0.67137600	1.41175900
C	2.94302700	-0.01620800	1.29939300
H	1.95845500	2.53542500	-0.82400300
C	5.34185400	1.27030400	0.98191500
C	5.16393700	0.24920000	1.88078300
H	6.28093300	1.78166500	0.82057500
H	5.99763900	-0.07981000	2.49228300
N	-5.43355800	1.45114700	-0.20895700
N	-5.36709300	-1.31723600	-0.39148600
N	4.27037300	1.68202300	0.23415200
N	3.99034400	-0.39270800	2.05583000
H	4.37429700	2.45987600	-0.40020600
H	-5.35545600	-2.32574500	-0.42371400
O	-3.08671700	2.87401200	0.00544500

O	1.55023500	-1.62874100	2.37029800
C	-2.50796500	3.44295700	1.22215800
H	-1.48550300	3.76181600	0.99779300
H	-3.11011800	4.33921900	1.37204100
C	-2.52596400	2.54590600	2.48391700
H	-3.02631500	3.09774100	3.28560900
H	-3.17194300	1.68574300	2.28788300
C	-1.13600800	2.05996500	2.97665300
H	-0.76824200	2.73252300	3.76139100
H	-0.41767900	2.14045300	2.15764600
C	-1.11184800	0.60590900	3.48393500
H	-1.76604800	0.50721100	4.35894700
H	-1.55519400	-0.02534500	2.71051400
C	0.30342500	0.06831800	3.82862300
H	1.06402600	0.69661900	3.35690800
H	0.48188900	0.16742500	4.90370700
C	0.56814600	-1.40424800	3.43000700
H	0.99001300	-1.96525500	4.26409900
H	-0.36703700	-1.89243000	3.13965800

***trans*-B-C1**

The lowest vibrational frequency: 50.25 cm^{-1}

C	-5.05478900	0.04292300	1.41942700
C	-2.99364900	-0.41329700	0.30689900
C	-3.58329200	0.22762400	-0.88631700
C	-5.59379000	0.45593500	0.22583900
C	-1.69165500	-0.86429500	0.27742300
C	-2.65088800	0.69046200	-1.85781500
C	-1.32507500	0.30171800	-1.74411700
C	-1.02572000	-0.92141500	-0.98286500
C	0.14843400	-1.62616600	-1.22807500
H	0.29805200	-2.60675500	-0.78670000
C	1.29497600	-0.83016000	-1.53255000
C	0.99296700	0.58074000	-1.28218800
C	-0.16427400	1.15371500	-1.75056900
H	-5.59738600	0.01734100	2.35423300
H	-6.63667000	0.74660200	0.17246400
H	-2.95345200	1.52185500	-2.48433000
H	-0.33309900	2.21843700	-1.62223400
C	1.61064600	0.94749800	-0.02475700
C	2.92870800	0.59248800	0.15870400
C	2.64901900	-1.17785900	-1.52867800
C	3.55729200	-0.37062000	-0.78955100
H	2.99797300	-2.14882100	-1.86127200
C	5.01032000	0.58177500	1.33397300
C	5.57449200	-0.14050500	0.31120900
H	5.54655400	0.91753000	2.21045000
H	6.63202400	-0.37850000	0.33680600
N	-4.85608100	0.60938900	-0.89801400
N	-3.74687200	-0.33738200	1.44855700
N	3.67851600	0.87960000	1.26707600
N	4.85238400	-0.66817000	-0.70147700
H	3.24111100	1.41196200	2.00752100
H	-3.30417300	-0.60642300	2.31737600
O	0.69292400	0.98092600	1.08349200

O	-0.97755200	-0.87966900	1.48130000
C	0.37307600	-0.34246100	1.59792700
H	1.07148600	-1.05731600	1.16643200
H	0.47611000	-0.28468300	2.67990400

***trans*-B-C2**

The lowest vibrational frequency: 46.19 cm^{-1}

C	-4.62182100	0.94720600	1.77795400
C	-2.58701500	0.26767700	0.72561800
C	-3.10525600	0.89005400	-0.50827000
C	-5.10119500	1.35341000	0.55888900
C	-1.33033400	-0.29014200	0.74265500
C	-2.13843700	1.19188300	-1.50649600
C	-0.84560100	0.69760900	-1.37746100
C	-0.64063900	-0.45782300	-0.49769100
C	0.45591500	-1.28288200	-0.68810500
H	0.53344100	-2.21764000	-0.14188500
C	1.65835400	-0.67482500	-1.16286600
C	1.54605800	0.78750500	-1.16416400
C	0.38197500	1.38864700	-1.61480300
H	-5.18268000	1.00375300	2.70058800
H	-6.11331400	1.73228200	0.47356300
H	-2.38531200	1.96735800	-2.22291200
H	0.34745300	2.46359400	-1.76126100
C	2.46580800	1.37667500	-0.24339900
C	3.73078500	0.84658300	-0.14699400
C	2.93384300	-1.22644100	-1.19822000
C	4.04864400	-0.43670700	-0.80276100
H	3.09242800	-2.29284700	-1.31334900
C	5.96761400	0.83228000	0.69294700
C	6.23565400	-0.27048500	-0.07701800
H	6.69403300	1.32142600	1.32700900
H	7.23668500	-0.68601700	-0.09854500
N	-4.33930000	1.38483600	-0.56124000
N	-3.34916800	0.45704200	1.85133200
N	4.70142200	1.34428800	0.68597900
N	5.28097100	-0.93747700	-0.76978200
H	4.46066100	2.14156000	1.25931600
H	-2.95239900	0.17236200	2.73669700
O	1.99302500	2.21807400	0.76968000

O	-0.62128500	-0.35208200	1.94761700
C	0.75238200	1.79402100	1.44681300
H	0.69593600	2.49371100	2.27987100
H	-0.08976100	1.99040600	0.78460600
C	0.69228800	0.32030000	1.97131200
H	1.40952500	-0.29804300	1.43330300
H	0.94658200	0.28608700	3.03007000

***trans*-B-C3**

The lowest vibrational frequency: 41.74 cm^{-1}

C	-4.86398000	-0.20493200	1.52389000
C	-2.68966000	-0.23482500	0.52443200
C	-3.13725200	0.89715000	-0.30551600
C	-5.24370900	0.77017600	0.63819000
C	-1.40789400	-0.71761700	0.41360700
C	-2.12568900	1.61316200	-0.99340000
C	-0.81982500	1.13307100	-1.02453700
C	-0.57818700	-0.26131700	-0.65469300
C	0.56263200	-0.90565600	-1.10046400
H	0.67086100	-1.97533100	-0.95538800
C	1.72988700	-0.12873700	-1.34684200
C	1.58961400	1.25963700	-0.90583900
C	0.37417700	1.90827200	-1.05240100
H	-5.51615400	-0.63348500	2.27224500
H	-6.26079800	1.14544100	0.65030000
H	-2.37140900	2.60538100	-1.35521500
H	0.30562800	2.97617400	-0.87089300
C	2.61498100	1.66463800	-0.00054800
C	3.88591600	1.16957200	-0.16777900
C	3.00864300	-0.60633500	-1.62014200
C	4.14474300	0.08660600	-1.13219100
H	3.16711400	-1.58637400	-2.05602700
C	6.20192500	1.05436100	0.40611000
C	6.39555600	0.15634700	-0.61467900
H	6.98883800	1.41586000	1.05357000
H	7.39269400	-0.21092300	-0.82978000
N	-4.38833900	1.35066700	-0.23778400
N	-3.57707700	-0.66335100	1.48271200
N	4.93980300	1.51282700	0.64313300
N	5.38125300	-0.36527200	-1.34241300
H	4.75200000	2.15479700	1.40161700
H	-3.26781400	-1.39420500	2.10896000
O	2.27618500	2.28619700	1.19922800

O	-0.81907100	-1.42293200	1.46687000
C	1.13537600	1.68029900	1.90517200
H	1.16024800	2.18445200	2.87239200
H	0.21924800	1.97889000	1.39541700
C	1.17194000	0.13800900	2.09065900
H	1.56373200	-0.34561200	1.19941300
H	1.88184100	-0.09688800	2.89028700
C	-0.19309400	-0.53413100	2.45420700
H	-0.04800900	-1.19431900	3.30949300
H	-0.93249200	0.22454200	2.73789000

***trans*-B-C4**

The lowest vibrational frequency: 38.33 cm^{-1}

C	-5.15873500	-0.11012100	0.49480000
C	-2.81010500	-0.51904900	0.29082000
C	-2.94578800	-0.16907900	-1.13018400
C	-5.22907600	0.07660000	-0.86423500
C	-1.58372200	-0.83495600	0.82265900
C	-1.75036200	0.08765500	-1.83355100
C	-0.50776600	-0.17165100	-1.24594600
C	-0.46453200	-1.00521100	-0.05040400
C	0.71115000	-1.65389200	0.28847700
H	0.70989500	-2.39006600	1.08547200
C	1.95220400	-1.10579900	-0.13070200
C	1.84161600	0.20131300	-0.76999300
C	0.70922400	0.49863200	-1.52198400
H	-6.01052900	-0.05909500	1.15878800
H	-6.18872000	0.26775400	-1.33189000
H	-1.82558900	0.60081100	-2.78589600
H	0.69588100	1.38035000	-2.15439700
C	2.78952500	1.16550700	-0.32895100
C	4.01917100	0.75152200	0.12737600
C	3.21110500	-1.55584800	0.27187500
C	4.30651500	-0.66970400	0.33415700
H	3.34849100	-2.55646200	0.66633000
C	6.22644900	1.20282500	0.92806700
C	6.45813200	-0.14966900	1.00144200
H	6.95795300	1.95759300	1.18167700
H	7.43167200	-0.51190100	1.31321400
N	-4.14389000	0.09367200	-1.66981800
N	-3.94027900	-0.35934100	1.06051200
N	4.99731800	1.63588400	0.52214600
N	5.51399200	-1.08202000	0.74662800
H	4.78044300	2.62139600	0.46274900
H	-3.84851600	-0.51175100	2.05551800
O	2.44198400	2.50165100	-0.19372300

O	-1.35832400	-0.66238200	2.19299400
C	1.22217800	2.76690900	0.57581300
H	1.17517700	3.85594200	0.55069700
H	0.36501400	2.38296200	0.02025900
C	1.19199700	2.29811100	2.05248100
H	2.20493600	2.40222700	2.45661300
H	0.59723600	3.04859900	2.59058300
C	0.66842300	0.88160300	2.43281100
H	1.10494700	0.13906400	1.77811200
H	1.05299100	0.64858900	3.43097200
C	-0.87075100	0.70070300	2.46092400
H	-1.25806500	0.93661800	3.45515800
H	-1.35653000	1.37187400	1.74520600

***trans*-B-C5**

The lowest vibrational frequency: 37.64 cm^{-1}

C	-5.58281300	-0.61285600	0.80963600
C	-3.27745000	-0.70010400	0.17899900
C	-3.50156200	0.53417600	-0.56950900
C	-5.73878300	0.49983700	0.01515100
C	-2.03430000	-1.28472100	0.22914000
C	-2.36591900	1.19683600	-1.06212800
C	-1.09235600	0.61961100	-0.96311100
C	-0.97618400	-0.77732200	-0.57304300
C	0.21426400	-1.46034500	-0.80920700
H	0.24782200	-2.53847200	-0.69192000
C	1.41883200	-0.74922800	-1.00192200
C	1.33064200	0.68661300	-0.79556500
C	0.12217000	1.34177000	-0.98726300
H	-6.38279700	-1.06841800	1.37670100
H	-6.71772100	0.95837700	-0.07587400
H	-2.49081400	2.20741300	-1.43482600
H	0.09325800	2.42568000	-0.96997900
C	2.46947300	1.30433500	-0.20356600
C	3.70906500	0.72687700	-0.32957700
C	2.68377400	-1.33504400	-1.16097400
C	3.85945400	-0.60961500	-0.90820500
H	2.78290900	-2.38735700	-1.40383700
C	6.08189800	0.73079000	-0.00186600
C	6.15230900	-0.49417600	-0.62167200
H	6.94083300	1.27006800	0.37281400
H	7.11850500	-0.96717500	-0.76181500
N	-4.72530000	1.09399400	-0.64676500
N	-4.34588700	-1.18309800	0.90415800
N	4.85537600	1.31150500	0.16941000
N	5.07220300	-1.17973200	-1.05082200
H	4.77034600	2.23418700	0.57181100
H	-4.18375500	-1.99969900	1.47704400
O	2.26036500	2.38515700	0.63674700

O	-1.80429700	-2.27050300	1.17310700
C	2.05347500	2.02214200	2.04965800
H	3.04524000	2.01328600	2.51596100
H	1.50389300	2.87315400	2.45673400
C	1.35799600	0.68800400	2.41626000
H	1.77434900	-0.11791900	1.80650200
H	1.69972500	0.47647200	3.43899900
C	-0.18372500	0.64925900	2.41446700
H	-0.56869800	0.90664500	1.43201300
H	-0.53861000	1.44187700	3.08569400
C	-0.72474400	-1.98611400	2.12122400
H	-0.79667600	-2.83092800	2.80697900
H	0.23106200	-2.06060400	1.60024800
C	-0.82681000	-0.67041100	2.92691500
H	-1.88807300	-0.47928100	3.12302500
H	-0.39030500	-0.89276300	3.90992100

***trans*-B-C6**

The lowest vibrational frequency: 38.76 cm^{-1}

C	-5.59703500	-0.73338000	0.43709400
C	-3.25174400	-0.78827000	-0.02967500
C	-3.39789100	0.55187800	-0.59038600
C	-5.67390200	0.49103400	-0.18638500
C	-2.02516100	-1.40353700	0.03244400
C	-2.21791200	1.24967500	-0.89178300
C	-0.96400500	0.62819100	-0.80726400
C	-0.89880700	-0.81261700	-0.61204600
C	0.28581400	-1.48692800	-0.88839400
H	0.29515900	-2.57208500	-0.90006300
C	1.50704400	-0.78635700	-1.01166700
C	1.46554500	0.62219700	-0.65062700
C	0.26715100	1.31698200	-0.71915500
H	-6.44584900	-1.24717000	0.86682000
H	-6.63573900	0.98422100	-0.27849500
H	-2.29904400	2.30586800	-1.12345200
H	0.26376000	2.39242200	-0.58069700
C	2.65682400	1.16344900	-0.08125100
C	3.87107500	0.57621800	-0.34082100
C	2.74679100	-1.38509900	-1.27839500
C	3.95284600	-0.71111400	-1.03069900
H	2.80461700	-2.41116500	-1.62475800
C	6.26170000	0.51656400	-0.18479300
C	6.26181700	-0.66288800	-0.89074000
H	7.15637700	1.01324500	0.16440300
H	7.20495000	-1.14367200	-1.12794000
N	-4.60286800	1.15198500	-0.67026900
N	-4.38039800	-1.34419500	0.53665000
N	5.06354000	1.10633200	0.11160600
N	5.13962600	-1.29314100	-1.29575600
H	5.02853200	2.00171100	0.57794000
H	-4.27495500	-2.23960000	0.99297500
O	2.54291000	2.17407000	0.86515000

O	-1.88461200	-2.51711900	0.84683000
C	2.51673000	1.64036900	2.23399400
H	3.52282800	1.26663400	2.45449700
H	2.34352300	2.52338200	2.85232500
C	1.48947100	0.52577000	2.54085500
H	1.35316300	-0.08057100	1.64649800
H	1.96548500	-0.14662400	3.26366900
C	0.12706800	0.99152000	3.10171100
H	-0.06021300	2.01862900	2.76759400
H	0.20126800	1.05073000	4.19513400
C	-0.90534500	-2.36744500	1.92382100
H	-0.88959900	-3.36238400	2.37178700
H	0.07539500	-2.18389200	1.48284000
C	-1.23067600	-1.33482700	3.02085000
H	-2.24046100	-1.55778200	3.38416900
H	-0.56706100	-1.58366900	3.86040100
C	-1.14132100	0.18993000	2.72026400
H	-1.35184200	0.37436200	1.67044000
H	-1.96648300	0.67032400	3.25765000

***cis*-C1**

The lowest vibrational frequency: 46.08 cm^{-1}

C	-5.55712200	-0.49548200	0.31830900
C	-3.58334900	-0.25369400	-0.86106400
C	-2.97723800	0.40746800	0.29861000
C	-5.00633900	-0.00808200	1.48015300
C	-2.68831300	-0.67606500	-1.86995300
C	-1.66493000	0.88203000	0.24547700
C	-1.02725400	0.92103800	-1.00749900
C	-1.35629600	-0.26570200	-1.79792400
C	-0.20064700	-1.11062800	-1.85904100
H	-0.37911400	-2.17603000	-1.75027800
C	0.98681700	-0.57408300	-1.38477700
C	1.29203400	0.84185900	-1.55213800
C	0.18078800	1.62538500	-1.25532200
H	-2.99537600	-1.49725700	-2.50722500
H	-6.59381600	-0.81514600	0.30921900
H	-5.52463100	0.06019200	2.42564700
H	0.30010000	2.63712000	-0.88066700
C	2.68952700	1.20499500	-1.51972300
C	3.49952700	0.41400500	-0.74523500
C	1.53851100	-0.89758800	-0.09746500
C	2.87093300	-0.53676800	0.21276300
H	3.04110900	2.12577500	-1.97362500
C	5.51569700	0.10583400	0.51201000
C	4.79899900	-0.55503700	1.47516500
H	6.57675100	0.30444700	0.57422700
H	5.28811200	-0.88058700	2.38630900
N	-3.70489800	0.41029900	1.44501100
N	-4.86317000	-0.65554500	-0.82469300
N	4.86180500	0.55727000	-0.60339700
N	3.48710600	-0.87213900	1.33966900
H	5.35591100	1.14373300	-1.26110200
H	-3.24299600	0.74507500	2.28163500
O	-0.95494700	1.00683900	1.41925000

O	0.55552700	-0.97799900	0.93442700
C	0.33268400	0.23737500	1.62740800
H	0.25729000	0.00349400	2.68665000
H	1.13452100	0.94321700	1.42447900

***cis*-C2**

The lowest vibrational frequency: 45.87 cm^{-1}

C	-4.21332300	1.10550800	3.25130900
C	-3.04664000	0.00624400	1.58194700
C	-2.07346400	1.10422900	1.55403600
C	-3.25954600	2.09355200	3.37198500
C	-2.68233400	-1.16830200	0.90927400
C	-1.01156400	1.08406200	0.65053100
C	-1.01359100	0.11211800	-0.36488900
C	-1.51795500	-1.17410000	0.11302100
C	-0.51034700	-2.15501500	0.05720700
H	-0.53965400	-2.97372700	0.76854300
C	0.71072200	-1.82644600	-0.56926400
C	0.69321100	-0.91125400	-1.70977300
C	-0.18975000	0.15063700	-1.51435700
H	-3.18941000	-2.08886800	1.17440800
H	-5.08825200	1.13153600	3.89347700
H	-3.29357900	2.90206100	4.08728100
H	-0.02847400	1.09242000	-2.02848000
C	1.78459600	-0.96668100	-2.62218000
C	2.96396300	-1.51420200	-2.16269100
C	1.97097600	-1.79233000	0.06337300
C	3.15273300	-1.78502200	-0.72288400
H	1.73564400	-0.45545200	-3.57892600
C	5.32887600	-1.87346100	-2.38723400
C	5.43339500	-1.96356200	-1.02310900
H	6.16190600	-1.94975300	-3.07187900
H	6.40664000	-2.09660800	-0.56319000
N	-2.18554900	2.04705200	2.52248100
N	-4.11644400	0.06810300	2.40653900
N	4.09073100	-1.65765900	-2.93215500
N	4.36941500	-1.90847600	-0.19232600
H	4.01062500	-1.49898400	-3.92688900
H	-1.44923700	2.73924100	2.58026000
O	0.14832300	1.79012600	0.95718400

O	2.05617900	-1.50720700	1.41398200
C	1.26273300	-0.37050100	1.88986100
H	0.21962800	-0.67335000	1.97506000
H	1.65305800	-0.22165700	2.89593700
C	1.37424800	0.96339800	1.07208000
H	1.74207600	0.76007800	0.06786400
H	2.06937900	1.64846300	1.55496900

***cis*-C3**

The lowest vibrational frequency: 43.15 cm^{-1}

C	-5.28803700	-1.09724200	-0.26139200
C	-3.09269200	-0.81805500	-0.93646800
C	-2.82894500	-0.01818500	0.26702900
C	-5.07249300	-0.47170300	0.94753300
C	-1.97277600	-1.22213000	-1.67669800
C	-1.57658900	0.53639300	0.48941300
C	-0.61706200	0.49172300	-0.54888400
C	-0.69882900	-0.71338200	-1.36425000
C	0.53669200	-1.38950400	-1.43854300
H	0.53412800	-2.46339200	-1.58734900
C	1.68811700	-0.76681800	-0.94604900
C	1.75736400	0.68649700	-0.91748600
C	0.53408400	1.29317900	-0.60983900
H	-2.09265800	-2.03581100	-2.38272200
H	-6.27451000	-1.48750500	-0.49053000
H	-5.81834300	-0.35283200	1.72008800
H	0.52058900	2.28528800	-0.17108300
C	3.03800700	1.29819700	-0.83677000
C	4.09860200	0.53052900	-0.40298900
C	2.60343400	-1.37603700	-0.05010700
C	3.87169000	-0.80979900	0.17379500
H	3.14458500	2.36961700	-0.98029500
C	6.34568300	0.35129100	0.42495200
C	6.00199500	-0.81543700	1.06722900
H	7.32484900	0.80704200	0.46392200
H	6.73469100	-1.32426200	1.68483900
N	-3.82390800	0.02743400	1.19604800
N	-4.32839800	-1.30198600	-1.17812100
N	5.38268400	0.99835800	-0.30014400
N	4.78831200	-1.38723700	0.96722000
H	5.59224100	1.90258400	-0.70016600
H	-3.61687200	0.49403800	2.06999800
O	-1.15050000	0.76969100	1.80126000

O	2.07633800	-2.35348300	0.77000900
C	1.73930300	-1.87846600	2.11536700
H	1.12432100	-2.68490300	2.52088600
H	2.67342900	-1.85157000	2.68093600
C	1.04017200	-0.49083600	2.26935600
H	1.38217900	0.17547500	1.48247800
H	1.42917700	-0.05269600	3.19429400
C	-0.50761100	-0.45496300	2.33827500
H	-0.83602500	-0.49291400	3.37921200
H	-0.94006700	-1.31197900	1.81600000

***cis*-C4**

The lowest vibrational frequency: 41.13 cm^{-1}

C	-5.36783800	-1.18145700	0.00300300
C	-3.18056000	-0.85433500	-0.68095900
C	-2.95196900	0.01842800	0.46658500
C	-5.18038300	-0.46945900	1.17317300
C	-2.06232900	-1.24704900	-1.41290000
C	-1.72464400	0.62366700	0.66568000
C	-0.72443500	0.51448600	-0.33023300
C	-0.79032100	-0.69070100	-1.13648700
C	0.44102300	-1.34303900	-1.30473000
H	0.45237400	-2.38825800	-1.59232900
C	1.62372000	-0.74306000	-0.84966700
C	1.66698300	0.69403100	-0.68232600
C	0.44730800	1.28969600	-0.34733900
H	-2.16865700	-2.07021600	-2.11041300
H	-6.34071300	-1.61983700	-0.19762400
H	-5.93858500	-0.33106200	1.93064700
H	0.43415400	2.28853200	0.07679300
C	2.93960700	1.32558500	-0.59299500
C	4.05624800	0.55149300	-0.37233900
C	2.68151900	-1.45917100	-0.22896500
C	3.94124300	-0.87259300	-0.04292300
H	3.00916900	2.41002900	-0.60355300
C	6.38487200	0.34828500	0.20102700
C	6.15667100	-0.94392000	0.61483300
H	7.34522000	0.84229600	0.24593800
H	6.97284000	-1.52039400	1.03854900
N	-3.95739900	0.09839600	1.39482700
N	-4.40830300	-1.40289600	-0.90349200
N	5.32945600	1.07393100	-0.29086500
N	4.96538600	-1.55901500	0.51912500
H	5.46211500	2.04763300	-0.52255000
H	-3.76438000	0.61795000	2.24052200
O	-1.42030700	1.09010300	1.93299600

O	2.33296300	-2.64863300	0.36062200
C	2.17829100	-2.59166300	1.81508700
H	1.53865800	-3.44765100	2.03959900
H	3.16633700	-2.77468100	2.24546000
C	1.62028300	-1.29465400	2.45163300
H	2.22462500	-0.45263300	2.10180300
H	1.85163600	-1.38578300	3.52030200
C	0.11542400	-0.96022600	2.27866600
H	-0.18698100	-1.23461500	1.27133600
H	-0.48520000	-1.58034600	2.95287100
C	-0.18985500	0.53800400	2.53282200
H	-0.32908500	0.74074100	3.59575400
H	0.64579900	1.14524400	2.18229500

***cis*-C5**

The lowest vibrational frequency: 37.65 cm^{-1}

C	-6.51493800	0.06345700	-0.29288100
C	-4.23185600	-0.13774700	-0.62565000
C	-4.03297300	1.21529200	-0.12144000
C	-6.39373100	1.32857400	0.24903600
C	-3.09645400	-0.89816800	-0.88397300
C	-2.77039800	1.76939300	-0.04836600
C	-1.66256100	1.09215900	-0.61117200
C	-1.79945900	-0.34128300	-0.78098800
C	-0.62685400	-1.08665700	-0.58866800
H	-0.69723700	-2.15489300	-0.41865900
C	0.60198400	-0.44521400	-0.39417000
C	0.75354500	0.93680500	-0.79009400
C	-0.41633700	1.69981800	-0.82021200
H	-3.22576700	-1.95386300	-1.09504500
H	-7.50206300	-0.38090500	-0.37731700
H	-7.22496100	1.91986400	0.60597800
H	-0.35421200	2.78198500	-0.85700400
C	2.06836300	1.47248300	-0.89360500
C	3.13171500	0.75707900	-0.39493800
C	1.63415900	-0.98649800	0.41960500
C	2.93113600	-0.46003800	0.39368100
H	2.21383500	2.47039200	-1.29896200
C	5.45190100	0.60763400	0.22935100
C	5.15069400	-0.46285200	1.04195500
H	6.44208500	1.02615800	0.11607900
H	5.93809000	-0.92133400	1.63193000
N	-5.14350300	1.87661100	0.34694500
N	-5.48250300	-0.67749100	-0.71494700
N	4.43725600	1.19813400	-0.47900800
N	3.92329400	-0.99534400	1.15075900
H	4.62705800	2.02823800	-1.02119900
H	-5.01017100	2.81463200	0.69869600
O	-2.56792200	2.92342600	0.69523200

O	1.24188100	-1.91196800	1.34813400
C	-2.27880500	2.65535500	2.10623900
H	-2.36197100	3.64710300	2.55384400
H	-3.08621700	2.03181600	2.50960900
C	-0.90081700	2.05395300	2.47008200
H	-0.15445900	2.46039900	1.78244000
H	-0.64966600	2.47054400	3.45518500
C	-0.75918800	0.51428900	2.55382400
H	-1.07225600	0.05231900	1.62236100
H	-1.44192800	0.13105000	3.32314400
C	0.68599000	0.08059700	2.89276300
H	0.88203800	0.29850500	3.95127500
H	1.39219000	0.70948100	2.34200100
C	1.09878200	-1.39652600	2.71145000
H	2.06325000	-1.54242100	3.20494600
H	0.37008100	-2.06928000	3.16900800

***cis*-C6**

The lowest vibrational frequency: 37.71 cm^{-1}

C	-5.81522900	-0.59716400	-0.04705800
C	-3.53207000	-0.63937100	-0.42955000
C	-3.41979600	0.72954300	0.04931700
C	-5.76840600	0.67595300	0.49058400
C	-2.35201100	-1.31952100	-0.70349200
C	-2.20478100	1.38488500	0.08417800
C	-1.04971200	0.76848700	-0.46094000
C	-1.09528800	-0.67164500	-0.63650800
C	0.12892600	-1.35018800	-0.58030900
H	0.13636100	-2.43101200	-0.50131400
C	1.34223500	-0.65729500	-0.49112100
C	1.36787300	0.76055200	-0.77319400
C	0.15265100	1.44976700	-0.69347700
H	-2.41026400	-2.38044500	-0.91984600
H	-6.77126400	-1.10835800	-0.10802300
H	-6.62898600	1.20579400	0.87367400
H	0.15029800	2.53396000	-0.73212100
C	2.62562700	1.39634800	-0.95407700
C	3.78567600	0.70581000	-0.69211300
C	2.52465700	-1.25487700	0.02521100
C	3.77169000	-0.63347400	-0.10967600
H	2.66178800	2.44173800	-1.25033400
C	6.18176900	0.63368700	-0.45100900
C	6.06971200	-0.59425900	0.16323300
H	7.11820900	1.14562100	-0.62234100
H	6.96547700	-1.09442400	0.51817300
N	-4.56020200	1.31250800	0.54795700
N	-4.74418200	-1.26736400	-0.48812100
N	5.03728600	1.26270900	-0.86938600
N	4.90447400	-1.23118100	0.35237200
H	5.09657500	2.18321800	-1.27904000
H	-4.46928200	2.24357700	0.93086400
O	-2.14553600	2.57653600	0.77894200

O	2.35868300	-2.41512400	0.72763700
C	2.60011100	-2.35047700	2.16435700
H	2.03730400	-3.20061400	2.55647700
H	3.66538000	-2.52783300	2.32911400
C	2.19659800	-1.04380100	2.86453600
H	2.77766500	-0.22742700	2.42431300
H	2.56894700	-1.13295900	3.89274600
C	-1.19031700	2.63225500	1.89718600
H	-0.23403700	2.97402600	1.49612000
H	-1.59406000	3.43281000	2.51770300
C	-0.99825700	1.32082700	2.70147700
H	-1.56993900	0.52617000	2.21697100
H	-1.44702800	1.43727500	3.69299000
C	0.47832900	0.86737700	2.83333500
H	1.03805900	1.25135200	1.97591400
H	0.93238800	1.33291700	3.71730900
C	0.69690000	-0.65999200	2.88022200
H	0.19385700	-1.10664900	2.02012700
H	0.21331600	-1.08547800	3.76792700