

Supporting Information for:

## Can a Wanzlick-like equilibrium exist between dicoordinate borylenes and diborenes?

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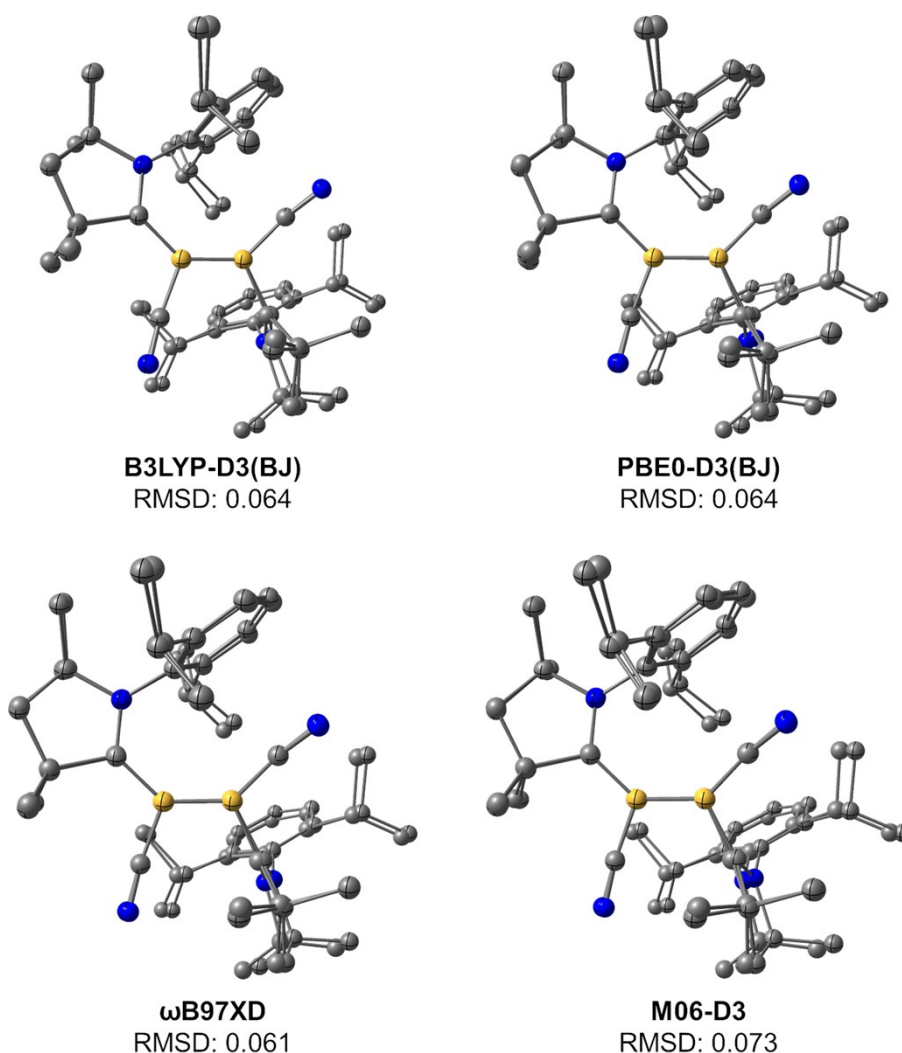
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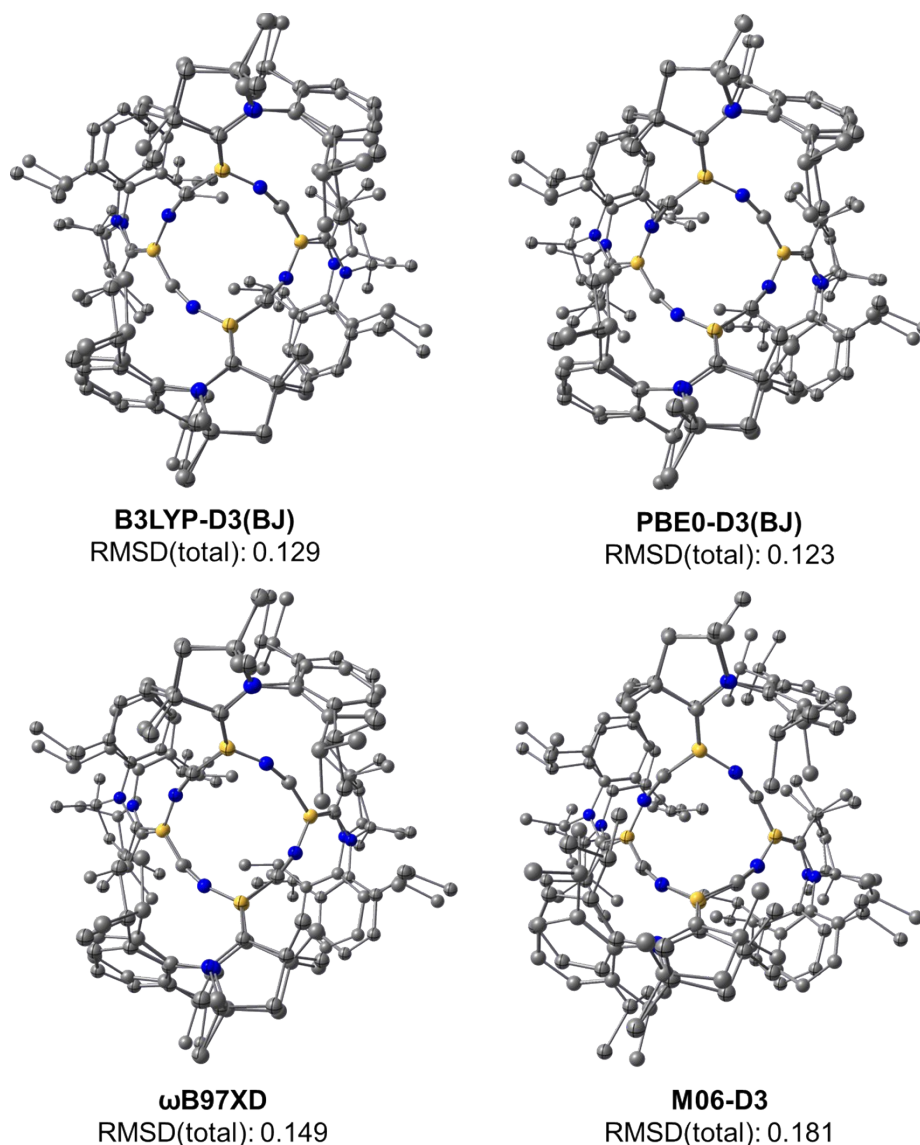
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## S1: Benchmark studies

In order to choose appropriate methods for optimising the structures investigated herein, we performed geometry optimisations of **2-dib** and **4cl** considering four distinct DFT functionals, namely B3LYP-D3(BJ), PBE0-D3(BJ),  $\omega$ B97XD, and M06-D3, and compared the optimised results with the X-ray crystal structures. Alrich's def2-SVP basis set was used in these calculations. A visual comparison of the geometries and the corresponding root-mean-square deviation (RMSD) values, which were obtained excluding hydrogen atoms and reported per unit of monomer, are shown in Figures S1 and S2. The RMSD values are further compared in Table S1. Our results show that, on average, B3LYP-D3(BJ) and PBE0-D3(BJ) presented the least RMSD values, followed by  $\omega$ B97XD. These three functionals are, therefore, fit for geometry optimisations of the target molecules of this investigation.



**Figure S1.** Comparison of the X-ray crystal structure of **2-dib** and the corresponding optimised geometries using the B3LYP-D3(BJ) (top left), PBE0-D3(BJ) (top right),  $\omega$ B97XD (bottom left), and M06-D3 (bottom right) functionals with the def2-SVP basis set. The RMSD values are reported per unit of monomer and were calculated considering all elements but hydrogen.



**Figure S2.** Comparison of the X-ray crystal structure of **4cl** and the corresponding optimised geometries using the B3LYP-D3(BJ) (top left), PBE0-D3(BJ) (top right),  $\omega$ B97XD (bottom left), and M06-D3 (bottom right) functionals with the def2-SVP basis set. The RMSD values are reported per unit of monomer and were calculated considering all elements but hydrogen.

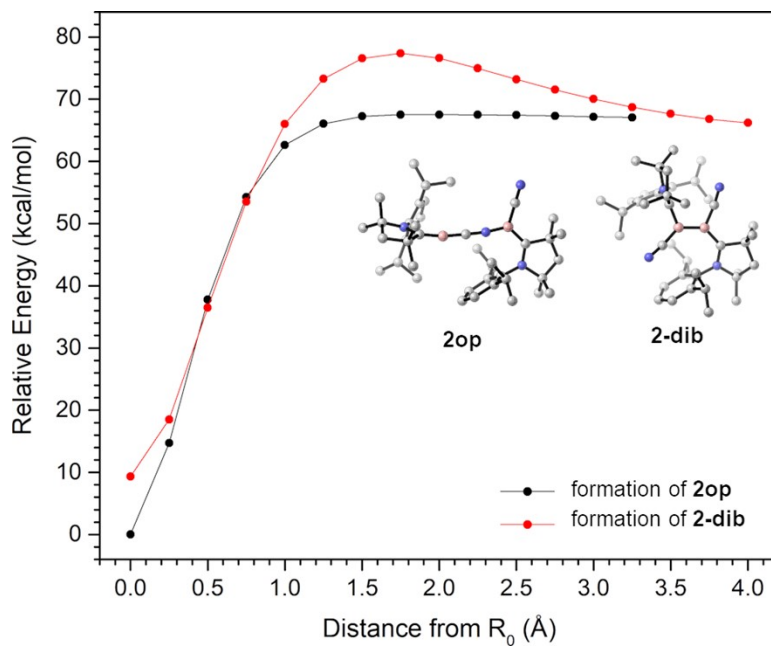
<b>Table S1.</b> Root-mean-square deviation (RMSD) values for each level of theory. The RMSD values are reported per unit of monomer and were calculated considering all elements but hydrogen. The average RMSD values are also shown.			
Functional	<b>2-dib</b>	<b>4cl</b>	Average
B3LYP-D3(BJ)	0.064	0.129	0.097
PBE0-D3(BJ)	0.064	0.123	0.093
$\omega$ B97XD	0.061	0.149	0.105
M06-D3	0.073	0.181	0.127

We then focused on energetic properties, aiming at choosing appropriate methods for depicting the free energies of the reaction pathways investigated herein. Free energy calculations for all species involved in the oligomerisation of **1** to **5cl** and the dimerisation of **1** to **2-dib** were calculated at distinct DFT/def2-TZVP+SMD(benzene)//B3LYP-D3(BJ)/def2-SVP levels of theory (DFT = B3LYP-D3(BJ),  $\omega$ B97XD, PBE0-D3(BJ), and M06-D3). Inspection of Table S2 shows that B3LYP-D3(BJ) and  $\omega$ B97XD present the least deviation energies. Furthermore, comparison of the electronic energies of the distinct DFT functionals with those obtained by high-level DLPNO-CCSD(T)/cc-pVDZ calculations evidences that the  $\omega$ B97XD is the most appropriate for computing the energies of the reaction pathways investigated herein.

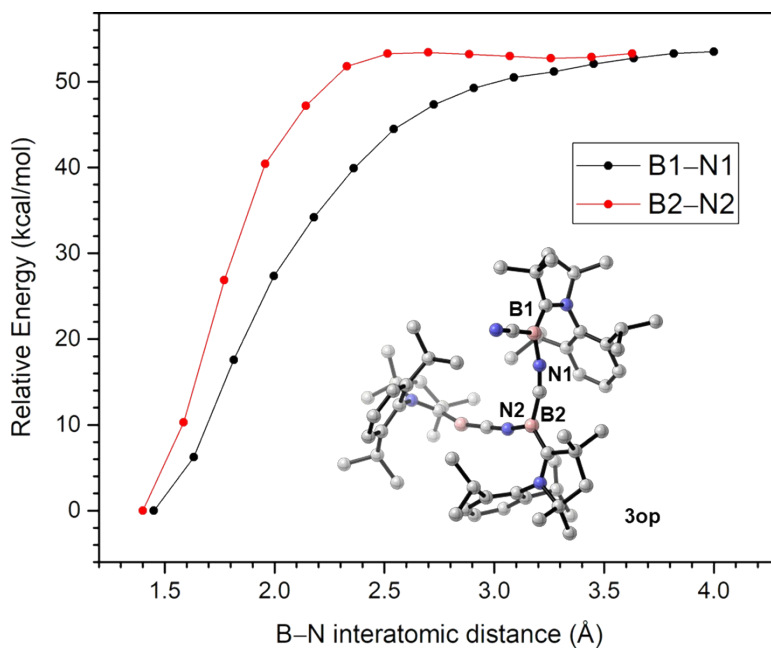
**Table S2.** Comparison between the free energy profile of the oligomerisation of **1** to **5cl** and the dimerisation of **1** to **2-dib** at distinct DFT/def2-TZVP+SMD(benzene)//B3LYP-D3(BJ)/def2-SVP levels of theory (DFT = B3LYP-D3(BJ),  $\omega$ B97XD, PBE0-D3(BJ), and M06-D3). The coupled-cluster values were obtained at the DLPNO-CCSD(T)/cc-pVDZ+SMD(benzene)//B3LYP-D3(BJ)/def2-SVP level.

	DLPNO-CCSD(T)	$\omega$ B97XD	B3LYP-D3(BJ)	PBE0-D3(BJ)	M06-D3
<b>1</b>	0	0	0	0	0
<b>2op</b>	-52	-56	-59	-63	-63
<b>TS2<sub>op-cl</sub></b>	-18	-11	-21	-24	-18
<b>2cl</b>	-26	-22	-28	-36	-26
<b>TS1-2-dib</b>	14	11	11	12	6
<b>2-dib</b>	-68	-67	-60	-66	-66
<b>Average deviation (kcal mol<sup>-1</sup>) with respect to DLPNO-CCSD(T)</b>	-	3.8	4.6	6.2	4.2
<b>3op</b>	-	-94	-96	-103	-107
<b>TS3<sub>op-cl</sub></b>	-	-76	-80	-88	-91
<b>3cl</b>	-	-113	-112	-125	-125
<b>4op</b>	-	-135	-134	-147	-153
<b>TS4<sub>op-cl</sub></b>	-	-126	-130	-141	-143
<b>4cl</b>	-	-173	-169	-185	-192
<b>5op</b>	-	-168	-166	-182	-197
<b>5cl</b>	-	-177	-170	-192	-203

## S2: CAAC-stabilised cyanoborylene systems I: geometry scans



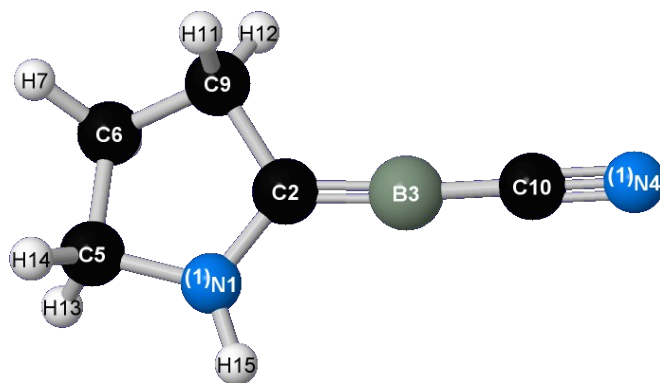
**Figure S3.** Geometry scan following the formation of **2op** (black) and **2-dib** (red) from two isolated **1** at the B3LYP/def2SVP level of theory.



**Figure S4.** Two distinct geometry scans following the formation of **3op** from isolated **1** and **2op** at the B3LYP/def2SVP level of theory.

**S3: CAAC-stabilised cyanoborylene systems II: NBO/NRT results**

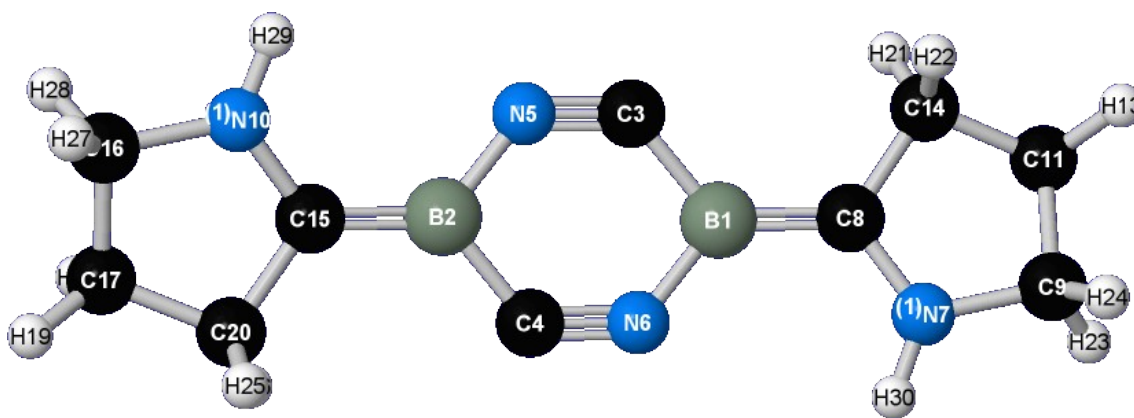
**Table S3.** NRT bond orders of a truncated model system of **1** at the B3LYP/def2SVP level.



**1**

Atom 1	Atom 2	NRT bond order
N1	C2	1.31
N1	C5	1.02
N1	H15	0.98
C2	B3	1.67
C2	C9	0.97
B3	C10	1.34
N4	C10	2.62
C5	C6	1.03
C5	H13	0.95
C5	H14	0.95
C6	H7	0.98
C6	H8	0.95
C6	C9	1.03
C9	H11	0.95
C9	H12	0.97

**Table S4.** NRT bond orders of a truncated model system of **2cl** at the B3LYP/def2SVP level.

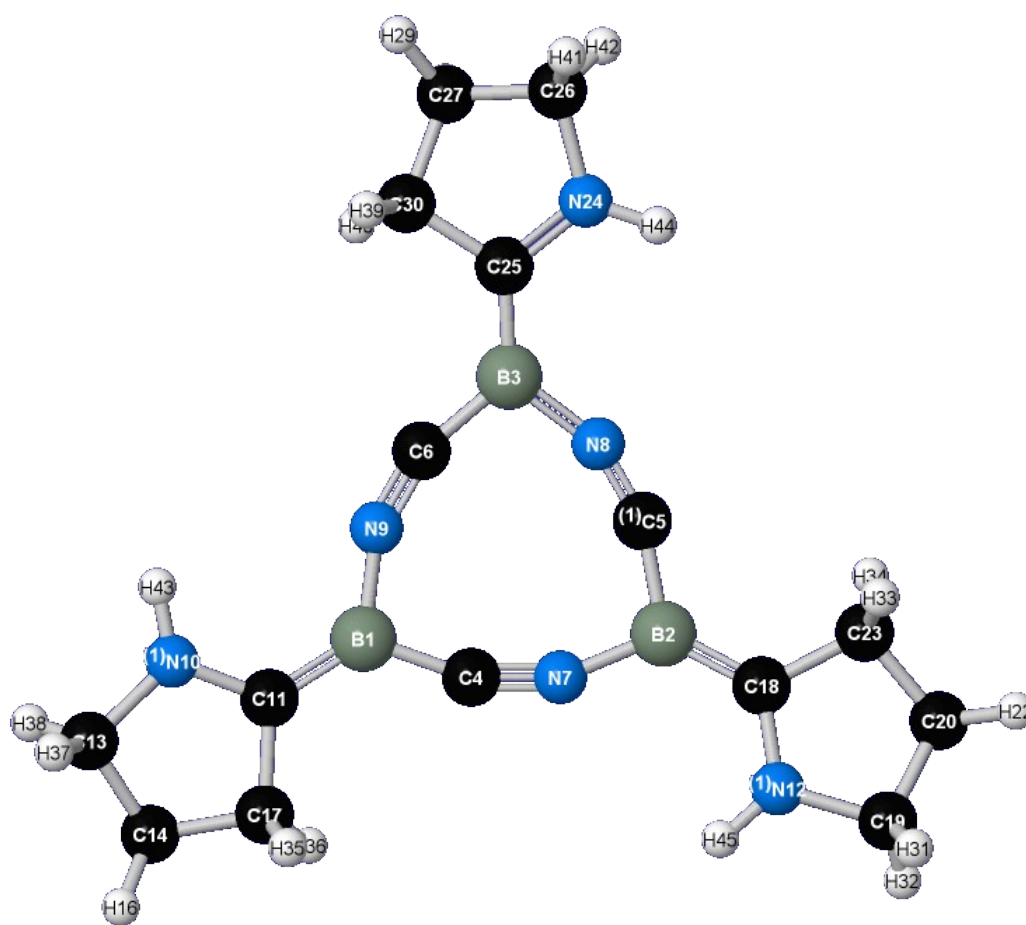


**2cl**

Atom 1	Atom 2	NRT bond order (alpha)	NRT bond order (beta)	NRT bond order (total)
B1	C3	0.62	0.63	1.25
B1	N6	0.59	0.58	1.18
B1	C8	0.70	0.68	1.38
B2	C4	0.63	0.62	1.25
B2	N5	0.58	0.59	1.18
B2	C15	0.68	0.70	1.38
C3	C4	0.01	0.01	0.02
C3	N5	1.22	1.20	2.41
C4	N6	1.20	1.22	2.41
N5	N6	0.01	0.01	0.02
N7	C8	0.79	0.80	1.59
N7	C9	0.51	0.51	1.01
N7	H30	0.50	0.50	1.00
C8	C14	0.50	0.50	1.01
C9	C11	0.51	0.51	1.02
C9	H23	0.49	0.49	0.99
C9	H24	0.49	0.49	0.98
N10	C15	0.80	0.79	1.59
N10	C16	0.51	0.51	1.01
N10	H29	0.50	0.50	1.00
C11	H12	0.49	0.49	0.98
C11	H13	0.50	0.50	1.00
C11	C14	0.50	0.50	1.01
C14	H21	0.50	0.50	1.00
C14	H22	0.49	0.49	0.98
C15	C20	0.50	0.50	1.01

C16	C17	0.51	0.51	1.02
C16	H27	0.49	0.49	0.98
C16	H28	0.49	0.49	0.99
C17	H18	0.49	0.49	0.98
C17	H19	0.50	0.50	1.00
C17	C20	0.50	0.50	1.01
C20	H25	0.49	0.49	0.98
C20	H26	0.50	0.50	1.00

**Table S5.** NRT bond orders of a truncated model system of **3cl** at the B3LYP/def2SVP level.

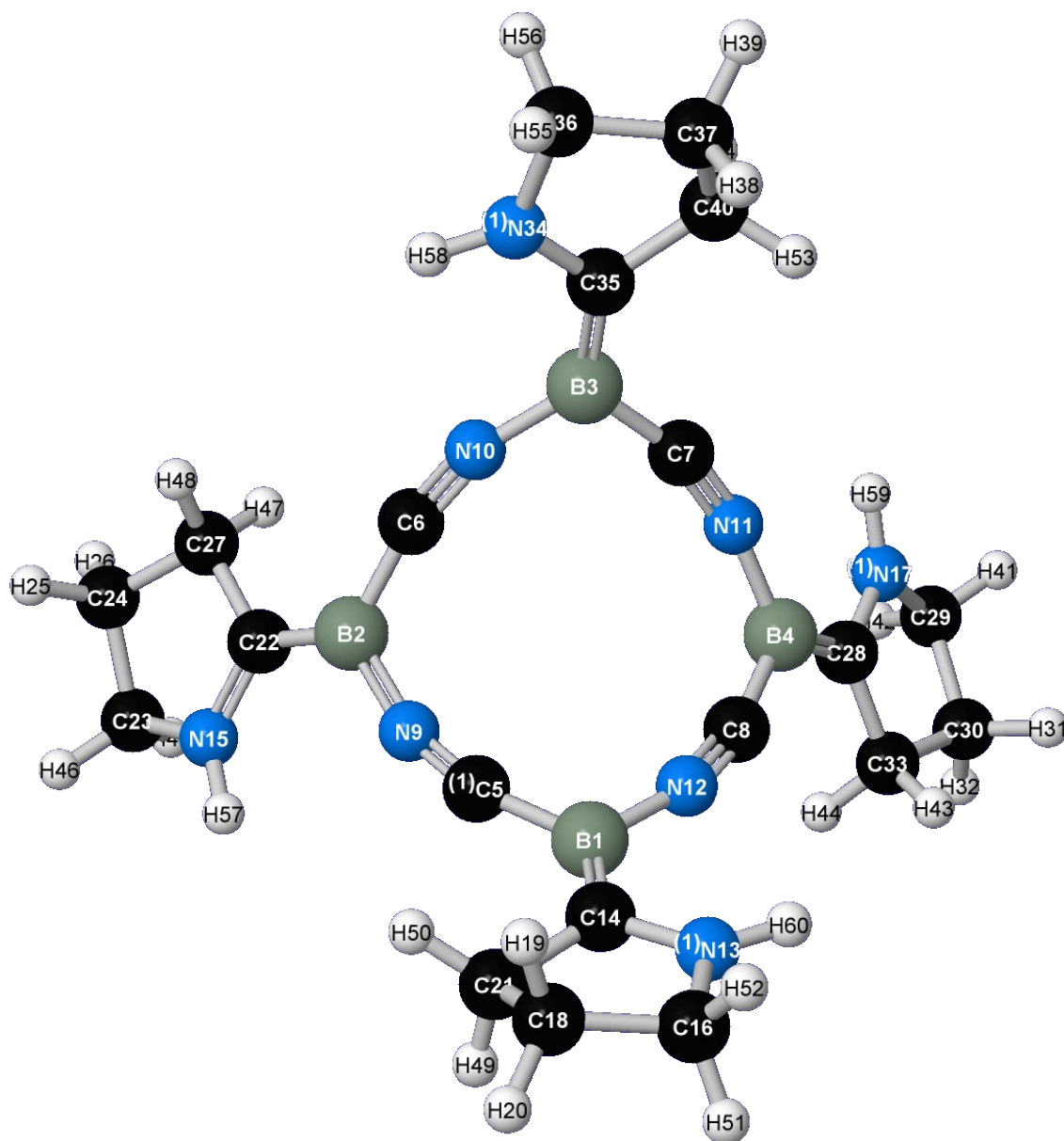


Atom 1	Atom 2	NRT bond order
B1	C4	1.18
B1	N9	1.13
B1	C11	1.49
B2	C5	1.18
B2	N7	1.13



B2	C18	1.49
B3	C6	1.18
B3	N8	1.13
B3	C25	1.49
C4	N7	2.67
C5	N8	2.67
C6	N9	2.67
N10	C11	1.29
N10	C13	1.00
N10	H43	1.00
C11	C17	1.01
N12	C18	1.29
N12	C19	1.00
N12	H45	1.00
C13	C14	1.03
C13	H37	0.98
C13	H38	0.99
C14	H15	0.98
C14	H16	1.00
C14	C17	1.00
C17	H35	0.98
C17	H36	1.00
C18	C23	1.01
C19	C20	1.03
C19	H31	0.98
C19	H32	0.99
C20	H21	0.98
C20	H22	1.00
C20	C23	1.00
C23	H33	0.98
C23	H34	1.00
N24	C25	1.29
N24	C26	1.00
N24	H44	1.00
C25	C30	1.01
C26	C27	1.03
C26	H41	0.98
C26	H42	0.99
C27	H28	0.98
C27	H29	1.00
C27	C30	1.00
C30	H39	0.98
C30	H40	1.00

**Table S6.** NRT bond orders of a truncated model system of **4cl** at the B3LYP/def2SVP level.



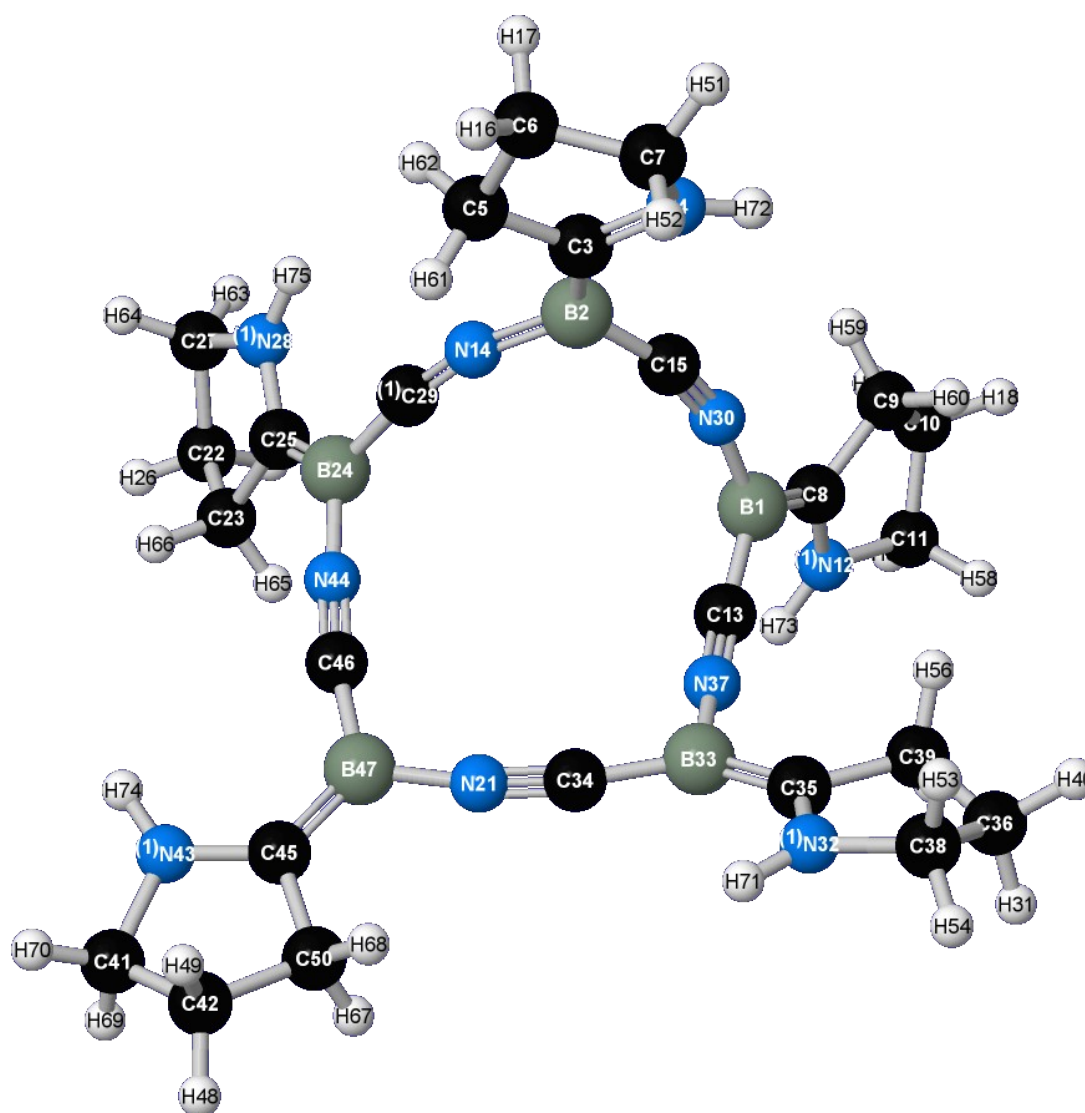
**4cl**

Atom 1	Atom 2	NRT bond order
B1	C5	1.17
B1	N12	1.06
B1	C14	1.58
B2	C6	1.17
B2	N9	1.06
B2	C22	1.58
B3	C7	1.17
B3	N10	1.06

B3	C35	1.58
B4	C8	1.17
B4	N11	1.06
B4	C28	1.58
C5	N9	2.73
C6	N10	2.73
C7	N11	2.73
C8	N12	2.73
N13	C14	1.30
N13	C16	0.96
N13	H60	1.00
C14	C21	1.04
N15	C22	1.29
N15	C23	0.96
N15	H57	1.00
C16	C18	1.04
C16	H51	1.00
C16	H52	1.00
N17	C28	1.29
N17	C29	0.96
N17	H59	1.00
C18	H19	1.00
C18	H20	1.00
C18	C21	0.96
C21	H49	1.00
C21	H50	1.00
C22	C27	1.04
C23	C24	1.04
C23	H45	1.00
C23	H46	1.00
C24	H25	1.00
C24	H26	1.00
C24	C27	0.96
C27	H47	1.00
C27	H48	1.00
C28	C33	1.04
C29	C30	1.04
C29	H41	1.00
C29	H42	1.00
C30	H31	1.00
C30	H32	1.00
C30	C33	0.96
C33	H43	1.00
C33	H44	1.00
N34	C35	1.30
N34	C36	0.96

N34	H58	1.00
C35	C40	1.04
C36	C37	1.04
C36	H55	1.00
C36	H56	1.00
C37	H38	1.00
C37	H39	1.00
C37	C40	0.96
C40	H53	1.00
C40	H54	1.00

**Table S7.** NRT bond orders of a truncated model system of **5cl** at the B3LYP/def2SVP level.



**5cl**

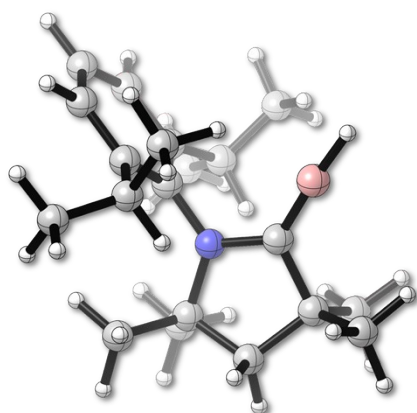
Atom 1	Atom 2	NRT bond order
B1	C8	1.59
B1	C13	1.21
B1	N30	1.05
B2	C3	1.59
B2	N14	1.09
B2	C15	1.18
C3	N4	1.25
C3	C5	1.05
N4	C7	0.95
N4	H72	1.00
C5	C6	0.95
C5	H61	1.00
C5	H62	1.00
C6	C7	1.05
C6	H16	1.00
C6	H17	1.00
C7	H51	1.00
C7	H52	1.00
C8	C9	1.05
C8	N12	1.23
C9	C10	0.95
C9	H59	1.00
C9	H60	1.00
C10	C11	1.05
C10	H18	1.00
C10	H19	1.00
C11	N12	0.95
C11	H57	0.99
C11	H58	1.00
N12	H73	1.00
C13	N37	2.75
N14	C29	2.70
C15	N30	2.74
H20	C22	1.00
N21	C34	2.79
N21	B47	1.04
C22	C23	0.95
C22	H26	1.00
C22	C27	1.05
C23	C25	1.05
C23	H65	1.00
C23	H66	1.00
B24	C25	1.58
B24	C29	1.17
B24	N44	1.05

C25	N28	1.28
C27	N28	0.95
C27	H63	1.00
C27	H64	1.00
N28	H75	1.00
H31	C36	1.00
N32	C35	1.24
N32	C38	0.95
N32	H71	1.00
B33	C34	1.17
B33	C35	1.59
B33	N37	1.04
C35	C39	1.05
C36	C38	1.05
C36	C39	0.95
C36	H40	1.00
C38	H53	1.00
C38	H54	1.00
C39	H55	1.00
C39	H56	1.00
C41	C42	1.05
C41	N43	0.95
C41	H69	1.00
C41	H70	1.00
C42	H48	1.00
C42	H49	1.00
C42	C50	0.95
N43	C45	1.23
N43	H74	1.00
N44	C46	2.78
C45	B47	1.61
C45	C50	1.05
C46	B47	1.16
C50	H67	1.00
C50	H68	1.00

**Table S8.** Most relevant NBO second-order perturbation energies  $E^{(2)}$  of **1** and the cyclooligomers **2cl**, **3cl**, **4cl** and **5cl**. For the *ncl* species, the values correspond to mean energies  $\langle E^{(2)} \rangle$  of the *n* individual donor–acceptor interactions. Values are in kcal mol<sup>-1</sup>.

	<b>1</b>	<b>2cl</b>	<b>3cl</b>	<b>4cl</b>	<b>5cl</b>
$CAACN(ip) \rightarrow CAAC C-B(\pi^*)$	35.3	30.3	32.7	34.2	33.1
$CAAC C-B(\pi) \rightarrow C-N(\pi^*)_{  }$	24.5	18.9	25.7	23.4	23.7
$CAAC C-B(\pi) \rightarrow C-N(\pi^*)_{\perp}$	0.0	0.0	2.8	7.2	5.7
$CAAC C-B(\pi) \rightarrow C-N(\pi^*)$ (total)	24.5	18.9	28.5	30.6	29.4
$CAAC C-B(\pi) \rightarrow N-C(\pi^*)_{  }$	-	9.7	13.8	10.6	15.0
$CAAC C-B(\pi) \rightarrow N-C(\pi^*)_{\perp}$	-	1.4	1.2	5.9	2.2
$CAAC C-B(\pi) \rightarrow N-C(\pi^*)$ (total)	-	11.1	15.0	16.5	17.1

**S4: CAAC- and NHC-stabilised [LHB:]**

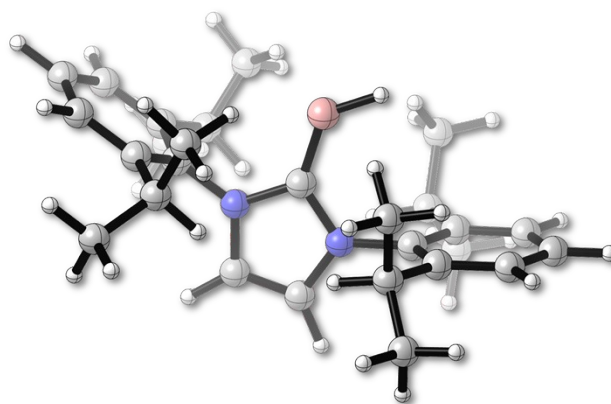


**[LHB:], L = CAAC**

GS: closed-shell singlet

Linear CBH

S-T gap (ad.): +11.0 kcal mol<sup>-1</sup>



**[LHB:], L = NHC**

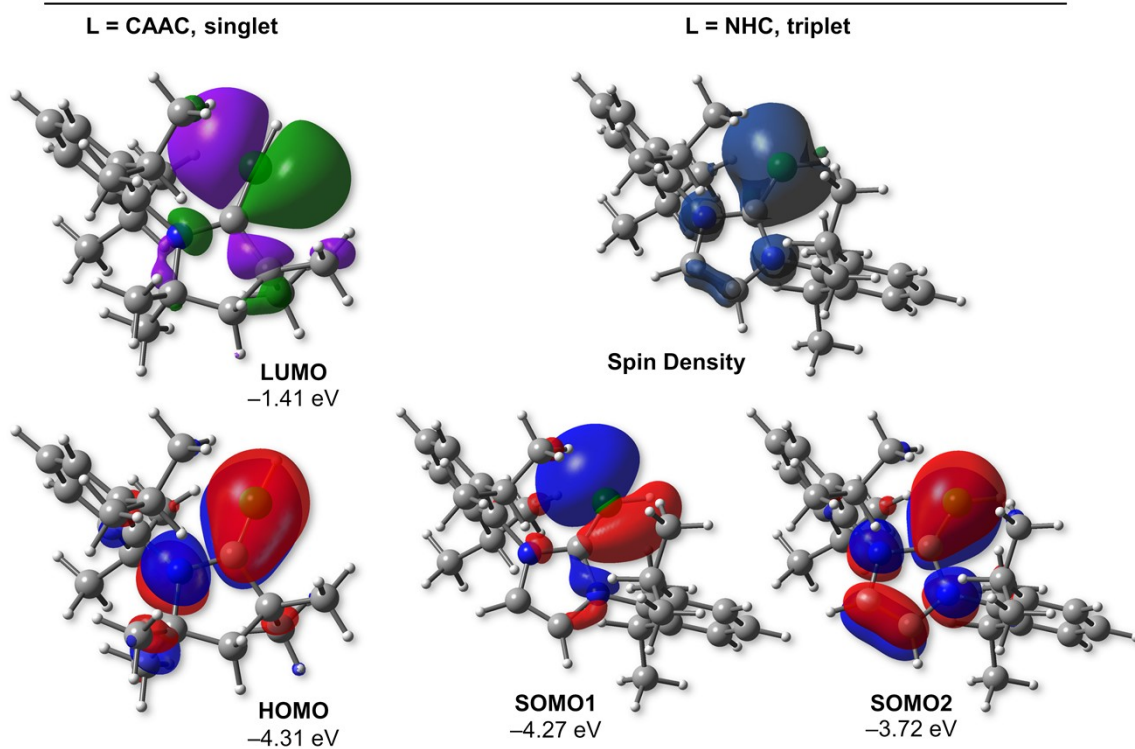
GS: triplet

Bent CBH

S-T gap (ad.): -12.0 kcal mol<sup>-1</sup>

**Figure S5.** Optimised structures and some properties of [LHB:] (L = CAAC, NHC) species. Adiabatic S-T gaps are obtained at the NEVPT2/CASSCF(2,2)/def2-SVP level of theory.

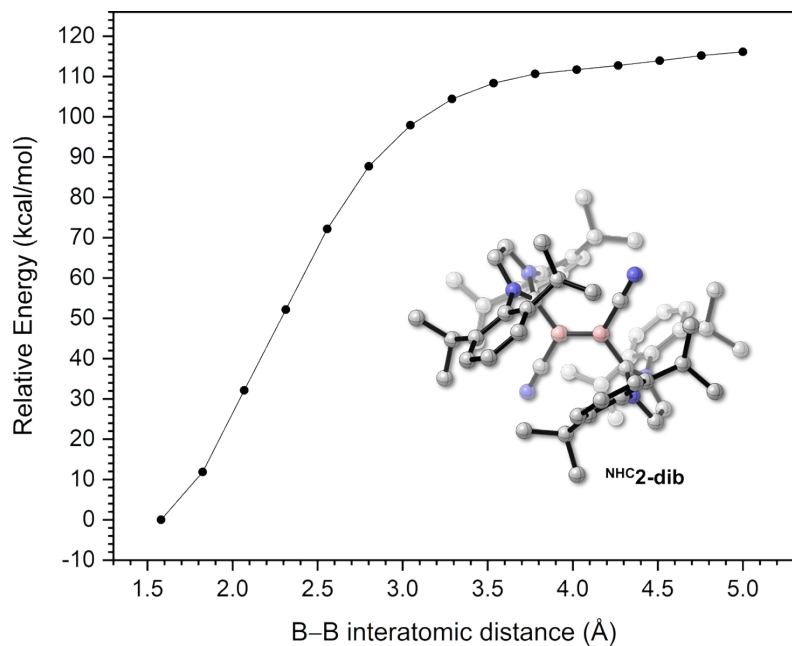
[LHB:] species



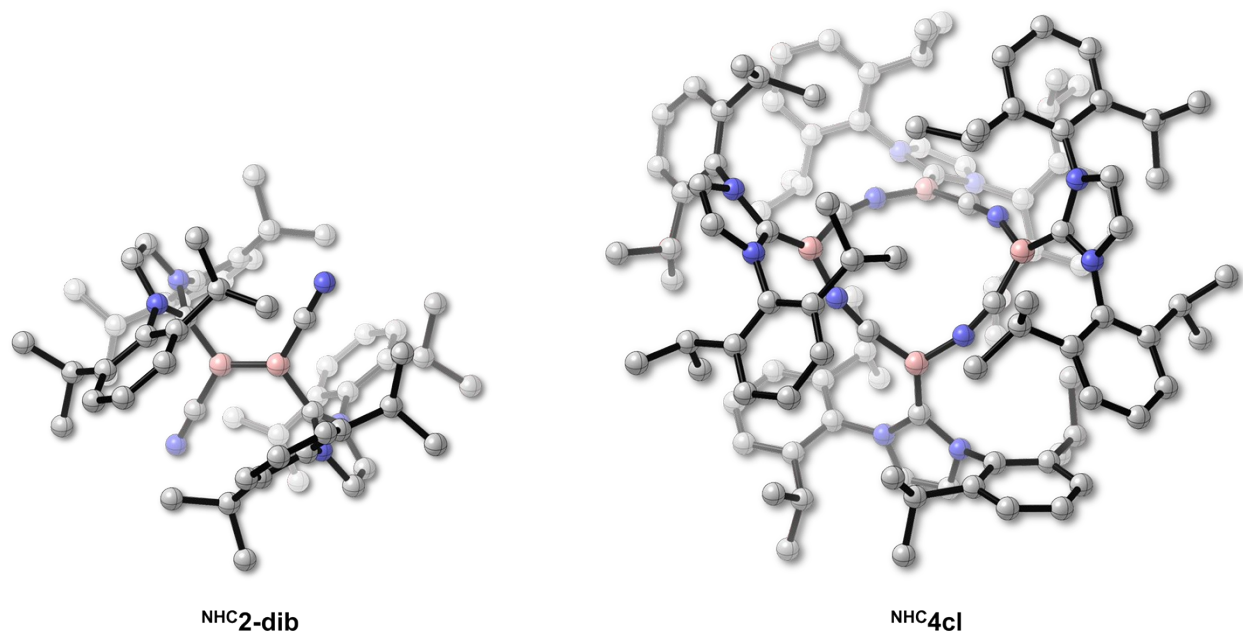
**Figure S6.** Frontier MOs and spin density plot of [LHB:] (L = CAAC, NHC) species at the B3LYP-D3(BJ)/def2-SVP level of theory.



## S5: NHC-stabilised cyanoborylene systems



**Figure S7.** Geometry scan following the formation of **NHC2-dib** from two isolated **NHC1**.



**Figure S8.** Optimised structures of **NHC2-dib** and **NHC4cl** at the B3LYP-D3(BJ)/def2SVP level of theory.

## S6: Multireference calculations

The multiradical character index  $y_i^{S1}$  is given by the following expression:

$$y_i = 1 - \frac{2T_i}{1 + T_i^2} \quad (S1)$$

where  $T_i$  is defined as:

$$T_i = \frac{\eta_{HOMO-i} - \eta_{LUMO+i}}{2} \quad (S2)$$

and  $\eta_{HOMO-i}$  and  $\eta_{LUMO+i}$  are the occupation numbers of the corresponding HOMO- $i$  and LUMO+ $i$  active space natural orbitals obtained from a complete active space self-consistent field (CASSCF)<sup>S2</sup> calculation.

The biradical character index,  $y_0$ , is obtained for  $i = 0$ :

$$y_0 = 1 - \frac{2T_0}{1 + T_0^2} \quad (S3)$$

in which

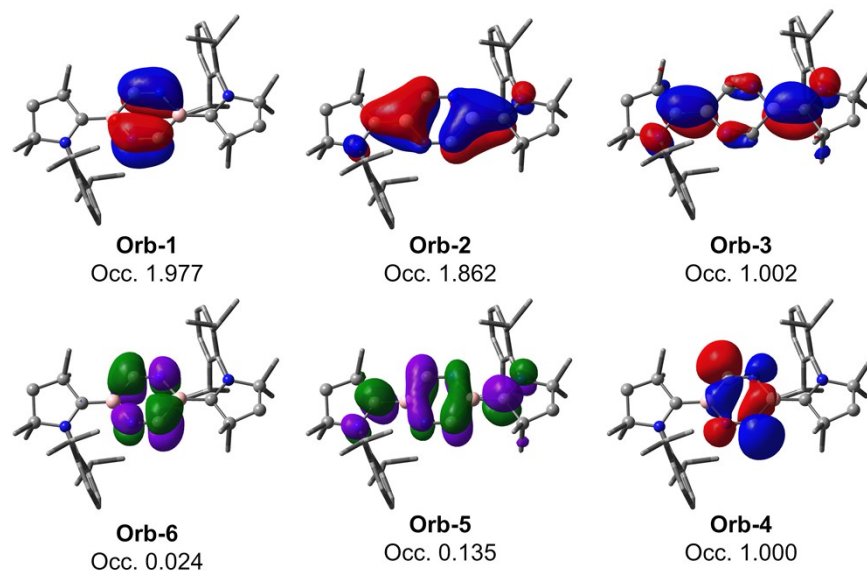
$$T_0 = \frac{\eta_{HOMO} - \eta_{LUMO}}{2} \quad (S4)$$

**Table S9.** Some properties of the CASSCF/NEVPT2 calculations of the open-shell singlet state of **2cl**. The triplet energy is obtained for the optimised triplet state, therefore the S-T gap shown herein is the adiabatic one.

	<b>2cl</b>
Active space	(6,6)
Dominant configuration	2 2 1 1 0 0
Weight of the dominant configuration	0.8624
CASSCF Energy	-1892.254553
$\eta_{HOMO}$	1.0016
$\eta_{LUMO}$	0.9999
$T_0$	0.00085
$y_0$	0.998
NEVPT2 Energy (singlet), hartree	-1899.134727
NEVPT2 Energy (triplet), hartree	-1899.135069
S-T gap, kcal mol <sup>-1</sup>	-0.2

**Table S10.** Comparison of the most stable singlet and triplet structures of **1**, <sup>NHC</sup>**1**, and [LHB:] (L = CAAC, NHC) species at the NEVPT2/CASSCF(2,2)/def2-SVP level of theory.

	Energy (hartree)	ST-gap (kcal mol <sup>-1</sup> )	$\eta_{HOMO}$	$\eta_{LUMO}$	$T_0$	$y_0$
<b>1</b> ( <b>S</b> <sub>0</sub> )	-949.496945	0.0	1.9913	0.0087	0.9913	0.000
<b>1</b> ( <b>T</b> <sub>1</sub> , <b>S</b> <sub>0</sub> geometry)	-949.4732494	14.9	1.0000	1.0000	0.0000	1.000
<b>1</b> ( <b>T</b> <sub>1</sub> )	-949.487931	5.7	1.0000	1.0000	0.0000	1.000
<sup>NHC</sup> <b>1</b> ( <b>S</b> <sub>1</sub> )	-1272.768949	0.0	1.9533	0.0467	0.9533	0.001
<sup>NHC</sup> <b>1</b> ( <b>T</b> <sub>0</sub> , <b>S</b> <sub>1</sub> geometry)	-1272.776002	-4.4	1.0000	1.0000	0.0000	1.000
<sup>NHC</sup> <b>1</b> ( <b>T</b> <sub>0</sub> )	-1272.790419	-13.5	1.0000	1.0000	0.0000	1.000
<sup>NHC</sup> <b>1</b> ( <b>S</b> <sub>1</sub> ')	-1272.7671	1.2	1.9669	0.0331	0.9669	0.001
[LHB:] (L = CAAC, <b>S</b> <sub>0</sub> )	-857.5426524	0.0	1.9258	0.0742	0.9258	0.003
[LHB:] (L = CAAC, <b>T</b> <sub>1</sub> )	-857.5250974	11.0	1.0000	1.0000	0.0000	1.000
[LHB:] (L = NHC, <b>S</b> <sub>1</sub> )	-1180.802597	0.0	1.9723	0.0277	0.9723	0.000
[LHB:] (L = NHC, <b>T</b> <sub>0</sub> )	-1180.821718	-12.0	1.0000	1.0000	0.0000	1.000



**Figure S9.** Active space orbitals of **2cl** at the CASSCF(6,6)/def2-SVP level of theory.

## S7: EDA-NOCV calculations

**Table S11.** EDA-NOCV results (PBE0-D3(BJ)/TZ2P) for **1** and <sup>NHC</sup>**1** (**S**<sub>1</sub><sup>'</sup>). Fragments: L + BCN at their singlet states, the latter in its excited configuration as described in the main text. Energy terms are given in kcal mol<sup>-1</sup>. For  $\Delta E_{\text{disp}}$ ,  $\Delta E_{\text{elstat}}$  and  $\Delta E_{\text{orb}}$ , the values in parentheses show the weight of each contribution with respect to the total attractive interaction. For  $\Delta E_{\text{orb}(1)}$ ,  $\Delta E_{\text{orb}(2)}$  and  $\Delta E_{\text{orb}(\text{rest})}$ , the values in parentheses show the weight of each contribution with respect to the total orbital interaction,  $\Delta E_{\text{orb}}$ .

	<b>1</b>	<sup>NHC</sup> <b>1</b> ( <b>S</b> <sub>1</sub> <sup>'</sup> )
$\Delta E_{\text{int}}$	-242.3	-211.6
$\Delta E_{\text{pauli}}$	142.7	135.9
$\Delta E_{\text{disp}}$	-4.4 (1.1%)	-5.4 (1.6%)
$\Delta E_{\text{elstat}}$	-160.7 (41.7%)	-149.5 (43.0%)
$\Delta E_{\text{orb}}$	-219.9 (57.1%)	-192.6 (55.4%)
$\Delta E_{\text{orb}(1)}$ (C→B $\sigma$ donation)	-114.6 (52.1%)	-110.3 (57.3%)
$\Delta E_{\text{orb}(2)}$ (B→C $\pi$ backdonation)	-83.9 (38.2%)	-61.8 (32.1%)
$\Delta E_{\text{orb}(\text{rest})}$	-21.4 (9.7%)	-20.5 (10.6%)

### S8: Cartesian coordinates (Ångstrom)

1			
N	-0.471796000	-0.086002000	0.514612000
C	-1.329682000	-0.286166000	-0.545007000
B	-0.997852000	-0.335642000	-1.924541000
N	-0.534912000	-0.449246000	-4.520697000
C	-1.122443000	-0.147659000	1.852622000
C	-0.352747000	-1.056377000	2.817317000
H	-0.853051000	-1.064549000	3.797544000
H	0.674981000	-0.692552000	2.966150000
H	-0.306291000	-2.089480000	2.451871000
C	-1.239418000	1.239532000	2.506757000
H	-1.743205000	1.152009000	3.481534000
H	-1.811269000	1.945580000	1.892505000
H	-0.241831000	1.666339000	2.681848000
C	-2.496330000	-0.748772000	1.480029000
H	-3.300465000	-0.375214000	2.130802000
H	-2.451195000	-1.841291000	1.604567000
C	-2.762469000	-0.427219000	-0.013062000
C	-3.530170000	0.897745000	-0.191926000
H	-4.506479000	0.846759000	0.317583000
H	-3.706311000	1.099471000	-1.258898000
H	-2.974627000	1.752621000	0.216111000
C	0.918676000	0.150867000	0.278159000
C	-3.536670000	-1.556189000	-0.705554000
H	-4.536747000	-1.670758000	-0.256753000
H	-3.002779000	-2.513950000	-0.619364000
H	-3.677257000	-1.341752000	-1.777527000
C	1.808894000	-0.948714000	0.185291000
C	1.328782000	-2.392984000	0.207784000
H	0.254572000	-2.379587000	0.432793000
C	1.489715000	-3.036540000	-1.180435000
H	1.079880000	-4.059538000	-1.179897000
H	2.550954000	-3.099532000	-1.470591000
H	0.959998000	-2.459757000	-1.952158000
C	2.037363000	-3.234688000	1.279026000
H	1.598659000	-4.244242000	1.327103000
H	1.958291000	-2.778963000	2.276719000
H	3.108610000	-3.354598000	1.052067000
C	3.171932000	-0.690035000	-0.010949000

H	3.871577000	-1.526189000	-0.073606000
C	3.646776000	0.612041000	-0.147106000
H	4.714208000	0.793261000	-0.294671000
C	2.752671000	1.679587000	-0.131637000
H	3.124205000	2.694359000	-0.289376000
C	1.380337000	1.473240000	0.061271000
C	0.431613000	2.656389000	-0.061560000
H	-0.574888000	2.296713000	0.179307000
C	0.775839000	3.797855000	0.905067000
H	0.017195000	4.594603000	0.845291000
H	1.748996000	4.253133000	0.661605000
H	0.823595000	3.450527000	1.947879000
C	0.391839000	3.163854000	-1.513411000
H	-0.349377000	3.972634000	-1.618411000
H	0.115240000	2.358067000	-2.208823000
H	1.370950000	3.562074000	-1.824960000
C	-0.747828000	-0.399309000	-3.368167000

## 2op

B	-2.374071000	1.690808000	-0.854562000
B	1.226210000	-0.013445000	-0.924879000
C	-2.430180000	3.037572000	-1.630192000
C	-0.071476000	0.493525000	-0.919803000
N	-2.472183000	4.045766000	-2.210835000
N	-1.178954000	0.986783000	-0.852323000
N	-3.769037000	-0.068927000	0.374669000
C	-3.628917000	1.153165000	-0.157545000
C	-5.148307000	-0.368106000	0.914043000
C	-5.100703000	-1.003373000	2.303002000
H	-6.131060000	-1.188841000	2.641672000
H	-4.619781000	-0.344050000	3.035195000
H	-4.568543000	-1.965018000	2.289680000
N	3.722341000	-0.084698000	-0.582246000
C	-5.902392000	-1.317781000	-0.026016000
H	-6.915627000	-1.484613000	0.369066000
H	-5.397960000	-2.291421000	-0.082854000
H	-5.995637000	-0.913118000	-1.041262000
C	-5.760635000	1.040326000	0.950023000
H	-5.668303000	1.446825000	1.968344000
H	-6.830747000	1.027876000	0.698820000
C	-4.942319000	1.919563000	-0.024724000
C	-5.612775000	2.035315000	-1.410349000

H	-6.596708000	2.520123000	-1.305775000
H	-5.765342000	1.050846000	-1.876218000
H	-4.999479000	2.642990000	-2.089856000
C	-4.746188000	3.326738000	0.567431000
H	-5.731965000	3.775524000	0.771911000
H	-4.202983000	3.988265000	-0.118219000
H	-4.188774000	3.278778000	1.515925000
C	-2.754798000	-1.092142000	0.364861000
C	-1.924647000	-1.236009000	1.499623000
C	-1.881940000	-0.223274000	2.637984000
H	-2.726794000	0.467175000	2.508419000
C	-0.595409000	0.621577000	2.572784000
H	-0.580048000	1.352295000	3.397614000
H	-0.517937000	1.169718000	1.626270000
H	0.302150000	-0.009376000	2.666142000
C	-2.006298000	-0.880962000	4.021637000
H	-2.095191000	-0.109891000	4.803305000
H	-1.113734000	-1.481225000	4.258282000
H	-2.880260000	-1.544438000	4.092457000
C	-1.038841000	-2.318125000	1.532338000
H	-0.401244000	-2.454979000	2.404899000
C	-0.933511000	-3.201922000	0.462364000
H	-0.231181000	-4.037030000	0.509219000
C	-1.692888000	-2.988979000	-0.683348000
H	-1.566972000	-3.651905000	-1.541676000
C	-2.610838000	-1.932185000	-0.764740000
C	-3.322419000	-1.695788000	-2.092110000
H	-4.038186000	-0.875690000	-1.954878000
C	-2.322853000	-1.244776000	-3.174146000
H	-2.854258000	-1.041208000	-4.117551000
H	-1.576076000	-2.030697000	-3.371424000
H	-1.786819000	-0.335764000	-2.876628000
C	-4.094965000	-2.930620000	-2.582744000
H	-4.670479000	-2.684387000	-3.489143000
H	-4.796339000	-3.313768000	-1.827719000
H	-3.409444000	-3.751855000	-2.845315000
C	2.569911000	-0.395339000	-1.257493000
C	4.957980000	-0.366839000	-1.364882000
C	6.116786000	-0.824812000	-0.477371000
H	7.013393000	-0.978814000	-1.096364000
H	5.896281000	-1.768258000	0.037711000
H	6.356458000	-0.064328000	0.280997000

C	5.415747000	0.871772000	-2.155931000
H	6.260806000	0.606855000	-2.810311000
H	5.750731000	1.667204000	-1.477124000
H	4.609967000	1.274073000	-2.783697000
C	4.445846000	-1.480128000	-2.304112000
H	4.625534000	-2.456903000	-1.828739000
H	4.977811000	-1.480625000	-3.266590000
C	2.917013000	-1.265700000	-2.476745000
C	2.156354000	-2.601853000	-2.409406000
H	2.474727000	-3.269591000	-3.227749000
H	1.071481000	-2.435840000	-2.495261000
H	2.340527000	-3.111165000	-1.451014000
C	2.559874000	-0.556230000	-3.793934000
H	2.843963000	-1.182099000	-4.655923000
H	3.068266000	0.413132000	-3.890496000
H	1.476809000	-0.367344000	-3.842394000
C	3.675687000	0.545001000	0.701328000
C	3.482052000	1.939813000	0.826291000
C	3.274390000	2.853199000	-0.372294000
H	3.309604000	2.231374000	-1.274230000
C	1.884262000	3.510750000	-0.333174000
H	1.705658000	4.090488000	-1.252505000
H	1.788742000	4.200359000	0.521005000
H	1.090714000	2.755048000	-0.253817000
C	4.376416000	3.918831000	-0.474626000
H	4.260648000	4.508056000	-1.398276000
H	5.381710000	3.470394000	-0.477180000
H	4.331977000	4.620469000	0.373938000
C	3.430580000	2.492237000	2.114565000
H	3.288270000	3.569218000	2.227092000
C	3.541807000	1.694116000	3.248988000
H	3.499292000	2.146092000	4.243203000
C	3.681535000	0.313589000	3.114037000
H	3.729529000	-0.311772000	4.007862000
C	3.739553000	-0.284285000	1.849698000
C	3.761803000	-1.801891000	1.738572000
H	4.010080000	-2.051796000	0.700510000
C	4.809567000	-2.460128000	2.644761000
H	4.855653000	-3.544354000	2.452734000
H	4.568324000	-2.329115000	3.711819000
H	5.812506000	-2.038314000	2.475240000
C	2.356429000	-2.362468000	1.995129000



H	2.339433000	-3.457744000	1.864899000
H	1.636763000	-1.919001000	1.294111000
H	2.022455000	-2.136370000	3.021562000

**TS2<sub>op-cl</sub>** (im. freq.: -405.5 cm<sup>-1</sup>)

B	-1.434233000	0.860815000	0.313152000
B	1.414798000	-0.609705000	0.594594000
C	-0.049931000	1.257887000	0.247689000
C	0.073662000	-1.300970000	0.953052000
N	1.072075000	0.734348000	0.197838000
N	-1.088811000	-1.018031000	0.947511000
N	-3.939332000	0.687375000	-0.105912000
C	-2.809824000	1.378677000	0.202417000
C	-5.135491000	1.548279000	-0.391588000
C	-6.265532000	1.343487000	0.625764000
H	-7.108762000	2.000416000	0.364229000
H	-5.956363000	1.582627000	1.650489000
H	-6.627782000	0.307364000	0.602532000
N	3.922591000	-0.658049000	0.131141000
C	-5.699040000	1.259564000	-1.787595000
H	-6.562657000	1.915922000	-1.974603000
H	-6.038512000	0.216885000	-1.872610000
H	-4.953891000	1.449707000	-2.569912000
C	-4.519366000	2.961085000	-0.313931000
H	-5.205477000	3.682036000	0.153974000
H	-4.309870000	3.321131000	-1.332467000
C	-3.184226000	2.840044000	0.456600000
C	-2.151685000	3.848496000	-0.058358000
H	-2.524661000	4.875943000	0.087609000
H	-1.951023000	3.696976000	-1.129307000
H	-1.196620000	3.742269000	0.474788000
C	-3.374716000	3.044984000	1.975278000
H	-3.754947000	4.059471000	2.179570000
H	-2.415514000	2.917961000	2.497729000
H	-4.083045000	2.320771000	2.401549000
C	-3.967357000	-0.742649000	-0.258944000
C	-4.354507000	-1.551086000	0.834948000
C	-4.602209000	-0.994787000	2.230722000
H	-4.568198000	0.098031000	2.160991000
C	-3.476150000	-1.412120000	3.191640000
H	-3.619177000	-0.934101000	4.174956000
H	-2.495701000	-1.130233000	2.787248000

H	-3.474635000	-2.503784000	3.345866000
C	-5.969639000	-1.399592000	2.800506000
H	-6.146998000	-0.896420000	3.764737000
H	-6.019445000	-2.484439000	2.985656000
H	-6.798083000	-1.141662000	2.124529000
C	-4.421360000	-2.937068000	0.644769000
H	-4.720188000	-3.575466000	1.478689000
C	-4.082666000	-3.516920000	-0.574232000
H	-4.139107000	-4.600916000	-0.701049000
C	-3.637285000	-2.713193000	-1.619627000
H	-3.326798000	-3.175891000	-2.558791000
C	-3.559354000	-1.321375000	-1.483425000
C	-2.951689000	-0.511709000	-2.621535000
H	-3.032212000	0.551465000	-2.360950000
C	-1.451777000	-0.823208000	-2.762909000
H	-0.995043000	-0.176407000	-3.528505000
H	-1.291057000	-1.870997000	-3.063981000
H	-0.920710000	-0.661065000	-1.815770000
C	-3.676076000	-0.731603000	-3.957744000
H	-3.261752000	-0.066685000	-4.732734000
H	-4.755025000	-0.534142000	-3.877976000
H	-3.553435000	-1.766205000	-4.315433000
C	2.765754000	-1.270867000	0.446986000
C	5.132994000	-1.549986000	0.169411000
C	5.960752000	-1.298218000	1.437858000
H	6.806217000	-2.001947000	1.465141000
H	5.372176000	-1.438180000	2.353016000
H	6.370366000	-0.279773000	1.439372000
C	6.042280000	-1.343009000	-1.043225000
H	6.914392000	-2.007957000	-0.953053000
H	6.408106000	-0.307528000	-1.098658000
H	5.531350000	-1.584641000	-1.982567000
C	4.469740000	-2.939266000	0.167453000
H	5.041480000	-3.665949000	0.761999000
H	4.433326000	-3.317459000	-0.865407000
C	3.024726000	-2.752953000	0.693107000
C	2.906495000	-3.075196000	2.197815000
H	3.186674000	-4.125774000	2.380237000
H	1.873579000	-2.921316000	2.539259000
H	3.560883000	-2.436202000	2.808499000
C	2.039391000	-3.635489000	-0.089567000
H	2.300725000	-4.698145000	0.043585000

H	2.071568000	-3.403132000	-1.165042000
H	1.008068000	-3.486189000	0.261699000
C	4.014087000	0.740938000	-0.193654000
C	3.889422000	1.131721000	-1.546188000
C	3.514352000	0.157027000	-2.654926000
H	3.564173000	-0.858853000	-2.241349000
C	2.059830000	0.382771000	-3.100240000
H	1.770658000	-0.361747000	-3.859711000
H	1.933553000	1.384248000	-3.542670000
H	1.371951000	0.301846000	-2.250324000
C	4.467685000	0.228660000	-3.856592000
H	4.224345000	-0.560570000	-4.585915000
H	5.519234000	0.107297000	-3.557132000
H	4.381335000	1.193296000	-4.381123000
C	4.033252000	2.488765000	-1.858879000
H	3.943170000	2.810187000	-2.898397000
C	4.263718000	3.437063000	-0.865810000
H	4.373963000	4.491677000	-1.129694000
C	4.319850000	3.041293000	0.467346000
H	4.453610000	3.794908000	1.246049000
C	4.182169000	1.696309000	0.834484000
C	4.120558000	1.348443000	2.316009000
H	4.045106000	0.257986000	2.403944000
C	5.370416000	1.806841000	3.082722000
H	5.331577000	1.455573000	4.126296000
H	5.440503000	2.905775000	3.109574000
H	6.298762000	1.428756000	2.630094000
C	2.854913000	1.938115000	2.963598000
H	2.779464000	1.615364000	4.014707000
H	1.948865000	1.618125000	2.433958000
H	2.882019000	3.039605000	2.952557000

### 2cl (open-shell singlet)

B	-1.414275000	0.661282000	0.455254000
B	1.414336000	-0.661467000	0.455529000
C	-0.004638000	1.309616000	0.487737000
C	0.004690000	-1.309780000	0.487688000
N	1.090649000	0.775950000	0.475071000
N	-1.090586000	-0.776084000	0.474753000
N	-3.937947000	0.690974000	0.115101000
C	-2.749241000	1.322943000	0.330843000
C	-5.119294000	1.604675000	-0.000660000

C	-6.292030000	1.137809000	0.866496000
H	-7.133030000	1.837526000	0.746390000
H	-6.025546000	1.110033000	1.930174000
H	-6.637263000	0.138161000	0.564632000
N	3.937979000	-0.690901000	0.115313000
C	-5.616922000	1.707389000	-1.450463000
H	-6.476399000	2.393267000	-1.493991000
H	-5.949690000	0.726307000	-1.816071000
H	-4.845931000	2.088126000	-2.131019000
C	-4.520146000	2.928269000	0.513639000
H	-4.765227000	3.040738000	1.580693000
H	-4.939719000	3.798660000	-0.011472000
C	-2.982182000	2.830190000	0.357823000
C	-2.491581000	3.460952000	-0.962891000
H	-2.727297000	4.538004000	-0.983901000
H	-2.959194000	2.992301000	-1.840565000
H	-1.403009000	3.339792000	-1.060153000
C	-2.272967000	3.520432000	1.532526000
H	-2.557337000	4.585116000	1.574843000
H	-1.180760000	3.458392000	1.426301000
H	-2.547087000	3.050138000	2.489289000
C	-4.030248000	-0.724161000	-0.108566000
C	-4.300617000	-1.579306000	0.984634000
C	-4.355148000	-1.079164000	2.421858000
H	-4.307684000	0.016892000	2.393361000
C	-3.121390000	-1.557338000	3.206948000
H	-3.131294000	-1.139721000	4.227053000
H	-2.192782000	-1.248438000	2.709889000
H	-3.108727000	-2.656061000	3.293268000
C	-5.646378000	-1.488368000	3.144996000
H	-5.687152000	-1.031253000	4.146818000
H	-5.699786000	-2.580080000	3.282668000
H	-6.544820000	-1.179416000	2.591251000
C	-4.426090000	-2.952863000	0.741563000
H	-4.639850000	-3.626037000	1.574439000
C	-4.254388000	-3.476902000	-0.536658000
H	-4.356027000	-4.551491000	-0.707449000
C	-3.918145000	-2.630708000	-1.589885000
H	-3.737638000	-3.052772000	-2.580788000
C	-3.784444000	-1.249324000	-1.400005000
C	-3.298736000	-0.397691000	-2.566637000
H	-3.308852000	0.649155000	-2.243798000

C	-1.841934000	-0.735307000	-2.929616000
H	-1.487145000	-0.074532000	-3.737138000
H	-1.750454000	-1.775496000	-3.281656000
H	-1.176197000	-0.611403000	-2.067127000
C	-4.198117000	-0.525152000	-3.805272000
H	-3.870923000	0.175127000	-4.590639000
H	-5.251862000	-0.310865000	-3.575289000
H	-4.151248000	-1.539771000	-4.231746000
C	2.749355000	-1.323011000	0.331166000
C	5.119409000	-1.604542000	-0.000520000
C	6.292254000	-1.137506000	0.866398000
H	7.133245000	-1.837234000	0.746287000
H	6.025923000	-1.109550000	1.930110000
H	6.637441000	-0.137911000	0.564315000
C	5.616779000	-1.707322000	-1.450398000
H	6.476254000	-2.393193000	-1.494060000
H	5.949468000	-0.726248000	-1.816090000
H	4.845671000	-2.088075000	-2.130810000
C	4.520434000	-2.928110000	0.514039000
H	4.765620000	-3.040353000	1.581093000
H	4.940068000	-3.798544000	-0.010952000
C	2.982459000	-2.830218000	0.358346000
C	2.273380000	-3.520300000	1.533245000
H	2.557800000	-4.584963000	1.575725000
H	1.181163000	-3.458316000	1.427079000
H	2.547554000	-3.049814000	2.489897000
C	2.491780000	-3.461309000	-0.962177000
H	2.727540000	-4.538356000	-0.982937000
H	2.959305000	-2.992879000	-1.840014000
H	1.403194000	-3.340225000	-1.059388000
C	4.030140000	0.724154000	-0.108914000
C	3.783875000	1.248876000	-1.400458000
C	3.297844000	0.396868000	-2.566673000
H	3.308045000	-0.649877000	-2.243504000
C	1.840946000	0.734334000	-2.929396000
H	1.485968000	0.073289000	-3.736612000
H	1.749333000	1.774405000	-3.281751000
H	1.175428000	0.610689000	-2.066700000
C	4.196884000	0.523956000	-3.805602000
H	3.869512000	-0.176625000	-4.590624000
H	5.250708000	0.309831000	-3.575846000
H	4.149820000	1.538428000	-4.232405000

C	3.917554000	2.630190000	-1.590861000
H	3.736675000	3.051906000	-2.581846000
C	4.254283000	3.476742000	-0.538083000
H	4.355936000	4.551258000	-0.709321000
C	4.426466000	2.953155000	0.740259000
H	4.640634000	3.626603000	1.572810000
C	4.300961000	1.579698000	0.983876000
C	4.355827000	1.080079000	2.421275000
H	4.308477000	-0.015990000	2.393179000
C	5.647090000	1.489665000	3.144106000
H	5.687994000	1.032938000	4.146099000
H	5.700451000	2.581432000	3.281370000
H	6.545500000	1.180554000	2.590395000
C	3.122103000	1.558416000	3.206332000
H	3.132128000	1.141142000	4.226578000
H	2.193473000	1.249295000	2.709452000
H	3.109377000	2.657170000	3.292274000

#### 2cl (triplet)

B	1.413370000	0.662581000	-0.456406000
B	-1.413457000	-0.662476000	-0.456437000
C	0.003543000	1.311116000	-0.490368000
C	-0.003636000	-1.311004000	-0.490709000
N	-1.090182000	0.775836000	-0.477128000
N	1.090089000	-0.775721000	-0.477439000
N	3.936102000	0.690978000	-0.113379000
C	2.748360000	1.322869000	-0.330892000
C	5.117708000	1.604223000	0.004708000
C	6.291775000	1.136934000	-0.860385000
H	7.132880000	1.836215000	-0.738509000
H	6.027241000	1.109598000	-1.924555000
H	6.635938000	0.137032000	-0.558152000
N	-3.936153000	-0.690944000	-0.113155000
C	5.612518000	1.706345000	1.455491000
H	6.471996000	2.392101000	1.500879000
H	5.944451000	0.725116000	1.821423000
H	4.840221000	2.086973000	2.134641000
C	4.519961000	2.928098000	-0.510382000
H	4.767596000	3.041109000	-1.576784000
H	4.938318000	3.798188000	0.016174000
C	2.981639000	2.830029000	-0.358197000
C	2.487690000	3.460914000	0.961209000

H	2.723297000	4.537979000	0.982398000
H	2.953260000	2.992520000	1.840107000
H	1.398904000	3.339592000	1.055736000
C	2.275063000	3.519676000	-1.534845000
H	2.559554000	4.584344000	-1.576774000
H	1.182669000	3.457235000	-1.431115000
H	2.551551000	3.049054000	-2.490761000
C	4.027808000	-0.724512000	0.108555000
C	4.299000000	-1.578221000	-0.985553000
C	4.355141000	-1.076256000	-2.422083000
H	4.308126000	0.019795000	-2.392318000
C	3.121979000	-1.552968000	-3.209008000
H	3.133029000	-1.133919000	-4.228513000
H	2.192991000	-1.244459000	-2.712438000
H	3.109125000	-2.651567000	-3.296881000
C	5.646943000	-1.485068000	-3.144435000
H	5.688893000	-1.026676000	-4.145622000
H	5.700025000	-2.576620000	-3.283478000
H	6.544975000	-1.177227000	-2.589398000
C	4.423913000	-2.952114000	-0.744110000
H	4.638344000	-3.624251000	-1.577647000
C	4.250850000	-3.477746000	0.533272000
H	4.352061000	-4.552578000	0.702776000
C	3.913779000	-2.632852000	1.587276000
H	3.732171000	-3.056156000	2.577447000
C	3.780551000	-1.251196000	1.399088000
C	3.293812000	-0.401024000	2.566335000
H	3.304038000	0.646240000	2.244821000
C	1.836751000	-0.739211000	2.927697000
H	1.481346000	-0.079465000	3.735781000
H	1.745040000	-1.779844000	3.278366000
H	1.171730000	-0.614077000	2.064842000
C	4.192184000	-0.530018000	3.805556000
H	3.864344000	0.169306000	4.591502000
H	5.246152000	-0.315529000	3.576777000
H	4.144888000	-1.545166000	4.230720000
C	-2.748440000	-1.322787000	-0.330960000
C	-5.117754000	-1.604216000	0.004810000
C	-6.291915000	-1.136692000	-0.860027000
H	-7.133008000	-1.836004000	-0.738243000
H	-6.027501000	-1.109071000	-1.924218000
H	-6.636043000	-0.136871000	-0.557486000

C	-5.612408000	-1.706734000	1.455617000
H	-6.471881000	-2.392503000	1.500910000
H	-5.944303000	-0.725605000	1.821850000
H	-4.840039000	-2.087546000	2.134581000
C	-4.520070000	-2.927952000	-0.510708000
H	-4.767812000	-3.040665000	-1.577117000
H	-4.938382000	-3.798185000	0.015648000
C	-2.981733000	-2.829938000	-0.358648000
C	-2.275276000	-3.519276000	-1.535548000
H	-2.559779000	-4.583931000	-1.577735000
H	-1.182871000	-3.456871000	-1.431906000
H	-2.551851000	-3.048395000	-2.491312000
C	-2.487663000	-3.461180000	0.960542000
H	-2.723276000	-4.538249000	0.981464000
H	-2.953149000	-2.993018000	1.839610000
H	-1.398867000	-3.339889000	1.054999000
C	-4.027819000	0.724481000	0.109213000
C	-3.780381000	1.250776000	1.399870000
C	-3.293506000	0.400249000	2.566802000
H	-3.303870000	-0.646927000	2.245005000
C	-1.836355000	0.738222000	2.927997000
H	-1.480855000	0.078222000	3.735831000
H	-1.744499000	1.778749000	3.278941000
H	-1.171501000	0.613278000	2.064986000
C	-4.191647000	0.528981000	3.806218000
H	-3.863726000	-0.170585000	4.591914000
H	-5.245674000	0.314643000	3.577570000
H	-4.144190000	1.544009000	4.231651000
C	-3.913537000	2.632381000	1.588483000
H	-3.731787000	3.055385000	2.578756000
C	-4.250717000	3.477599000	0.534774000
H	-4.351870000	4.552384000	0.704609000
C	-4.423953000	2.952351000	-0.742743000
H	-4.638459000	3.624743000	-1.576055000
C	-4.299112000	1.578526000	-0.984610000
C	-4.355409000	1.077001000	-2.421288000
H	-4.308475000	-0.019062000	-2.391861000
C	-5.647234000	1.486139000	-3.143415000
H	-5.689300000	1.028052000	-4.144737000
H	-5.700235000	2.577737000	-3.282127000
H	-6.545249000	1.178207000	-2.588403000
C	-3.122272000	1.553859000	-3.208164000



H	-3.133435000	1.135122000	-4.227796000
H	-2.193269000	1.245124000	-2.711761000
H	-3.109338000	2.652483000	-3.295702000

### 3op

B	-2.419434000	-0.662293000	0.999537000
B	0.452051000	1.784098000	-0.281592000
B	3.162541000	-0.982401000	-1.677607000
C	-1.456980000	0.290679000	0.646297000
C	1.677500000	0.941601000	-0.696611000
C	2.750846000	-1.170716000	-3.156821000
N	-0.631410000	1.077347000	0.237450000
N	2.424843000	0.102558000	-1.041214000
N	2.420055000	-1.285061000	-4.270393000
N	-3.571362000	-2.847091000	0.517136000
C	-3.008237000	-1.927393000	1.362320000
N	-0.672238000	4.076708000	-0.389807000
C	-3.874401000	-4.165243000	1.155843000
C	-3.175187000	-5.309874000	0.415788000
H	-3.379529000	-6.261594000	0.929924000
H	-2.088525000	-5.162977000	0.387221000
H	-3.543359000	-5.396339000	-0.616948000
C	-5.378454000	-4.479317000	1.194309000
H	-5.530170000	-5.480194000	1.625880000
H	-5.801164000	-4.484585000	0.179627000
H	-5.944456000	-3.764129000	1.803520000
C	-3.272736000	-3.962153000	2.566477000
H	-2.268094000	-4.410126000	2.596472000
H	-3.876026000	-4.453849000	3.343783000
C	-3.144423000	-2.438860000	2.797458000
C	-4.420834000	-1.840178000	3.426482000
H	-4.609657000	-2.294908000	4.412946000
H	-5.306872000	-2.004430000	2.798792000
H	-4.306125000	-0.754097000	3.557332000
C	-1.946237000	-2.086915000	3.683447000
H	-2.098669000	-2.471083000	4.704885000
H	-1.815387000	-0.994835000	3.747926000
H	-1.015849000	-2.512518000	3.286993000
C	-3.794177000	-2.549917000	-0.869983000
C	-2.767321000	-2.739657000	-1.827209000
C	-1.350325000	-3.170474000	-1.474414000
H	-1.303070000	-3.307241000	-0.385317000

C	-0.340335000	-2.074582000	-1.847809000
H	0.670430000	-2.353074000	-1.518061000
H	-0.598463000	-1.116956000	-1.380306000
H	-0.282939000	-1.922037000	-2.935645000
C	-0.949842000	-4.489712000	-2.154897000
H	0.051868000	-4.800403000	-1.817603000
H	-0.899072000	-4.368687000	-3.248239000
H	-1.655015000	-5.304992000	-1.940729000
C	-3.050417000	-2.450900000	-3.171042000
H	-2.268848000	-2.595172000	-3.919256000
C	-4.292457000	-1.964511000	-3.564234000
H	-4.487778000	-1.747661000	-4.617272000
C	-5.274550000	-1.725215000	-2.605599000
H	-6.234131000	-1.303088000	-2.911302000
C	-5.044089000	-1.998571000	-1.252419000
C	-6.099797000	-1.600692000	-0.231536000
H	-5.808876000	-2.035991000	0.727934000
C	-6.095576000	-0.078264000	-0.034552000
H	-6.815708000	0.216865000	0.746792000
H	-6.373078000	0.443095000	-0.965538000
H	-5.097629000	0.264380000	0.269693000
C	-7.501972000	-2.117005000	-0.575756000
H	-8.205021000	-1.890410000	0.241948000
H	-7.506627000	-3.205613000	-0.737372000
H	-7.899529000	-1.643275000	-1.487323000
C	0.393361000	3.289344000	-0.561001000
C	-0.481259000	5.510851000	-0.819554000
C	-1.198030000	5.791132000	-2.146044000
H	-0.991326000	6.828048000	-2.450283000
H	-2.284548000	5.682117000	-2.040262000
H	-0.854568000	5.126840000	-2.949443000
C	-1.002888000	6.488397000	0.234374000
H	-0.834959000	7.516346000	-0.120137000
H	-0.478585000	6.372639000	1.190497000
H	-2.081053000	6.358761000	0.406415000
C	1.047995000	5.572551000	-0.965784000
H	1.480583000	6.022165000	-0.059738000
H	1.350450000	6.198854000	-1.816494000
C	1.553436000	4.115178000	-1.104621000
C	2.818906000	3.915258000	-0.259826000
H	3.606916000	4.604697000	-0.603457000
H	3.200478000	2.892504000	-0.335829000

H	2.620150000	4.119491000	0.803032000
C	1.833574000	3.727106000	-2.570904000
H	2.632404000	4.366540000	-2.978848000
H	0.940952000	3.848215000	-3.202107000
H	2.159703000	2.680574000	-2.648707000
C	-1.916676000	3.630176000	0.181097000
C	-2.054641000	3.658074000	1.588512000
C	-0.903554000	3.989421000	2.532454000
H	-0.067558000	4.369123000	1.929665000
C	-0.395628000	2.727397000	3.253334000
H	0.447139000	2.982022000	3.916478000
H	-0.052584000	1.968144000	2.539798000
H	-1.189424000	2.280875000	3.873059000
C	-1.278125000	5.073703000	3.554573000
H	-0.393170000	5.370878000	4.139541000
H	-2.032759000	4.708641000	4.268711000
H	-1.688047000	5.972093000	3.070257000
C	-3.291566000	3.294195000	2.133978000
H	-3.421439000	3.303019000	3.217823000
C	-4.354658000	2.914786000	1.318972000
H	-5.315676000	2.643060000	1.761037000
C	-4.176054000	2.837514000	-0.058391000
H	-4.995642000	2.489420000	-0.686221000
C	-2.951950000	3.161114000	-0.656892000
C	-2.779557000	2.891428000	-2.147394000
H	-1.800140000	3.278827000	-2.452453000
C	-3.856834000	3.583255000	-2.997100000
H	-3.627832000	3.472253000	-4.068601000
H	-3.941595000	4.657385000	-2.774533000
H	-4.847060000	3.131744000	-2.827646000
C	-2.771629000	1.379546000	-2.441724000
H	-2.663671000	1.205921000	-3.523870000
H	-3.706580000	0.897120000	-2.119015000
H	-1.942879000	0.872003000	-1.935744000
N	4.695731000	-1.706314000	0.258635000
C	4.153768000	-1.850894000	-1.006709000
C	5.721375000	-2.722398000	0.630364000
C	7.157355000	-2.172284000	0.559798000
H	7.869363000	-2.972854000	0.812788000
H	7.300607000	-1.357128000	1.282202000
H	7.412396000	-1.801024000	-0.440154000
C	5.511902000	-3.269882000	2.047344000

H	6.308275000	-3.992055000	2.283345000
H	4.550036000	-3.786935000	2.148447000
H	5.555675000	-2.463678000	2.795141000
C	5.464889000	-3.794436000	-0.442737000
H	4.777545000	-4.549815000	-0.031576000
H	6.388148000	-4.317742000	-0.732432000
C	4.781734000	-3.096326000	-1.645876000
C	3.742830000	-4.047974000	-2.263346000
H	4.232921000	-4.986083000	-2.575052000
H	3.256481000	-3.607370000	-3.142502000
H	2.959714000	-4.296165000	-1.529757000
C	5.796752000	-2.686934000	-2.732556000
H	6.321747000	-3.574702000	-3.124080000
H	6.550898000	-1.987298000	-2.344058000
H	5.281205000	-2.192912000	-3.568113000
C	4.353640000	-0.589352000	1.078441000
C	3.274833000	-0.708484000	1.987151000
C	2.452645000	-1.983713000	2.101439000
H	2.943700000	-2.742484000	1.481388000
C	1.046116000	-1.783481000	1.527055000
H	0.474582000	-2.724510000	1.564247000
H	1.084619000	-1.459976000	0.483083000
H	0.481039000	-1.029103000	2.092219000
C	2.378904000	-2.505453000	3.543523000
H	1.859587000	-3.477256000	3.574300000
H	1.815959000	-1.814441000	4.191531000
H	3.377577000	-2.637806000	3.985077000
C	2.908181000	0.408853000	2.748294000
H	2.069337000	0.333931000	3.443719000
C	3.583668000	1.619668000	2.617455000
H	3.283565000	2.481653000	3.218900000
C	4.626582000	1.734325000	1.700937000
H	5.133476000	2.694462000	1.581672000
C	5.017661000	0.650242000	0.904463000
C	6.090319000	0.859697000	-0.156080000
H	6.275012000	-0.111167000	-0.624516000
C	7.409144000	1.368606000	0.443900000
H	8.195561000	1.403847000	-0.327242000
H	7.763801000	0.726054000	1.263144000
H	7.298764000	2.388249000	0.847254000
C	5.618443000	1.797889000	-1.277952000
H	6.378046000	1.844202000	-2.074859000

H	5.462601000	2.822868000	-0.907649000
H	4.682550000	1.437424000	-1.725511000

**TS3<sub>op-cl</sub>** (im. freq.: -112.2 cm<sup>-1</sup>)

B	-2.600183000	-0.230375000	0.535966000
B	0.633265000	2.068553000	0.612898000
B	1.782036000	-1.630020000	-0.001217000
C	-1.590694000	0.762308000	0.578078000
C	1.584341000	0.858562000	0.684365000
C	0.293340000	-1.834332000	-0.363827000
N	-0.685855000	1.557682000	0.533359000
N	1.930494000	-0.243721000	0.467446000
N	-0.855390000	-1.816935000	-0.576129000
N	-4.435361000	-2.002105000	0.344619000
C	-3.844000000	-0.882422000	0.860880000
N	0.189403000	4.490999000	-0.004137000
C	-5.865289000	-2.153182000	0.740531000
C	-6.264557000	-3.616133000	0.940694000
H	-7.328582000	-3.665928000	1.217185000
H	-5.685071000	-4.097439000	1.737321000
H	-6.125659000	-4.194030000	0.015382000
C	-6.800862000	-1.540931000	-0.317941000
H	-7.839803000	-1.553794000	0.046761000
H	-6.763710000	-2.118373000	-1.251545000
H	-6.531447000	-0.501816000	-0.547995000
C	-5.883350000	-1.349547000	2.055733000
H	-5.670062000	-2.032657000	2.891943000
H	-6.864683000	-0.891325000	2.246948000
C	-4.755355000	-0.289830000	1.956940000
C	-5.288445000	1.095797000	1.552769000
H	-5.972467000	1.483957000	2.325720000
H	-5.831068000	1.064536000	0.597797000
H	-4.456980000	1.802599000	1.430879000
C	-3.996861000	-0.165051000	3.288868000
H	-4.681616000	0.153556000	4.092646000
H	-3.189005000	0.577530000	3.211426000
H	-3.544767000	-1.126277000	3.575339000
C	-3.722238000	-2.954770000	-0.451412000
C	-3.039472000	-4.001884000	0.210900000
C	-2.974735000	-4.092350000	1.730002000
H	-3.741135000	-3.418503000	2.133002000
C	-1.622748000	-3.583768000	2.256835000

H	-1.609865000	-3.607494000	3.359296000
H	-1.431623000	-2.556636000	1.921700000
H	-0.794655000	-4.210511000	1.892634000
C	-3.273057000	-5.503654000	2.253842000
H	-3.330866000	-5.499873000	3.354274000
H	-2.481150000	-6.216026000	1.973391000
H	-4.224927000	-5.893348000	1.860536000
C	-2.341978000	-4.932848000	-0.565737000
H	-1.804734000	-5.746617000	-0.075285000
C	-2.297082000	-4.822193000	-1.954321000
H	-1.739866000	-5.555361000	-2.542854000
C	-2.935634000	-3.759756000	-2.586374000
H	-2.860565000	-3.654529000	-3.671023000
C	-3.646190000	-2.802697000	-1.850234000
C	-4.215254000	-1.585724000	-2.562226000
H	-4.743727000	-0.983609000	-1.813780000
C	-3.084596000	-0.705801000	-3.119344000
H	-3.496546000	0.224763000	-3.544056000
H	-2.528712000	-1.224672000	-3.917138000
H	-2.366469000	-0.445075000	-2.331241000
C	-5.215864000	-1.964300000	-3.662549000
H	-5.669783000	-1.061530000	-4.102946000
H	-6.026785000	-2.600666000	-3.275224000
H	-4.724634000	-2.518029000	-4.478680000
C	1.025120000	3.500200000	0.384506000
C	0.838477000	5.835124000	-0.160390000
C	1.008179000	6.202230000	-1.642237000
H	1.495740000	7.185417000	-1.721123000
H	0.029618000	6.269400000	-2.137255000
H	1.621614000	5.475577000	-2.187283000
C	0.030619000	6.950323000	0.507491000
H	0.543298000	7.910999000	0.348744000
H	-0.067017000	6.795694000	1.588928000
H	-0.975220000	7.027960000	0.070123000
C	2.182703000	5.591713000	0.553416000
H	2.104151000	5.940601000	1.594391000
H	3.004155000	6.149710000	0.081461000
C	2.430470000	4.063522000	0.548827000
C	3.100546000	3.607027000	1.853571000
H	4.063037000	4.128248000	1.984649000
H	3.307582000	2.528068000	1.845475000
H	2.463599000	3.828919000	2.723228000

C	3.298597000	3.618451000	-0.645220000
H	4.305885000	4.058321000	-0.565592000
H	2.866168000	3.924061000	-1.607812000
H	3.407457000	2.527402000	-0.657010000
C	-1.162252000	4.215553000	-0.406914000
C	-2.207953000	4.393301000	0.528064000
C	-1.958580000	4.770477000	1.982931000
H	-0.889826000	4.993135000	2.089435000
C	-2.256099000	3.585895000	2.918643000
H	-2.010386000	3.852114000	3.959379000
H	-1.669066000	2.701151000	2.640024000
H	-3.321793000	3.309893000	2.888644000
C	-2.757169000	6.007945000	2.417291000
H	-2.483502000	6.302523000	3.443169000
H	-3.839919000	5.804876000	2.413746000
H	-2.578899000	6.867612000	1.755494000
C	-3.516975000	4.106970000	0.121143000
H	-4.338451000	4.245460000	0.826578000
C	-3.784118000	3.611758000	-1.152157000
H	-4.810404000	3.377412000	-1.444371000
C	-2.735565000	3.378758000	-2.037583000
H	-2.946582000	2.945171000	-3.016964000
C	-1.409696000	3.664082000	-1.687859000
C	-0.304363000	3.296587000	-2.670699000
H	0.651512000	3.598325000	-2.229439000
C	-0.459557000	4.025434000	-4.014690000
H	0.399877000	3.808794000	-4.669318000
H	-0.527861000	5.115823000	-3.890393000
H	-1.366703000	3.693882000	-4.544335000
C	-0.229216000	1.777317000	-2.900791000
H	0.634866000	1.535715000	-3.539913000
H	-1.132559000	1.404470000	-3.405835000
H	-0.119188000	1.224989000	-1.959756000
N	4.198656000	-2.456653000	0.044840000
C	2.840465000	-2.633205000	-0.165362000
C	5.036825000	-3.665237000	-0.189404000
C	5.881883000	-3.557249000	-1.470305000
H	6.482426000	-4.471308000	-1.595788000
H	6.575200000	-2.706818000	-1.406075000
H	5.264575000	-3.434503000	-2.368323000
C	5.996989000	-3.936177000	0.975123000
H	6.586176000	-4.842307000	0.765553000

H	5.456162000	-4.095109000	1.916525000
H	6.700425000	-3.101224000	1.111825000
C	3.955348000	-4.757628000	-0.293711000
H	3.838896000	-5.237660000	0.690067000
H	4.234207000	-5.545040000	-1.009770000
C	2.623838000	-4.062468000	-0.669747000
C	1.447532000	-4.782407000	0.005910000
H	1.428416000	-5.842819000	-0.299074000
H	0.484623000	-4.334948000	-0.271550000
H	1.539629000	-4.738387000	1.101683000
C	2.384725000	-4.054697000	-2.194572000
H	2.331373000	-5.085770000	-2.583912000
H	3.185253000	-3.528322000	-2.733587000
H	1.436744000	-3.547767000	-2.426968000
C	4.750887000	-1.171436000	0.326755000
C	4.952696000	-0.775260000	1.671410000
C	4.486710000	-1.621504000	2.848527000
H	4.120810000	-2.571870000	2.440438000
C	3.300255000	-0.959383000	3.569804000
H	2.959844000	-1.593877000	4.404273000
H	2.454458000	-0.809290000	2.887095000
H	3.582536000	0.020906000	3.988119000
C	5.618414000	-1.918748000	3.843382000
H	5.271129000	-2.614767000	4.623968000
H	5.957180000	-1.001388000	4.351439000
H	6.492428000	-2.367610000	3.350118000
C	5.537194000	0.473389000	1.924705000
H	5.704874000	0.786643000	2.957583000
C	5.892500000	1.326819000	0.883848000
H	6.353219000	2.294010000	1.099739000
C	5.624094000	0.958076000	-0.432366000
H	5.862098000	1.650218000	-1.242833000
C	5.032778000	-0.274590000	-0.735905000
C	4.648508000	-0.568906000	-2.180321000
H	4.273878000	-1.596633000	-2.214243000
C	5.836547000	-0.453169000	-3.146050000
H	5.540029000	-0.771184000	-4.158623000
H	6.686915000	-1.074197000	-2.829909000
H	6.193524000	0.586625000	-3.221830000
C	3.494417000	0.334966000	-2.647718000
H	3.173935000	0.045514000	-3.661697000
H	3.802750000	1.392030000	-2.685911000



H 2.625676000 0.250563000 -1.982949000

**3cl**

B	-1.821335000	1.392288000	0.554357000
B	2.116413000	0.880685000	0.556266000
B	-0.295821000	-2.273593000	0.557356000
C	-0.341122000	1.739774000	0.610144000
C	1.677011000	-0.574877000	0.613360000
C	-1.336959000	-1.165459000	0.612867000
N	0.829919000	1.611887000	0.596808000
N	0.980492000	-1.524926000	0.599961000
N	-1.811655000	-0.087369000	0.597631000
N	-4.263609000	1.948301000	0.116434000
C	-2.951629000	2.305518000	0.342611000
N	3.819283000	2.717587000	0.117907000
C	-5.201621000	3.094782000	-0.058864000
C	-6.456480000	2.954274000	0.810161000
H	-7.112907000	3.823536000	0.650857000
H	-6.207807000	2.909966000	1.877862000
H	-7.024067000	2.050220000	0.544372000
C	-5.662345000	3.245672000	-1.518314000
H	-6.346153000	4.103883000	-1.605147000
H	-6.206432000	2.347843000	-1.844163000
H	-4.825136000	3.409934000	-2.206729000
C	-4.319741000	4.269494000	0.410910000
H	-4.526449000	4.466507000	1.474049000
H	-4.538262000	5.194809000	-0.142438000
C	-2.843979000	3.826546000	0.261306000
C	-2.257585000	4.241784000	-1.104925000
H	-2.256200000	5.340048000	-1.208308000
H	-2.831465000	3.821670000	-1.942189000
H	-1.221905000	3.890037000	-1.200064000
C	-1.979730000	4.430994000	1.376887000
H	-2.024897000	5.532445000	1.341376000
H	-0.923859000	4.146568000	1.271598000
H	-2.325391000	4.097727000	2.366802000
C	-4.657205000	0.588973000	-0.085983000
C	-5.159486000	-0.160376000	1.005582000
C	-5.137548000	0.367599000	2.433671000
H	-4.834050000	1.420959000	2.388203000
C	-4.072492000	-0.367944000	3.265772000
H	-4.034797000	0.042940000	4.287765000

H	-3.076307000	-0.263521000	2.816981000
H	-4.299515000	-1.443657000	3.344209000
C	-6.507811000	0.283577000	3.120954000
H	-6.470343000	0.763586000	4.112097000
H	-6.815340000	-0.762829000	3.277407000
H	-7.294446000	0.776944000	2.532100000
C	-5.606750000	-1.467980000	0.773611000
H	-6.002605000	-2.054333000	1.605449000
C	-5.528327000	-2.041334000	-0.492013000
H	-5.881445000	-3.062281000	-0.655069000
C	-4.952631000	-1.325634000	-1.538764000
H	-4.842266000	-1.800916000	-2.515717000
C	-4.491597000	-0.015350000	-1.358301000
C	-3.767532000	0.668939000	-2.511473000
H	-3.545382000	1.694941000	-2.199288000
C	-2.416538000	-0.010752000	-2.800549000
H	-1.886608000	0.522280000	-3.606509000
H	-2.553590000	-1.055756000	-3.122892000
H	-1.770371000	-0.011015000	-1.914719000
C	-4.616125000	0.727780000	-3.790189000
H	-4.099080000	1.315006000	-4.566136000
H	-5.598253000	1.188793000	-3.612134000
H	-4.790311000	-0.278339000	-4.204009000
C	3.472555000	1.402933000	0.345498000
C	5.281406000	2.956927000	-0.054584000
C	5.645468000	3.278953000	-1.513656000
H	6.730747000	3.442221000	-1.598355000
H	5.140480000	4.198645000	-1.841448000
H	5.370849000	2.471100000	-2.202024000
C	5.784796000	4.115172000	0.814155000
H	6.866259000	4.248791000	0.657733000
H	5.619021000	3.923585000	1.881666000
H	5.286403000	5.058337000	0.545547000
C	5.857151000	1.606568000	0.417976000
H	6.128703000	1.688262000	1.481651000
H	6.769026000	1.332836000	-0.133110000
C	4.736280000	0.549564000	0.266927000
C	4.825960000	-0.500697000	1.382954000
H	5.802755000	-1.011817000	1.349484000
H	4.052317000	-1.273335000	1.276160000
H	4.707949000	-0.034535000	2.372516000
C	4.805151000	-0.166343000	-1.098915000

H	5.756274000	-0.715771000	-1.200842000
H	4.728593000	0.540365000	-1.936514000
H	3.983507000	-0.888226000	-1.194680000
C	2.839190000	3.737795000	-0.087646000
C	2.439201000	4.548909000	1.002087000
C	2.882558000	4.268066000	2.431544000
H	3.643358000	3.478692000	2.388982000
C	1.711526000	3.714216000	3.262052000
H	2.046670000	3.477385000	4.284947000
H	1.304927000	2.798664000	2.813581000
H	0.893076000	4.448531000	3.338183000
C	3.493041000	5.497969000	3.118318000
H	3.888276000	5.227065000	4.110575000
H	2.739921000	6.287342000	3.272270000
H	4.314507000	5.932123000	2.530399000
C	1.530692000	5.589577000	0.766914000
H	1.219009000	6.226645000	1.597258000
C	0.997417000	5.806618000	-0.500071000
H	0.290021000	6.622587000	-0.665582000
C	1.331545000	4.948899000	-1.545071000
H	0.866592000	5.089572000	-2.523115000
C	2.235533000	3.894814000	-1.361354000
C	2.468267000	2.923891000	-2.512530000
H	3.244837000	2.218664000	-2.197647000
C	2.946330000	3.627112000	-3.791448000
H	3.198030000	2.884351000	-4.565540000
H	3.836248000	4.247452000	-3.612545000
H	2.163026000	4.280302000	-4.208128000
C	1.204274000	2.093952000	-2.802453000
H	1.402307000	1.365753000	-3.605599000
H	0.369182000	2.734865000	-3.128864000
H	0.878311000	1.537742000	-1.915549000
N	0.444337000	-4.666038000	0.116876000
C	-0.521189000	-3.708916000	0.344579000
C	-0.079118000	-6.051754000	-0.058266000
C	0.019597000	-6.525731000	-1.517922000
H	-0.380021000	-7.547722000	-1.604480000
H	1.068826000	-6.546047000	-1.845113000
H	-0.543278000	-5.883699000	-2.205510000
C	0.671331000	-7.067930000	0.809946000
H	0.246541000	-8.071119000	0.651692000
H	0.587097000	-6.829990000	1.877702000

H	1.737616000	-7.107480000	0.542406000
C	-1.537039000	-5.876136000	0.412881000
H	-1.603438000	-6.154286000	1.475906000
H	-2.229257000	-6.527959000	-0.140363000
C	-1.892065000	-4.376674000	0.264185000
C	-2.846940000	-3.931173000	1.380672000
H	-3.778037000	-4.521363000	1.345754000
H	-3.129032000	-2.874605000	1.275922000
H	-2.384614000	-4.064007000	2.370151000
C	-2.546191000	-4.076334000	-1.101379000
H	-3.498233000	-4.624091000	-1.203638000
H	-1.896468000	-4.363457000	-1.939413000
H	-2.759454000	-3.003546000	-1.196407000
C	1.817833000	-4.326590000	-0.088181000
C	2.720461000	-4.388100000	1.001229000
C	2.255693000	-4.634272000	2.430263000
H	1.191667000	-4.898345000	2.387108000
C	2.361722000	-3.344590000	3.262916000
H	1.989045000	-3.517947000	4.285553000
H	1.772251000	-2.533919000	2.815709000
H	3.406927000	-3.003200000	3.339479000
C	3.015657000	-5.779045000	3.115038000
H	2.583588000	-5.987474000	4.107027000
H	4.075865000	-5.521777000	3.269214000
H	2.980817000	-6.706588000	2.525656000
C	4.076046000	-4.121698000	0.766424000
H	4.783691000	-4.172521000	1.596564000
C	4.530500000	-3.765666000	-0.499834000
H	5.590863000	-3.560921000	-0.665106000
C	3.620401000	-3.623478000	-1.544276000
H	3.974544000	-3.289137000	-2.521673000
C	2.255548000	-3.879569000	-1.361008000
C	1.298435000	-3.593310000	-2.511740000
H	0.299415000	-3.913951000	-2.197721000
C	1.668685000	-4.356458000	-3.792068000
H	0.900067000	-4.201054000	-4.566239000
H	1.760226000	-5.437740000	-3.615295000
H	2.626441000	-4.004359000	-4.207500000
C	1.211374000	-2.083109000	-2.798753000
H	0.482061000	-1.889222000	-3.601894000
H	2.183971000	-1.679335000	-3.123944000
H	0.891968000	-1.524486000	-1.910967000

**4op**

B	1.477728000	-1.405728000	1.293247000
B	-1.895686000	-1.133280000	-1.123092000
B	-3.362575000	2.531810000	0.055720000
B	4.360002000	0.385135000	-0.790361000
C	0.195658000	-1.490104000	0.438326000
C	-2.612803000	0.131129000	-0.682497000
C	-2.255880000	3.492839000	-0.445784000
C	3.460272000	-0.356270000	-0.016739000
N	-0.721766000	-1.422967000	-0.288535000
N	-3.079110000	1.133715000	-0.272205000
N	-1.398579000	4.199215000	-0.806736000
N	2.604915000	-0.879962000	0.662035000
N	2.516322000	-1.698641000	3.605542000
C	1.464592000	-1.764761000	2.780547000
N	-1.723800000	-3.047053000	-2.830744000
C	2.247142000	-2.136706000	5.025184000
C	2.280045000	-0.953247000	6.000205000
H	2.075956000	-1.324269000	7.015495000
H	1.529657000	-0.190129000	5.762975000
H	3.270585000	-0.480016000	6.007164000
N	4.766364000	2.353481000	-2.274174000
C	3.274434000	-3.169474000	5.493418000
H	3.029729000	-3.472358000	6.522495000
H	4.291806000	-2.753122000	5.494229000
H	3.261339000	-4.068648000	4.865665000
C	0.845371000	-2.750681000	4.878810000
H	0.214936000	-2.551219000	5.756734000
H	0.936485000	-3.843060000	4.781561000
C	0.233955000	-2.179481000	3.579660000
C	-0.640675000	-3.235533000	2.893837000
H	-1.413643000	-3.582921000	3.597917000
H	-0.044138000	-4.103598000	2.577337000
H	-1.151913000	-2.842080000	2.009454000
C	-0.597271000	-0.904328000	3.844843000
H	-1.429937000	-1.137474000	4.525903000
H	-1.018386000	-0.508608000	2.910876000
H	0.006116000	-0.108520000	4.302594000
C	3.816963000	-1.211621000	3.220810000
C	4.099908000	0.168654000	3.336961000
C	3.047332000	1.225102000	3.655064000
H	2.127405000	0.709335000	3.953464000

C	2.704597000	2.064307000	2.410225000
H	1.961543000	2.835504000	2.665664000
H	2.285341000	1.449829000	1.605935000
H	3.590978000	2.578190000	2.010353000
C	3.469645000	2.149119000	4.807656000
H	2.636779000	2.813580000	5.086225000
H	4.312806000	2.793429000	4.513031000
H	3.775847000	1.589334000	5.703688000
C	5.404434000	0.591575000	3.055221000
H	5.649824000	1.648345000	3.152542000
C	6.379702000	-0.300454000	2.621073000
H	7.386315000	0.058272000	2.395385000
C	6.054623000	-1.640324000	2.429844000
H	6.808325000	-2.325466000	2.036913000
C	4.772913000	-2.124486000	2.720114000
C	4.448443000	-3.577747000	2.394108000
H	3.435051000	-3.789951000	2.760575000
C	4.428045000	-3.805562000	0.872345000
H	4.163278000	-4.851536000	0.647621000
H	5.416886000	-3.607142000	0.429518000
H	3.697613000	-3.151672000	0.381386000
C	5.417687000	-4.563686000	3.064131000
H	5.090155000	-5.601247000	2.890771000
H	5.487518000	-4.403031000	4.149330000
H	6.433299000	-4.469000000	2.648862000
C	-2.297441000	-1.902288000	-2.330806000
C	-2.270394000	-3.490375000	-4.151837000
C	-1.397931000	-3.044035000	-5.340315000
H	-1.935798000	-3.248411000	-6.278869000
H	-0.449304000	-3.593150000	-5.376331000
H	-1.178261000	-1.969143000	-5.304568000
C	-2.426905000	-5.010790000	-4.221053000
H	-2.821878000	-5.292649000	-5.208723000
H	-3.121482000	-5.386956000	-3.460465000
H	-1.458859000	-5.516505000	-4.086476000
C	-3.619383000	-2.753445000	-4.160254000
H	-4.390851000	-3.417194000	-3.740227000
H	-3.939741000	-2.484107000	-5.176984000
C	-3.468424000	-1.513195000	-3.243543000
C	-4.771193000	-1.309451000	-2.458886000
H	-5.616389000	-1.192493000	-3.156435000
H	-4.743182000	-0.416827000	-1.826078000

H	-4.982902000	-2.170073000	-1.808529000
C	-3.150580000	-0.228286000	-4.033495000
H	-3.965746000	-0.003057000	-4.740601000
H	-2.214405000	-0.314265000	-4.603009000
H	-3.045152000	0.626274000	-3.350606000
C	-0.811935000	-3.815103000	-2.039130000
C	-1.338261000	-4.642054000	-1.015134000
C	-2.835243000	-4.816267000	-0.794972000
H	-3.349743000	-4.312405000	-1.622017000
C	-3.307506000	-4.133636000	0.494719000
H	-4.402093000	-4.214293000	0.593877000
H	-3.050048000	-3.067483000	0.483743000
H	-2.853742000	-4.596656000	1.385432000
C	-3.248390000	-6.295657000	-0.814169000
H	-4.345579000	-6.387924000	-0.770836000
H	-2.839373000	-6.840463000	0.051584000
H	-2.895879000	-6.806095000	-1.723163000
C	-0.443315000	-5.309565000	-0.170460000
H	-0.834361000	-5.941406000	0.630039000
C	0.935062000	-5.177041000	-0.329495000
H	1.619180000	-5.697389000	0.345525000
C	1.438226000	-4.375929000	-1.350218000
H	2.517876000	-4.269841000	-1.468125000
C	0.582106000	-3.680732000	-2.214594000
C	1.181795000	-2.775521000	-3.275958000
H	0.349468000	-2.296528000	-3.800139000
C	2.005668000	-3.575598000	-4.296244000
H	2.340487000	-2.925335000	-5.120605000
H	1.430426000	-4.409274000	-4.727721000
H	2.905364000	-4.006188000	-3.827416000
C	2.021937000	-1.654082000	-2.662694000
H	2.391437000	-0.975478000	-3.445796000
H	2.897768000	-2.044798000	-2.125676000
H	1.437430000	-1.057533000	-1.956557000
C	4.974995000	1.054556000	-1.912841000
C	5.300109000	2.679717000	-3.629534000
C	5.820563000	4.114493000	-3.721658000
H	6.159582000	4.312795000	-4.749479000
H	6.666477000	4.293508000	-3.046990000
H	5.026256000	4.836504000	-3.481489000
C	4.219699000	2.485460000	-4.707610000
H	4.662050000	2.615240000	-5.707503000

H	3.415934000	3.223637000	-4.593162000
H	3.769814000	1.485438000	-4.657200000
C	6.418983000	1.625688000	-3.749675000
H	7.357382000	2.056219000	-3.368021000
H	6.594112000	1.328468000	-4.793670000
C	6.005205000	0.422058000	-2.859498000
C	7.204304000	-0.103899000	-2.050689000
H	8.000524000	-0.456040000	-2.727775000
H	6.902821000	-0.942532000	-1.404285000
H	7.618988000	0.684188000	-1.404338000
C	5.408954000	-0.735595000	-3.676386000
H	6.169249000	-1.147492000	-4.359499000
H	4.547655000	-0.414901000	-4.276948000
H	5.067709000	-1.543889000	-3.013728000
C	4.045121000	3.262815000	-1.428753000
C	2.633648000	3.334822000	-1.456965000
C	1.766529000	2.441586000	-2.331530000
H	2.430721000	1.762950000	-2.881956000
C	0.828386000	1.577121000	-1.474011000
H	0.236295000	0.902171000	-2.110983000
H	0.120200000	2.199181000	-0.912821000
H	1.394369000	0.965970000	-0.762295000
C	0.944117000	3.261084000	-3.340825000
H	0.429546000	2.588669000	-4.046824000
H	1.573574000	3.952275000	-3.922889000
H	0.174388000	3.853145000	-2.823727000
C	1.994741000	4.256272000	-0.609399000
H	0.904791000	4.336127000	-0.627356000
C	2.730608000	5.059772000	0.255463000
H	2.213793000	5.770128000	0.905553000
C	4.119835000	4.946100000	0.308609000
H	4.684315000	5.559917000	1.013937000
C	4.799961000	4.048542000	-0.520636000
C	6.307153000	3.885243000	-0.372778000
H	6.663553000	3.307561000	-1.234104000
C	7.058147000	5.222536000	-0.362839000
H	8.146951000	5.052232000	-0.364978000
H	6.823177000	5.815337000	0.535193000
H	6.804084000	5.835930000	-1.240766000
C	6.635577000	3.050415000	0.873265000
H	7.722424000	2.882861000	0.959248000
H	6.136592000	2.073329000	0.822609000



H	6.298830000	3.563043000	1.789502000
N	-5.612174000	2.325838000	1.305004000
C	-4.521258000	3.039555000	0.808481000
C	-6.427275000	3.113604000	2.277240000
C	-7.918219000	2.787857000	2.181535000
H	-8.477166000	3.431058000	2.878566000
H	-8.121242000	1.739895000	2.446682000
H	-8.306076000	2.961866000	1.169454000
C	-5.961690000	2.896701000	3.730963000
H	-6.419941000	3.652712000	4.388044000
H	-4.870765000	2.986295000	3.816494000
H	-6.255355000	1.909754000	4.106533000
C	-6.120479000	4.549530000	1.820822000
H	-6.195432000	5.274534000	2.644800000
H	-6.861125000	4.843532000	1.060869000
C	-4.709984000	4.526432000	1.182334000
C	-3.624628000	5.010049000	2.164931000
H	-3.825332000	6.049517000	2.475391000
H	-2.634841000	4.979708000	1.689364000
H	-3.581826000	4.385745000	3.068241000
C	-4.700125000	5.456536000	-0.047576000
H	-4.987131000	6.478104000	0.256174000
H	-5.418377000	5.114082000	-0.807579000
H	-3.709125000	5.506664000	-0.514963000
C	-6.102605000	1.115479000	0.729473000
C	-5.966952000	-0.115921000	1.410684000
C	-5.169714000	-0.241990000	2.697164000
H	-4.757384000	0.750116000	2.918214000
C	-3.987522000	-1.204502000	2.535758000
H	-3.405213000	-1.251279000	3.467442000
H	-3.319329000	-0.884460000	1.724626000
H	-4.328672000	-2.225359000	2.309282000
C	-6.054259000	-0.684627000	3.873571000
H	-5.494605000	-0.642842000	4.822477000
H	-6.401804000	-1.721767000	3.738262000
H	-6.948636000	-0.052445000	3.976017000
C	-6.580680000	-1.260906000	0.881847000
H	-6.483071000	-2.212419000	1.409877000
C	-7.310813000	-1.205070000	-0.300132000
H	-7.791231000	-2.103639000	-0.695105000
C	-7.403680000	0.001253000	-0.991415000
H	-7.954323000	0.037610000	-1.933652000

C	-6.802058000	1.167405000	-0.506584000
C	-6.906023000	2.444405000	-1.326813000
H	-6.559191000	3.268158000	-0.693784000
C	-8.344371000	2.765682000	-1.756430000
H	-8.383849000	3.752617000	-2.244820000
H	-9.032418000	2.782828000	-0.896987000
H	-8.732632000	2.029511000	-2.478263000
C	-5.970493000	2.387373000	-2.545210000
H	-6.004957000	3.336494000	-3.104421000
H	-6.263037000	1.576845000	-3.232677000
H	-4.931840000	2.219369000	-2.229701000

**TS4<sub>op-cl</sub>** (im. freq.: -21.4 cm<sup>-1</sup>)

B	3.193536000	-0.618242000	-0.968985000
B	1.145299000	2.109241000	1.144456000
B	-2.191365000	1.267003000	-1.071087000
B	-1.680225000	-2.362059000	0.730582000
C	2.563103000	0.343731000	-0.137519000
C	-0.195200000	2.170778000	0.374858000
C	-2.330085000	-0.139169000	-0.488369000
C	-0.167785000	-2.461229000	0.376518000
N	2.034060000	1.159910000	0.577919000
N	-1.113557000	1.960126000	-0.333408000
N	-2.244811000	-1.136655000	0.139047000
N	0.971882000	-2.439980000	0.114027000
N	4.267564000	-2.456214000	-2.435060000
C	4.101211000	-1.185945000	-1.943968000
N	2.473608000	2.882736000	3.227071000
C	5.429214000	-2.596554000	-3.381168000
C	5.089121000	-3.446759000	-4.612531000
H	5.970870000	-3.492344000	-5.270776000
H	4.261279000	-3.019777000	-5.191736000
H	4.824537000	-4.477383000	-4.333774000
N	-3.675114000	-3.368122000	2.068502000
C	6.659005000	-3.233139000	-2.703075000
H	7.506630000	-3.235489000	-3.406610000
H	6.456798000	-4.276091000	-2.424183000
H	6.970732000	-2.690730000	-1.801050000
C	5.676384000	-1.124525000	-3.764918000
H	5.109981000	-0.895390000	-4.681194000
H	6.737522000	-0.926420000	-3.979887000
C	5.142778000	-0.246220000	-2.607090000

C	6.254435000	0.134406000	-1.605183000
H	7.038691000	0.721912000	-2.112276000
H	6.728941000	-0.748478000	-1.154458000
H	5.842383000	0.737597000	-0.783697000
C	4.510972000	1.044833000	-3.155125000
H	5.268562000	1.637755000	-3.695252000
H	4.106678000	1.669407000	-2.345226000
H	3.688382000	0.821677000	-3.850698000
C	3.388012000	-3.561002000	-2.138895000
C	2.235835000	-3.759326000	-2.946195000
C	1.773297000	-2.756048000	-4.002001000
H	2.583645000	-2.028279000	-4.148345000
C	0.547020000	-1.966225000	-3.505696000
H	0.268444000	-1.191285000	-4.239594000
H	0.745883000	-1.479291000	-2.541724000
H	-0.322975000	-2.628646000	-3.368338000
C	1.473979000	-3.405654000	-5.365001000
H	1.253388000	-2.630247000	-6.117087000
H	0.593066000	-4.065515000	-5.316149000
H	2.317568000	-4.008604000	-5.734854000
C	1.451896000	-4.898005000	-2.718243000
H	0.563114000	-5.067383000	-3.330006000
C	1.772436000	-5.811251000	-1.717547000
H	1.150352000	-6.696397000	-1.562216000
C	2.865876000	-5.570918000	-0.891726000
H	3.081092000	-6.263698000	-0.074902000
C	3.680517000	-4.443093000	-1.068456000
C	4.773658000	-4.168808000	-0.038742000
H	5.348517000	-3.300839000	-0.385937000
C	4.145185000	-3.776160000	1.312369000
H	4.927751000	-3.457357000	2.021678000
H	3.610001000	-4.627742000	1.764078000
H	3.419920000	-2.960363000	1.189599000
C	5.749081000	-5.344250000	0.143888000
H	6.563796000	-5.064464000	0.832150000
H	6.204264000	-5.662156000	-0.806862000
H	5.246635000	-6.223819000	0.577706000
C	1.391981000	2.921405000	2.413394000
C	2.379216000	3.777339000	4.448579000
C	2.053800000	2.984795000	5.727697000
H	1.920720000	3.694095000	6.559195000
H	2.873399000	2.307450000	5.999203000

H	1.130994000	2.397485000	5.637768000
C	3.670953000	4.563133000	4.704254000
H	3.530160000	5.192431000	5.596581000
H	3.924288000	5.226408000	3.868428000
H	4.524048000	3.895886000	4.896515000
C	1.220107000	4.700066000	4.039595000
H	1.631466000	5.622933000	3.601552000
H	0.607746000	4.997957000	4.903448000
C	0.392762000	3.952529000	2.965242000
C	-0.078526000	4.957182000	1.898959000
H	-0.661265000	5.759312000	2.382517000
H	-0.718940000	4.494998000	1.138846000
H	0.774395000	5.422607000	1.381661000
C	-0.837093000	3.238936000	3.571500000
H	-1.511229000	3.979609000	4.032370000
H	-0.555560000	2.508762000	4.343868000
H	-1.402163000	2.700179000	2.798474000
C	3.649264000	2.076908000	2.974923000
C	4.699255000	2.631294000	2.193992000
C	4.609158000	3.990989000	1.497661000
H	3.702579000	4.495034000	1.859101000
C	4.449560000	3.834829000	-0.026921000
H	4.330912000	4.823038000	-0.501319000
H	3.570245000	3.226286000	-0.278637000
H	5.335955000	3.356211000	-0.473720000
C	5.810406000	4.902423000	1.809990000
H	5.646182000	5.908016000	1.389537000
H	6.740203000	4.514500000	1.364180000
H	5.982782000	5.009102000	2.891309000
C	5.862009000	1.869743000	2.013807000
H	6.684102000	2.280790000	1.423801000
C	5.988621000	0.596131000	2.563164000
H	6.905543000	0.021134000	2.410770000
C	4.933134000	0.050315000	3.285970000
H	5.024935000	-0.962583000	3.683338000
C	3.744402000	0.764110000	3.503354000
C	2.608668000	0.061018000	4.245497000
H	1.799500000	0.787363000	4.385965000
C	3.039211000	-0.448395000	5.634104000
H	2.166723000	-0.834023000	6.185955000
H	3.510212000	0.335182000	6.247348000
H	3.760342000	-1.277244000	5.551122000

C	2.023696000	-1.100550000	3.422431000
H	1.165281000	-1.543989000	3.951382000
H	2.766536000	-1.898798000	3.270824000
H	1.677155000	-0.779740000	2.431989000
C	-2.352963000	-3.347716000	1.605651000
C	-3.914013000	-4.380103000	3.147023000
C	-5.300475000	-5.030217000	3.056039000
H	-5.397717000	-5.789598000	3.848043000
H	-5.458295000	-5.530180000	2.091681000
H	-6.106048000	-4.293750000	3.197626000
C	-3.759621000	-3.792388000	4.568565000
H	-3.758715000	-4.608558000	5.309185000
H	-4.590784000	-3.121686000	4.821358000
H	-2.820287000	-3.234294000	4.680768000
C	-2.788967000	-5.387593000	2.849917000
H	-3.171884000	-6.149926000	2.152489000
H	-2.456172000	-5.918803000	3.755075000
C	-1.637819000	-4.601680000	2.170361000
C	-1.016431000	-5.480072000	1.062909000
H	-0.650200000	-6.427823000	1.496733000
H	-0.169660000	-4.984252000	0.570728000
H	-1.760976000	-5.726900000	0.289992000
C	-0.524841000	-4.236574000	3.177702000
H	-0.092118000	-5.151694000	3.618267000
H	-0.899351000	-3.610138000	4.000243000
H	0.283597000	-3.684300000	2.679496000
C	-4.741330000	-2.616937000	1.473721000
C	-5.198984000	-1.405128000	2.056364000
C	-4.523014000	-0.756552000	3.261709000
H	-3.704618000	-1.418212000	3.569779000
C	-3.888689000	0.599200000	2.903072000
H	-3.373023000	1.022206000	3.781427000
H	-4.647536000	1.331002000	2.580636000
H	-3.154868000	0.494766000	2.092593000
C	-5.488006000	-0.589531000	4.450300000
H	-4.945765000	-0.240959000	5.344998000
H	-5.997367000	-1.530937000	4.707678000
H	-6.271055000	0.155069000	4.231565000
C	-6.307018000	-0.755119000	1.489440000
H	-6.671404000	0.171561000	1.940039000
C	-6.945616000	-1.260329000	0.361740000
H	-7.809748000	-0.741517000	-0.061919000

C	-6.464250000	-2.424314000	-0.234408000
H	-6.957181000	-2.806840000	-1.131373000
C	-5.368078000	-3.118262000	0.295597000
C	-4.889817000	-4.379733000	-0.423259000
H	-4.166925000	-4.877050000	0.236258000
C	-6.028200000	-5.376986000	-0.705839000
H	-5.618689000	-6.319040000	-1.106172000
H	-6.737861000	-4.989906000	-1.454961000
H	-6.604393000	-5.615861000	0.201542000
C	-4.144553000	-4.037646000	-1.726657000
H	-3.775791000	-4.956823000	-2.212011000
H	-3.279166000	-3.390659000	-1.525810000
H	-4.806460000	-3.523109000	-2.443093000
N	-2.955308000	3.022825000	-2.825333000
C	-2.946377000	1.761962000	-2.259599000
C	-3.882539000	3.179384000	-4.002918000
C	-5.173480000	3.944325000	-3.648304000
H	-5.829431000	3.977839000	-4.532289000
H	-4.952236000	4.982100000	-3.362992000
H	-5.736118000	3.471113000	-2.833912000
C	-3.233216000	3.914561000	-5.184381000
H	-3.961920000	3.982096000	-6.007289000
H	-2.352148000	3.384128000	-5.565741000
H	-2.939047000	4.940316000	-4.915747000
C	-4.160050000	1.707763000	-4.348772000
H	-3.451411000	1.385406000	-5.127998000
H	-5.173230000	1.562465000	-4.753410000
C	-3.915150000	0.873379000	-3.068281000
C	-3.318625000	-0.489567000	-3.466392000
H	-3.995957000	-0.997601000	-4.174138000
H	-3.184735000	-1.151800000	-2.602035000
H	-2.339805000	-0.369157000	-3.954900000
C	-5.222990000	0.632824000	-2.283357000
H	-5.949918000	0.088502000	-2.910103000
H	-5.693745000	1.572430000	-1.959189000
H	-5.037133000	0.031302000	-1.383750000
C	-2.212106000	4.142477000	-2.309901000
C	-0.918874000	4.423363000	-2.831192000
C	-0.200220000	3.509483000	-3.824130000
H	-0.917703000	2.742920000	-4.145066000
C	0.974797000	2.766845000	-3.162362000
H	1.459139000	2.097356000	-3.891172000

H	0.643105000	2.154261000	-2.314525000
H	1.740519000	3.470704000	-2.796266000
C	0.293792000	4.259603000	-5.075167000
H	0.688379000	3.545447000	-5.816400000
H	1.112268000	4.956686000	-4.832693000
H	-0.505163000	4.842164000	-5.556779000
C	-0.251045000	5.574141000	-2.386582000
H	0.739061000	5.805448000	-2.786164000
C	-0.822047000	6.427277000	-1.446507000
H	-0.290453000	7.326828000	-1.124676000
C	-2.064750000	6.115252000	-0.902108000
H	-2.492552000	6.769927000	-0.139260000
C	-2.775007000	4.972912000	-1.301269000
C	-4.089335000	4.655892000	-0.586491000
H	-4.550083000	3.805052000	-1.100852000
C	-5.086078000	5.828809000	-0.611924000
H	-6.056352000	5.514442000	-0.193909000
H	-5.263293000	6.205322000	-1.630317000
H	-4.731786000	6.676642000	-0.003414000
C	-3.844870000	4.208626000	0.867034000
H	-4.799801000	3.942436000	1.349363000
H	-3.383071000	5.012039000	1.463956000
H	-3.191131000	3.326955000	0.908517000

#### 4cl; B3LYP-D3(BJ)/def2-SVP

B	0.600764000	-2.543116000	-0.743981000
B	2.481515000	0.574607000	1.007884000
B	-0.601176000	2.543251000	-0.743947000
B	-2.481870000	-0.574567000	1.007814000
C	1.633661000	-1.635667000	-0.106885000
C	1.568353000	1.608814000	0.380573000
C	-1.634295000	1.635811000	-0.107101000
C	-1.568720000	-1.608838000	0.380599000
N	2.153813000	-0.760113000	0.489089000
N	0.722572000	2.170423000	-0.223618000
N	-2.154090000	0.760043000	0.488869000
N	-0.723139000	-2.170423000	-0.223912000
N	-0.069543000	-4.125651000	-2.631665000
C	0.865439000	-3.473513000	-1.866850000
N	4.249926000	-0.065850000	2.724110000
C	0.481869000	-4.929533000	-3.766082000
C	-0.184181000	-4.568130000	-5.098667000

H	0.259266000	-5.173721000	-5.903760000
H	-0.036245000	-3.511308000	-5.351206000
H	-1.264032000	-4.775559000	-5.074541000
N	-4.250177000	0.065897000	2.724180000
C	0.304644000	-6.442956000	-3.559264000
H	0.721914000	-6.981106000	-4.423955000
H	-0.761032000	-6.701291000	-3.486269000
H	0.812741000	-6.809108000	-2.659592000
C	1.958653000	-4.492956000	-3.741926000
H	2.104477000	-3.681247000	-4.471394000
H	2.637550000	-5.312097000	-4.021617000
C	2.246640000	-3.947143000	-2.325998000
C	2.725177000	-5.062230000	-1.370835000
H	3.670733000	-5.499779000	-1.733277000
H	1.988174000	-5.871317000	-1.278039000
H	2.893485000	-4.648346000	-0.368853000
C	3.320115000	-2.855921000	-2.378267000
H	4.240980000	-3.262586000	-2.828648000
H	3.578731000	-2.490786000	-1.376662000
H	2.989185000	-1.999482000	-2.980718000
C	-1.475327000	-4.039024000	-2.375659000
C	-2.238072000	-2.999326000	-2.958821000
C	-1.618225000	-1.871348000	-3.774682000
H	-0.551434000	-2.098048000	-3.898471000
C	-1.709898000	-0.530056000	-3.030971000
H	-1.296234000	0.282641000	-3.647806000
H	-1.149818000	-0.549121000	-2.091179000
H	-2.753961000	-0.275414000	-2.794771000
C	-2.254911000	-1.742326000	-5.167644000
H	-1.706859000	-1.000721000	-5.771165000
H	-3.298975000	-1.397564000	-5.097359000
H	-2.256139000	-2.695841000	-5.714599000
C	-3.618937000	-2.973727000	-2.720980000
H	-4.222120000	-2.175538000	-3.158145000
C	-4.233471000	-3.936192000	-1.925496000
H	-5.312670000	-3.900815000	-1.757882000
C	-3.462217000	-4.918947000	-1.309910000
H	-3.941701000	-5.638220000	-0.643037000
C	-2.076222000	-4.975574000	-1.499089000
C	-1.255209000	-5.970360000	-0.688228000
H	-0.232474000	-5.941931000	-1.076262000
C	-1.172279000	-5.548472000	0.789019000



H	-0.509928000	-6.233607000	1.343024000
H	-2.161918000	-5.576436000	1.270518000
H	-0.770488000	-4.531751000	0.888804000
C	-1.770907000	-7.410541000	-0.808343000
H	-1.089600000	-8.106411000	-0.292758000
H	-1.854583000	-7.730440000	-1.857565000
H	-2.764069000	-7.524246000	-0.345195000
C	3.449521000	0.853619000	2.091235000
C	5.021092000	0.481382000	3.880866000
C	4.336581000	0.185418000	5.227348000
H	4.859079000	0.725861000	6.031965000
H	4.370924000	-0.884188000	5.467691000
H	3.286663000	0.507073000	5.227686000
C	6.446463000	-0.072001000	3.930053000
H	6.982337000	0.373883000	4.781790000
H	7.005510000	0.164592000	3.016381000
H	6.446793000	-1.164161000	4.061770000
C	4.988384000	1.986887000	3.563496000
H	5.893370000	2.250521000	2.994644000
H	4.985985000	2.602039000	4.475063000
C	3.741135000	2.238240000	2.678924000
C	4.081513000	3.252935000	1.578477000
H	4.407913000	4.207907000	2.025083000
H	3.218048000	3.456223000	0.936742000
H	4.888742000	2.879272000	0.931429000
C	2.540752000	2.763219000	3.488878000
H	2.788463000	3.726560000	3.964906000
H	2.236327000	2.058499000	4.275627000
H	1.674224000	2.917687000	2.831722000
C	4.457370000	-1.381560000	2.201854000
C	5.368234000	-1.544148000	1.126806000
C	6.063925000	-0.365518000	0.456288000
H	5.877929000	0.522866000	1.072726000
C	5.464866000	-0.080147000	-0.931549000
H	5.939283000	0.809395000	-1.377222000
H	4.386282000	0.111870000	-0.863051000
H	5.626088000	-0.928510000	-1.615882000
C	7.584422000	-0.559000000	0.357399000
H	8.063024000	0.358017000	-0.022407000
H	7.845424000	-1.373826000	-0.336317000
H	8.030953000	-0.800338000	1.333929000
C	5.604113000	-2.835682000	0.641994000

H	6.305575000	-2.979204000	-0.182360000
C	4.954772000	-3.940850000	1.187806000
H	5.160307000	-4.941640000	0.801895000
C	4.021435000	-3.760692000	2.204284000
H	3.482287000	-4.624894000	2.598416000
C	3.744811000	-2.486631000	2.718914000
C	2.660277000	-2.340878000	3.775896000
H	2.615805000	-1.281406000	4.052400000
C	2.983063000	-3.160143000	5.035566000
H	2.263276000	-2.936427000	5.839392000
H	3.995711000	-2.952831000	5.413954000
H	2.925049000	-4.241665000	4.832597000
C	1.270153000	-2.716623000	3.237208000
H	0.517500000	-2.611655000	4.034254000
H	1.237426000	-3.759072000	2.881860000
H	0.972351000	-2.069411000	2.403673000
C	-3.449720000	-0.853512000	2.091341000
C	-5.021397000	-0.481301000	3.880931000
C	-6.446901000	0.071782000	3.929838000
H	-6.982738000	-0.373908000	4.781700000
H	-7.005846000	-0.165248000	3.016220000
H	-6.447465000	1.163987000	4.061189000
C	-4.337169000	-0.184897000	5.227457000
H	-4.859740000	-0.725183000	6.032134000
H	-4.371708000	0.884781000	5.467474000
H	-3.287209000	-0.506405000	5.228074000
C	-4.988318000	-1.986842000	3.563814000
H	-5.893234000	-2.250775000	2.994983000
H	-4.985825000	-2.601847000	4.475481000
C	-3.741013000	-2.238100000	2.679291000
C	-4.081183000	-3.253149000	1.579101000
H	-4.407392000	-4.208060000	2.025969000
H	-3.217679000	-3.456447000	0.937419000
H	-4.888477000	-2.879807000	0.931950000
C	-2.540481000	-2.762578000	3.489347000
H	-2.787979000	-3.725834000	3.965659000
H	-2.236185000	-2.057565000	4.275884000
H	-1.673951000	-2.917049000	2.832194000
C	-4.457378000	1.381693000	2.202003000
C	-3.744548000	2.486577000	2.719089000
C	-2.659856000	2.340509000	3.775880000
H	-2.615732000	1.281054000	4.052495000

C	-1.269707000	2.715620000	3.236816000
H	-0.516937000	2.610592000	4.033739000
H	-1.236667000	3.757962000	2.881175000
H	-0.972299000	2.068070000	2.403395000
C	-2.982053000	3.160026000	5.035532000
H	-2.262220000	2.936052000	5.839244000
H	-3.994726000	2.953169000	5.414112000
H	-2.923606000	4.241504000	4.832479000
C	-4.020999000	3.760727000	2.204593000
H	-3.481637000	4.624799000	2.598716000
C	-4.954414000	3.941135000	1.188236000
H	-5.159851000	4.941999000	0.802465000
C	-5.603976000	2.836132000	0.642350000
H	-6.305432000	2.979865000	-0.181972000
C	-5.368261000	1.544507000	1.127003000
C	-6.064051000	0.366036000	0.456317000
H	-5.878100000	-0.522467000	1.072596000
C	-7.584538000	0.559674000	0.357483000
H	-8.063245000	-0.357235000	-0.022449000
H	-7.845450000	1.374640000	-0.336107000
H	-8.031002000	0.800916000	1.334067000
C	-5.465026000	0.080817000	-0.931565000
H	-5.939494000	-0.808650000	-1.377331000
H	-4.386443000	-0.111257000	-0.863099000
H	-5.626204000	0.929255000	-1.615808000
N	0.069539000	4.125622000	-2.631670000
C	-0.865586000	3.473617000	-1.866907000
C	-0.481670000	4.929660000	-3.766069000
C	-0.304348000	6.443060000	-3.559180000
H	-0.721675000	6.981248000	-4.423820000
H	0.761336000	6.701365000	-3.486273000
H	-0.812360000	6.809202000	-2.659461000
C	0.184491000	4.568260000	-5.098598000
H	-0.258644000	5.174055000	-5.903710000
H	0.036342000	3.511502000	-5.351287000
H	1.264388000	4.775416000	-5.074251000
C	-1.958513000	4.493263000	-3.742076000
H	-2.104342000	3.681609000	-4.471595000
H	-2.637290000	5.312496000	-4.021786000
C	-2.246707000	3.947379000	-2.326228000
C	-3.320259000	2.856258000	-2.378738000
H	-4.241033000	3.263035000	-2.829202000

H	-3.579033000	2.491055000	-1.377201000
H	-2.989300000	1.999852000	-2.981217000
C	-2.725270000	5.062392000	-1.371018000
H	-3.670625000	5.500253000	-1.733619000
H	-1.988101000	5.871295000	-1.277831000
H	-2.893915000	4.648387000	-0.369150000
C	1.475316000	4.038765000	-2.375626000
C	2.237847000	2.998892000	-2.958744000
C	1.617759000	1.870937000	-3.774452000
H	0.551028000	2.097887000	-3.898310000
C	1.709110000	0.529747000	-3.030519000
H	1.295479000	-0.283005000	-3.647291000
H	1.148835000	0.549042000	-2.090841000
H	2.753085000	0.275007000	-2.794035000
C	2.254442000	1.741574000	-5.167387000
H	1.706202000	1.000031000	-5.770813000
H	3.298425000	1.396577000	-5.097072000
H	2.255881000	2.695033000	-5.714441000
C	3.618740000	2.973119000	-2.721024000
H	4.221767000	2.174803000	-3.158165000
C	4.233471000	3.935580000	-1.925697000
H	5.312678000	3.900093000	-1.758174000
C	3.462405000	4.918490000	-1.310110000
H	3.942062000	5.637754000	-0.643349000
C	2.076402000	4.975300000	-1.499168000
C	1.255608000	5.970275000	-0.688344000
H	0.232867000	5.942104000	-1.076386000
C	1.771690000	7.410326000	-0.808388000
H	1.090485000	8.106373000	-0.292913000
H	1.855618000	7.730204000	-1.857591000
H	2.764807000	7.523788000	-0.345079000
C	1.172557000	5.548374000	0.788904000
H	0.510452000	6.233734000	1.342926000
H	2.162226000	5.575983000	1.270364000
H	0.770420000	4.531790000	0.888652000

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B	-0.644800000	2.530158000	-0.752103000
B	-2.475282000	-0.620981000	0.994582000
B	0.644767000	-2.530174000	-0.752228000
B	2.475266000	0.620878000	0.994600000
C	-1.655452000	1.597939000	-0.114501000

C	-1.542118000	-1.636623000	0.364382000
C	1.655437000	-1.597987000	-0.114604000
C	1.542094000	1.636550000	0.364450000
N	-2.164347000	0.716096000	0.478471000
N	-0.684724000	-2.181984000	-0.234724000
N	2.164328000	-0.716182000	0.478434000
N	0.684696000	2.181930000	-0.234633000
N	-0.041375000	4.153115000	-2.625709000
C	-0.943782000	3.460301000	-1.868289000
N	-4.241468000	-0.027987000	2.727103000
C	-0.621878000	4.947778000	-3.739336000
C	0.056522000	4.641201000	-5.071931000
H	-0.411809000	5.241850000	-5.865872000
H	-0.045409000	3.583592000	-5.344776000
H	1.126590000	4.895637000	-5.042582000
N	4.241505000	0.027829000	2.727058000
C	-0.511605000	6.457741000	-3.510044000
H	-0.943970000	6.989630000	-4.370662000
H	0.542120000	6.759632000	-3.425935000
H	-1.042156000	6.791721000	-2.610273000
C	-2.070593000	4.446890000	-3.723592000
H	-2.174322000	3.631645000	-4.457004000
H	-2.786278000	5.234082000	-4.004021000
C	-2.338159000	3.882371000	-2.319118000
C	-2.854386000	4.962515000	-1.355833000
H	-3.806591000	5.381271000	-1.722020000
H	-2.140225000	5.788935000	-1.237509000
H	-3.023967000	4.526121000	-0.362763000
C	-3.364176000	2.756227000	-2.384352000
H	-4.297296000	3.131437000	-2.835859000
H	-3.614733000	2.373859000	-1.386013000
H	-2.998245000	1.917260000	-2.991998000
C	1.360986000	4.112776000	-2.375370000
C	2.155998000	3.111020000	-2.974787000
C	1.576832000	1.980854000	-3.806822000
H	0.500271000	2.173320000	-3.919171000
C	1.720033000	0.636877000	-3.091989000
H	1.322594000	-0.177086000	-3.718123000
H	1.172870000	0.620924000	-2.143041000
H	2.775428000	0.409997000	-2.876051000
C	2.209587000	1.902812000	-5.197092000
H	1.692009000	1.149127000	-5.811397000

H	3.267032000	1.600604000	-5.135970000
H	2.170293000	2.863749000	-5.729046000
C	3.534435000	3.129765000	-2.741142000
H	4.163084000	2.359488000	-3.194235000
C	4.116982000	4.098062000	-1.934443000
H	5.197507000	4.098153000	-1.771191000
C	3.316057000	5.042711000	-1.304575000
H	3.772365000	5.771122000	-0.630087000
C	1.931443000	5.055471000	-1.489854000
C	1.084319000	6.012803000	-0.671850000
H	0.061993000	5.952613000	-1.063026000
C	1.017137000	5.574428000	0.792992000
H	0.337466000	6.233017000	1.357012000
H	2.006863000	5.624938000	1.272986000
H	0.643626000	4.545327000	0.881855000
C	1.553189000	7.462162000	-0.777940000
H	0.853593000	8.131491000	-0.253156000
H	1.625269000	7.797483000	-1.822928000
H	2.543223000	7.601499000	-0.315773000
C	-3.427184000	-0.922350000	2.087111000
C	-4.975525000	-0.592087000	3.888044000
C	-4.278649000	-0.290204000	5.219276000
H	-4.771867000	-0.850961000	6.027900000
H	-4.337434000	0.776190000	5.470667000
H	-3.220294000	-0.582942000	5.199354000
C	-6.405539000	-0.072580000	3.962369000
H	-6.919242000	-0.535795000	4.817814000
H	-6.972124000	-0.314067000	3.053982000
H	-6.427505000	1.018501000	4.102161000
C	-4.916009000	-2.088237000	3.562850000
H	-5.818278000	-2.363394000	2.993927000
H	-4.900870000	-2.710621000	4.469684000
C	-3.674716000	-2.309422000	2.675353000
C	-3.997332000	-3.329306000	1.583437000
H	-4.292555000	-4.291790000	2.034799000
H	-3.134945000	-3.510712000	0.931127000
H	-4.821673000	-2.978717000	0.944737000
C	-2.459360000	-2.800273000	3.470972000
H	-2.677948000	-3.769169000	3.949013000
H	-2.162475000	-2.088992000	4.254337000
H	-1.595699000	-2.933737000	2.804696000
C	-4.506183000	1.267566000	2.197696000

C	-5.427370000	1.381413000	1.128758000
C	-6.079284000	0.174487000	0.478336000
H	-5.846580000	-0.699535000	1.102894000
C	-5.487010000	-0.094673000	-0.906801000
H	-5.930372000	-1.004160000	-1.343065000
H	-4.400260000	-0.244721000	-0.847143000
H	-5.688168000	0.742475000	-1.594527000
C	-7.600104000	0.304550000	0.397173000
H	-8.045257000	-0.632270000	0.026966000
H	-7.902444000	1.103827000	-0.297421000
H	-8.047080000	0.532985000	1.376313000
C	-5.722081000	2.654494000	0.636102000
H	-6.435216000	2.758591000	-0.185154000
C	-5.124393000	3.790099000	1.169973000
H	-5.377308000	4.777875000	0.777937000
C	-4.185301000	3.660364000	2.184320000
H	-3.687479000	4.551536000	2.574712000
C	-3.849058000	2.406954000	2.705664000
C	-2.767179000	2.321960000	3.763446000
H	-2.668612000	1.263723000	4.037825000
C	-3.139558000	3.119089000	5.014278000
H	-2.409982000	2.942293000	5.820186000
H	-4.138853000	2.854605000	5.392010000
H	-3.146017000	4.201327000	4.808504000
C	-1.406217000	2.771827000	3.230177000
H	-0.646464000	2.696564000	4.023487000
H	-1.427826000	3.818605000	2.887184000
H	-1.078469000	2.150748000	2.387212000
C	3.427163000	0.922200000	2.087147000
C	4.975536000	0.591873000	3.888043000
C	6.405583000	0.072447000	3.962308000
H	6.919266000	0.535619000	4.817788000
H	6.972144000	0.314048000	3.053936000
H	6.427619000	-1.018646000	4.102003000
C	4.278690000	0.289823000	5.219253000
H	4.771882000	0.850538000	6.027923000
H	4.337547000	-0.776590000	5.470547000
H	3.220317000	0.582495000	5.199370000
C	4.915927000	2.088048000	3.562979000
H	5.818180000	2.363309000	2.994080000
H	4.900750000	2.710354000	4.469866000
C	3.674626000	2.309235000	2.675500000

C	3.997183000	3.329223000	1.583667000
H	4.292343000	4.291691000	2.035105000
H	3.134786000	3.510622000	0.931369000
H	4.821550000	2.978735000	0.944944000
C	2.459237000	2.799953000	3.471155000
H	2.677765000	3.768825000	3.949273000
H	2.162388000	2.088594000	4.254462000
H	1.595571000	2.933417000	2.804884000
C	4.506340000	-1.267646000	2.197524000
C	3.849372000	-2.407150000	2.705428000
C	2.767525000	-2.322359000	3.763256000
H	2.668831000	-1.264150000	4.037696000
C	1.406600000	-2.772372000	3.230022000
H	0.646876000	-2.697263000	4.023374000
H	1.428332000	-3.819126000	2.886958000
H	1.078727000	-2.151281000	2.387113000
C	3.140062000	-3.119505000	5.014030000
H	2.410495000	-2.942851000	5.819977000
H	4.139338000	-2.854908000	5.391737000
H	3.146658000	-4.201731000	4.808197000
C	4.185756000	-3.660482000	2.183986000
H	3.688054000	-4.551743000	2.574326000
C	5.124841000	-3.790027000	1.169608000
H	5.377871000	-4.777743000	0.777496000
C	5.722378000	-2.654310000	0.635807000
H	6.435513000	-2.758259000	-0.185467000
C	5.427523000	-1.381301000	1.128563000
C	6.079292000	-0.174246000	0.478232000
H	5.846479000	0.699702000	1.102853000
C	7.600129000	-0.304115000	0.397068000
H	8.045168000	0.632789000	0.026937000
H	7.902572000	-1.103300000	-0.297588000
H	8.047129000	-0.532571000	1.376192000
C	5.486996000	0.094948000	-0.906890000
H	5.930266000	1.004512000	-1.343087000
H	4.400230000	0.244880000	-0.847231000
H	5.688249000	-0.742130000	-1.594674000
N	0.041262000	-4.153049000	-2.625869000
C	0.943715000	-3.460338000	-1.868412000
C	0.621729000	-4.947896000	-3.739382000
C	0.511248000	-6.457817000	-3.509914000
H	0.943612000	-6.989866000	-4.370432000



H	-0.542522000	-6.759565000	-3.425849000
H	1.041685000	-6.791753000	-2.610059000
C	-0.056551000	-4.641391000	-5.072056000
H	0.411746000	-5.242208000	-5.865889000
H	0.045541000	-3.583833000	-5.345036000
H	-1.126655000	-4.895679000	-5.042741000
C	2.070506000	-4.447183000	-3.723598000
H	2.174379000	-3.632000000	-4.457059000
H	2.786108000	-5.234484000	-4.003934000
C	2.338064000	-3.882616000	-2.319141000
C	3.364245000	-2.756622000	-2.384376000
H	4.297342000	-3.131991000	-2.835798000
H	3.614789000	-2.374229000	-1.386042000
H	2.998473000	-1.917643000	-2.992098000
C	2.854080000	-4.962786000	-1.355776000
H	3.806248000	-5.381690000	-1.721892000
H	2.139798000	-5.789101000	-1.237462000
H	3.023666000	-4.526372000	-0.362715000
C	-1.361111000	-4.112520000	-2.375627000
C	-2.155978000	-3.110679000	-2.975103000
C	-1.576653000	-1.980580000	-3.807125000
H	-0.500110000	-2.173158000	-3.919436000
C	-1.719729000	-0.636586000	-3.092301000
H	-1.322122000	0.177323000	-3.718402000
H	-1.172638000	-0.620710000	-2.143311000
H	-2.775107000	-0.409552000	-2.876443000
C	-2.209354000	-1.902475000	-5.197414000
H	-1.691651000	-1.148871000	-5.811715000
H	-3.266759000	-1.600116000	-5.136334000
H	-2.170178000	-2.863425000	-5.729353000
C	-3.534427000	-3.129256000	-2.741510000
H	-4.162967000	-2.358912000	-3.194640000
C	-4.117120000	-4.097457000	-1.934802000
H	-5.197649000	-4.097409000	-1.771583000
C	-3.316331000	-5.042180000	-1.304874000
H	-3.772749000	-5.770504000	-0.630367000
C	-1.931714000	-5.055116000	-1.490110000
C	-1.084718000	-6.012510000	-0.672048000
H	-0.062368000	-5.952412000	-1.063179000
C	-1.553706000	-7.461831000	-0.778141000
H	-0.854188000	-8.131208000	-0.253315000
H	-1.625766000	-7.797163000	-1.823128000

H	-2.543771000	-7.601081000	-0.316016000
C	-1.017572000	-5.574112000	0.792791000
H	-0.337983000	-6.232746000	1.356856000
H	-2.007327000	-5.624536000	1.272731000
H	-0.643984000	-4.545039000	0.881656000

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B	-0.485931000	2.588014000	-0.726148000
B	-2.523887000	-0.461663000	0.997461000
B	0.486019000	-2.587877000	-0.726282000
B	2.524015000	0.461718000	0.997430000
C	-1.561627000	1.718359000	-0.090680000
C	-1.644147000	-1.534164000	0.373391000
C	1.561722000	-1.718252000	-0.090790000
C	1.644280000	1.534250000	0.373401000
N	-2.124278000	0.860806000	0.478515000
N	-0.820190000	-2.138684000	-0.204840000
N	2.124388000	-0.860724000	0.478429000
N	0.820294000	2.138793000	-0.204765000
N	0.250900000	4.086139000	-2.652682000
C	-0.706832000	3.505317000	-1.862583000
N	-4.251750000	0.225618000	2.730262000
C	-0.263619000	4.887838000	-3.794171000
C	0.355792000	4.453541000	-5.125517000
H	-0.065421000	5.061332000	-5.940094000
H	0.142137000	3.400466000	-5.347395000
H	1.446645000	4.598148000	-5.124034000
N	4.251683000	-0.225689000	2.730374000
C	0.007789000	6.390707000	-3.634237000
H	-0.379443000	6.929448000	-4.511724000
H	1.088969000	6.581152000	-3.574025000
H	-0.469543000	6.816785000	-2.743666000
C	-1.760444000	4.542890000	-3.741259000
H	-1.965984000	3.723913000	-4.448493000
H	-2.393020000	5.394233000	-4.034155000
C	-2.061497000	4.052193000	-2.313001000
C	-2.453610000	5.212913000	-1.379073000
H	-3.375849000	5.699616000	-1.737379000
H	-1.667880000	5.977593000	-1.312251000
H	-2.629665000	4.829700000	-0.365410000
C	-3.201609000	3.033895000	-2.324454000
H	-4.095134000	3.484427000	-2.787102000

H	-3.481539000	2.723310000	-1.308809000
H	-2.931240000	2.136369000	-2.897131000
C	1.650003000	3.923384000	-2.412684000
C	2.341989000	2.828642000	-2.975097000
C	1.650857000	1.715352000	-3.751177000
H	0.592879000	1.991526000	-3.857484000
C	1.692455000	0.392240000	-2.978770000
H	1.246866000	-0.419333000	-3.575022000
H	1.131756000	0.453962000	-2.039981000
H	2.726663000	0.103294000	-2.734549000
C	2.248688000	1.523964000	-5.150326000
H	1.642704000	0.809372000	-5.729240000
H	3.269806000	1.114678000	-5.094303000
H	2.298870000	2.465834000	-5.714282000
C	3.719397000	2.730266000	-2.755703000
H	4.270183000	1.887198000	-3.179553000
C	4.399091000	3.673969000	-1.997742000
H	5.476775000	3.581818000	-1.845166000
C	3.695624000	4.711530000	-1.398844000
H	4.225739000	5.416901000	-0.754601000
C	2.315588000	4.841606000	-1.569284000
C	1.567100000	5.897195000	-0.767588000
H	0.534982000	5.912245000	-1.133268000
C	1.497647000	5.512617000	0.716372000
H	0.881287000	6.238653000	1.269582000
H	2.498864000	5.503671000	1.175178000
H	1.050284000	4.517848000	0.847557000
C	2.150914000	7.302947000	-0.933024000
H	1.514383000	8.043628000	-0.424488000
H	2.231325000	7.593173000	-1.990529000
H	3.156186000	7.378861000	-0.489372000
C	-3.497733000	-0.713110000	2.075759000
C	-5.057272000	-0.301875000	3.859763000
C	-4.382940000	-0.063639000	5.219742000
H	-4.954117000	-0.574212000	6.009868000
H	-4.353960000	1.005324000	5.467117000
H	-3.355570000	-0.451397000	5.239123000
C	-6.455266000	0.314314000	3.905244000
H	-7.018355000	-0.117711000	4.745723000
H	-7.016903000	0.113923000	2.984243000
H	-6.407304000	1.403860000	4.051509000
C	-5.094553000	-1.797195000	3.512256000

H	-6.007574000	-2.005083000	2.932390000
H	-5.129926000	-2.431038000	4.410581000
C	-3.858487000	-2.092407000	2.632772000
C	-4.243029000	-3.066745000	1.514657000
H	-4.629893000	-4.006960000	1.943140000
H	-3.383904000	-3.313134000	0.879350000
H	-5.018450000	-2.635787000	0.863564000
C	-2.693024000	-2.688822000	3.437599000
H	-2.992673000	-3.643626000	3.899312000
H	-2.354558000	-2.011607000	4.234478000
H	-1.832285000	-2.881103000	2.781442000
C	-4.348843000	1.569694000	2.259737000
C	-5.242169000	1.847678000	1.198600000
C	-6.038841000	0.759437000	0.490739000
H	-5.916238000	-0.168268000	1.065731000
C	-5.483113000	0.488464000	-0.913749000
H	-6.025095000	-0.347637000	-1.383614000
H	-4.418236000	0.220996000	-0.873135000
H	-5.596687000	1.371463000	-1.563037000
C	-7.536345000	1.079264000	0.424576000
H	-8.094291000	0.218100000	0.025251000
H	-7.738946000	1.934217000	-0.239348000
H	-7.947332000	1.325542000	1.414789000
C	-5.358496000	3.166487000	0.755239000
H	-6.046630000	3.400823000	-0.060443000
C	-4.604350000	4.185823000	1.324703000
H	-4.716954000	5.212645000	0.970550000
C	-3.685416000	3.888293000	2.321976000
H	-3.061621000	4.686239000	2.732220000
C	-3.529727000	2.582618000	2.798120000
C	-2.454657000	2.304098000	3.836924000
H	-2.515976000	1.239837000	4.092606000
C	-2.677122000	3.123698000	5.113783000
H	-1.987615000	2.797855000	5.908010000
H	-3.706002000	3.027579000	5.492010000
H	-2.492538000	4.195294000	4.937203000
C	-1.041680000	2.541527000	3.289140000
H	-0.298082000	2.360345000	4.080162000
H	-0.908442000	3.576256000	2.934338000
H	-0.813162000	1.866785000	2.454560000
C	3.497798000	0.713096000	2.075801000
C	5.057054000	0.301730000	3.860022000

C	6.455005000	-0.314534000	3.905767000
H	7.017953000	0.117436000	4.746371000
H	7.016835000	-0.114142000	2.984886000
H	6.406958000	-1.404082000	4.051991000
C	4.382457000	0.063524000	5.219872000
H	4.953500000	0.574077000	6.010108000
H	4.353389000	-1.005437000	5.467239000
H	3.355095000	0.451319000	5.239051000
C	5.094487000	1.797052000	3.512549000
H	6.007613000	2.004885000	2.932830000
H	5.129764000	2.430876000	4.410890000
C	3.858576000	2.092362000	2.632876000
C	4.243362000	3.066672000	1.514821000
H	4.630216000	4.006864000	1.943363000
H	3.384357000	3.313112000	0.879370000
H	5.018860000	2.635663000	0.863854000
C	2.693039000	2.688868000	3.437523000
H	2.992708000	3.643625000	3.899320000
H	2.354363000	2.011663000	4.234322000
H	1.832436000	2.881262000	2.781222000
C	4.348722000	-1.569767000	2.259842000
C	3.529465000	-2.582636000	2.798125000
C	2.454363000	-2.304067000	3.836887000
H	2.515812000	-1.239839000	4.092683000
C	1.041390000	-2.541261000	3.288991000
H	0.297763000	-2.360084000	4.079988000
H	0.908051000	-3.575934000	2.934062000
H	0.813000000	-1.866393000	2.454480000
C	2.676624000	-3.123830000	5.113675000
H	1.987111000	-2.797973000	5.907891000
H	3.705492000	-3.027897000	5.491981000
H	2.491902000	-4.195381000	4.936971000
C	3.685069000	-3.888308000	2.321945000
H	3.061170000	-4.686212000	2.732114000
C	4.604056000	-4.185889000	1.324736000
H	4.716597000	-5.212710000	0.970560000
C	5.358359000	-3.166607000	0.755383000
H	6.046555000	-3.400985000	-0.060235000
C	5.242124000	-1.847802000	1.198780000
C	6.039008000	-0.759620000	0.491060000
H	5.916545000	0.168045000	1.066146000
C	7.536460000	-1.079697000	0.424899000

H	8.094569000	-0.218576000	0.025708000
H	7.738930000	-1.934593000	-0.239138000
H	7.947380000	-1.326186000	1.415087000
C	5.483381000	-0.488391000	-0.913417000
H	6.025510000	0.347686000	-1.383153000
H	4.418543000	-0.220769000	-0.872817000
H	5.596850000	-1.371327000	-1.562808000
N	-0.250815000	-4.086041000	-2.652806000
C	0.706909000	-3.505155000	-1.862744000
C	0.263719000	-4.887712000	-3.794310000
C	-0.007604000	-6.390598000	-3.634383000
H	0.379601000	-6.929306000	-4.511901000
H	-1.088772000	-6.581095000	-3.574108000
H	0.469801000	-6.816666000	-2.743848000
C	-0.355739000	-4.453451000	-5.125644000
H	0.065455000	-5.061263000	-5.940216000
H	-0.142095000	-3.400383000	-5.347559000
H	-1.446590000	-4.598064000	-5.124123000
C	1.760526000	-4.542687000	-3.741437000
H	1.966003000	-3.723692000	-4.448670000
H	2.393140000	-5.393994000	-4.034354000
C	2.061580000	-4.051988000	-2.313180000
C	3.201647000	-3.033641000	-2.324633000
H	4.095189000	-3.484126000	-2.787293000
H	3.481567000	-2.723056000	-1.308985000
H	2.931231000	-2.136119000	-2.897295000
C	2.453740000	-5.212699000	-1.379259000
H	3.375976000	-5.699389000	-1.737591000
H	1.668022000	-5.977389000	-1.312416000
H	2.629814000	-4.829481000	-0.365602000
C	-1.649920000	-3.923384000	-2.412756000
C	-2.342017000	-2.828711000	-2.975168000
C	-1.651011000	-1.715381000	-3.751303000
H	-0.593023000	-1.991488000	-3.857692000
C	-1.692627000	-0.392274000	-2.978888000
H	-1.247168000	0.419339000	-3.575182000
H	-1.131821000	-0.453953000	-2.040159000
H	-2.726831000	-0.103410000	-2.734552000
C	-2.248966000	-1.524030000	-5.150404000
H	-1.643057000	-0.809424000	-5.729380000
H	-3.270094000	-1.114782000	-5.094301000
H	-2.299160000	-2.465911000	-5.714341000

C	-3.719420000	-2.730432000	-2.755702000
H	-4.270293000	-1.887415000	-3.179541000
C	-4.399007000	-3.674169000	-1.997688000
H	-5.476689000	-3.582092000	-1.845056000
C	-3.695434000	-4.711661000	-1.398797000
H	-4.225463000	-5.417047000	-0.754501000
C	-2.315394000	-4.841631000	-1.569295000
C	-1.566779000	-5.897099000	-0.767558000
H	-0.534658000	-5.912041000	-1.133233000
C	-2.150424000	-7.302929000	-0.932937000
H	-1.513808000	-8.043512000	-0.424366000
H	-2.230794000	-7.593209000	-1.990431000
H	-3.155690000	-7.378944000	-0.489288000
C	-1.497380000	-5.512450000	0.716386000
H	-0.880944000	-6.238393000	1.269635000
H	-2.498603000	-5.503596000	1.175181000
H	-1.050131000	-4.517624000	0.847533000

#### 4cl; M06-D3/def2-SVP

B	-0.254034000	2.611413000	-0.738045000
B	-2.576147000	-0.246703000	0.973929000
B	0.254057000	-2.611301000	-0.738432000
B	2.576455000	0.246609000	0.973554000
C	-1.399329000	1.840858000	-0.101478000
C	-1.791484000	-1.385763000	0.353818000
C	1.399429000	-1.840867000	-0.101838000
C	1.791673000	1.385745000	0.353742000
N	-2.047244000	1.034993000	0.466575000
N	-1.010822000	-2.054301000	-0.226695000
N	2.047562000	-1.035024000	0.465989000
N	1.010923000	2.054316000	-0.226627000
N	0.626990000	4.029058000	-2.672957000
C	-0.384110000	3.551203000	-1.873946000
N	-4.228116000	0.585253000	2.722497000
C	0.174574000	4.860772000	-3.826162000
C	0.740677000	4.356804000	-5.146937000
H	0.337986000	4.966221000	-5.972585000
H	0.463278000	3.309861000	-5.339250000
H	1.840260000	4.441388000	-5.174660000
N	4.228515000	-0.585544000	2.721975000
C	0.575412000	6.329743000	-3.695798000
H	0.235712000	6.882167000	-4.587181000

H	1.671862000	6.431479000	-3.642551000
H	0.138723000	6.823648000	-2.816021000
C	-1.339509000	4.646410000	-3.756989000
H	-1.614743000	3.815272000	-4.432896000
H	-1.905756000	5.536330000	-4.084194000
C	-1.670541000	4.231554000	-2.318154000
C	-1.922807000	5.443370000	-1.411843000
H	-2.806680000	6.008669000	-1.760534000
H	-1.068478000	6.136292000	-1.374518000
H	-2.110351000	5.103077000	-0.381416000
C	-2.912184000	3.355405000	-2.283836000
H	-3.765016000	3.901932000	-2.726482000
H	-3.195363000	3.089863000	-1.252650000
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C	2.005051000	3.720307000	-2.457906000
C	2.565744000	2.545972000	-3.007218000
C	1.756376000	1.499024000	-3.749249000
H	0.719689000	1.871227000	-3.833382000
C	1.702312000	0.185415000	-2.974130000
H	1.178161000	-0.591590000	-3.559909000
H	1.171685000	0.286032000	-2.015470000
H	2.716121000	-0.194382000	-2.752590000
C	2.293212000	1.238663000	-5.154174000
H	1.607869000	0.574967000	-5.709052000
H	3.273568000	0.733030000	-5.119912000
H	2.419541000	2.163904000	-5.737934000
C	3.930183000	2.308202000	-2.814964000
H	4.379106000	1.401585000	-3.234851000
C	4.723857000	3.190406000	-2.095421000
H	5.791426000	2.987425000	-1.964666000
C	4.148363000	4.310631000	-1.509553000
H	4.765798000	4.974961000	-0.894681000
C	2.786586000	4.583809000	-1.656347000
C	2.179679000	5.732515000	-0.874297000
H	1.156743000	5.881471000	-1.249354000
C	2.052817000	5.378094000	0.606414000
H	1.542172000	6.187518000	1.155291000
H	3.044189000	5.233905000	1.071892000
H	1.471080000	4.452843000	0.749568000
C	2.939332000	7.041595000	-1.047038000
H	2.402456000	7.868363000	-0.552579000
H	3.070470000	7.309338000	-2.108399000



H	3.943542000	6.994593000	-0.591862000
C	-3.584477000	-0.416253000	2.043473000
C	-5.100470000	0.120392000	3.834838000
C	-4.417183000	0.246470000	5.196285000
H	-5.067704000	-0.180779000	5.977451000
H	-4.236983000	1.301413000	5.456480000
H	-3.455437000	-0.287527000	5.232480000
C	-6.412018000	0.888371000	3.898802000
H	-7.022579000	0.500521000	4.730342000
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H	-6.241272000	1.962731000	4.082892000
C	-5.302843000	-1.342848000	3.437833000
H	-6.227508000	-1.424635000	2.838142000
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C	-4.099208000	-1.752680000	2.566582000
C	-4.567892000	-2.657825000	1.432781000
H	-5.068675000	-3.556833000	1.839355000
H	-3.729071000	-2.994870000	0.804129000
H	-5.280295000	-2.133642000	0.772380000
C	-3.025025000	-2.484494000	3.372657000
H	-3.431803000	-3.418801000	3.799445000
H	-2.635288000	-1.870832000	4.201268000
H	-2.168066000	-2.747450000	2.731132000
C	-4.086175000	1.952144000	2.343941000
C	-4.935265000	2.459779000	1.333500000
C	-5.938478000	1.586204000	0.602418000
H	-6.007133000	0.632418000	1.152101000
C	-5.468841000	1.242420000	-0.810597000
H	-6.188378000	0.561000000	-1.296586000
H	-4.485035000	0.743232000	-0.802387000
H	-5.392082000	2.147619000	-1.438692000
C	-7.330022000	2.207856000	0.563249000
H	-8.060980000	1.496094000	0.144590000
H	-7.356138000	3.106878000	-0.076048000
H	-7.678707000	2.507140000	1.565568000
C	-4.804865000	3.801855000	0.970137000
H	-5.456514000	4.216981000	0.192882000
C	-3.849836000	4.616879000	1.567787000
H	-3.772499000	5.669967000	1.280630000
C	-2.976261000	4.085444000	2.507217000
H	-2.193605000	4.721023000	2.935916000
C	-3.066435000	2.747791000	2.904692000

C	-2.043058000	2.203704000	3.882333000
H	-2.316972000	1.159965000	4.103191000
C	-2.046869000	2.988902000	5.190937000
H	-1.410825000	2.495122000	5.944639000
H	-3.060255000	3.092809000	5.613634000
H	-1.648018000	4.008187000	5.048646000
C	-0.633186000	2.170612000	3.295250000
H	0.086407000	1.830385000	4.059257000
H	-0.309397000	3.171165000	2.955857000
H	-0.553560000	1.481804000	2.439536000
C	3.584843000	0.416014000	2.043076000
C	5.100927000	-0.120816000	3.834331000
C	6.412520000	-0.888746000	3.898077000
H	7.023143000	-0.500989000	4.729615000
H	7.001829000	-0.783893000	2.975308000
H	6.241837000	-1.963141000	4.082029000
C	4.417762000	-0.247136000	5.195809000
H	5.068315000	0.180049000	5.976984000
H	4.237667000	-1.302130000	5.455867000
H	3.455985000	0.286795000	5.232165000
C	5.303216000	1.342494000	3.437536000
H	6.227877000	1.424433000	2.837865000
H	5.429454000	1.999196000	4.315853000
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C	4.568192000	2.657700000	1.432687000
H	5.068916000	3.556690000	1.839376000
H	3.729367000	2.994764000	0.804054000
H	5.280638000	2.133624000	0.772246000
C	3.025356000	2.484035000	3.372585000
H	3.432116000	3.418272000	3.799545000
H	2.635676000	1.870192000	4.201091000
H	2.168361000	2.747082000	2.731148000
C	4.086435000	-1.952412000	2.343374000
C	3.066637000	-2.747976000	2.904132000
C	2.043288000	-2.203835000	3.881766000
H	2.317385000	-1.160189000	4.102841000
C	0.633494000	-2.170354000	3.294525000
H	-0.086151000	-1.830260000	4.058542000
H	0.309618000	-3.170764000	2.954792000
H	0.554067000	-1.481276000	2.439015000
C	2.046741000	-2.989281000	5.190220000
H	1.410692000	-2.495503000	5.943919000

H	3.060035000	-3.093504000	5.613059000
H	1.647674000	-4.008445000	5.047673000
C	2.976339000	-4.085612000	2.506623000
H	2.193650000	-4.721144000	2.935334000
C	3.849838000	-4.617102000	1.567156000
H	3.772401000	-5.670178000	1.279979000
C	4.804892000	-3.802140000	0.969462000
H	5.456441000	-4.217287000	0.192135000
C	4.935407000	-2.460081000	1.332842000
C	5.938536000	-1.586533000	0.601617000
H	6.007349000	-0.632766000	1.151310000
C	7.330032000	-2.208276000	0.562156000
H	8.060946000	-1.496565000	0.143333000
H	7.355950000	-3.107305000	-0.077138000
H	7.678919000	-2.507572000	1.564402000
C	5.468666000	-1.242675000	-0.811302000
H	6.188151000	-0.561256000	-1.297375000
H	4.484880000	-0.743453000	-0.802913000
H	5.391754000	-2.147836000	-1.439433000
N	-0.627233000	-4.028679000	-2.673421000
C	0.383976000	-3.550917000	-1.874475000
C	-0.174981000	-4.860354000	-3.826706000
C	-0.575836000	-6.329314000	-3.696310000
H	-0.236200000	-6.881758000	-4.587706000
H	-1.672286000	-6.431024000	-3.642996000
H	-0.139112000	-6.823224000	-2.816552000
C	-0.741268000	-4.356339000	-5.147393000
H	-0.338707000	-4.965721000	-5.973129000
H	-0.463886000	-3.309387000	-5.339691000
H	-1.840855000	-4.440917000	-5.174953000
C	1.339117000	-4.646009000	-3.757741000
H	1.614280000	-3.814891000	-4.433699000
H	1.905306000	-5.535943000	-4.085014000
C	1.670371000	-4.231162000	-2.318955000
C	2.911949000	-3.354912000	-2.284862000
H	3.764722000	-3.901371000	-2.727704000
H	3.195328000	-3.089370000	-1.253733000
H	2.769754000	-2.421204000	-2.852541000
C	1.922908000	-5.442992000	-1.412734000
H	2.806881000	-6.008086000	-1.761509000
H	1.068732000	-6.136104000	-1.375461000
H	2.110429000	-5.102742000	-0.382289000

C	-2.005270000	-3.720020000	-2.458076000
C	-2.566153000	-2.545689000	-3.007204000
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H	-0.720217000	-1.870575000	-3.833299000
C	-1.703211000	-0.184982000	-2.973997000
H	-1.178988000	0.592108000	-3.559605000
H	-1.172815000	-0.285611000	-2.015210000
H	-2.717130000	0.194687000	-2.752744000
C	-2.293806000	-1.238240000	-5.154123000
H	-1.608622000	-0.574310000	-5.708915000
H	-3.274311000	-0.732897000	-5.119873000
H	-2.419844000	-2.163469000	-5.737966000
C	-3.930601000	-2.308089000	-2.814786000
H	-4.379681000	-1.401512000	-3.234587000
C	-4.724089000	-3.190414000	-2.095188000
H	-5.791662000	-2.987552000	-1.964285000
C	-4.148396000	-4.310607000	-1.509454000
H	-4.765683000	-4.975038000	-0.894543000
C	-2.786615000	-4.583647000	-1.656465000
C	-2.179520000	-5.732377000	-0.874602000
H	-1.156562000	-5.881113000	-1.249692000
C	-2.938977000	-7.041547000	-1.047540000
H	-2.401987000	-7.868309000	-0.553193000
H	-3.070063000	-7.309159000	-2.108940000
H	-3.943199000	-6.994755000	-0.592373000
C	-2.052707000	-5.378164000	0.606163000
H	-1.542002000	-6.187632000	1.154919000
H	-3.044093000	-5.234121000	1.071657000
H	-1.471042000	-4.452896000	0.749461000

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B	2.601571000	-2.667712000	-1.948020000
B	4.785790000	0.567063000	-1.272966000
C	5.444584000	1.837337000	-1.089105000
N	5.962078000	2.365653000	0.060472000
C	5.669876000	2.822870000	-2.243710000
C	6.819265000	3.694382000	-1.688033000
C	6.749090000	3.629407000	-0.147979000
C	2.733992000	-3.862177000	-2.884847000
C	3.963718000	-4.180608000	-3.731291000
C	3.431175000	-5.269603000	-4.698033000
C	2.182029000	-5.883912000	-4.040738000

N	1.763593000	-4.755056000	-3.131932000
C	1.503627000	-2.519782000	-0.886408000
N	-4.234359000	4.339667000	0.865429000
C	4.129632000	-0.616510000	-1.608326000
H	6.769479000	4.729234000	-2.056471000
H	7.780581000	3.273505000	-2.019832000
H	4.190292000	-6.029891000	-4.928672000
H	3.142504000	-4.796713000	-5.648898000
H	1.489643000	2.903430000	-1.583708000
N	-2.281599000	-1.689467000	1.108335000
C	0.774327000	3.054561000	-2.404793000
C	-0.470182000	2.178215000	-2.140034000
B	-2.552886000	2.737602000	-0.535962000
C	-1.379707000	3.122117000	-1.341907000
H	1.284834000	2.779816000	-3.340130000
C	0.309669000	4.518858000	-2.402616000
N	-0.921261000	4.420529000	-1.574846000
C	-3.487539000	3.692166000	0.243617000
N	3.580210000	-1.668024000	-1.889830000
H	3.349163000	-3.348391000	4.291622000
N	0.948574000	-1.752315000	3.895306000
B	0.342258000	-2.129873000	1.436567000
C	-1.152436000	-1.884617000	1.387749000
C	1.275067000	-2.052787000	2.606134000
C	3.228412000	-2.291723000	4.008760000
N	0.924669000	-2.341344000	0.118274000
C	2.101410000	-1.674546000	4.849860000
C	2.800528000	-2.209539000	2.524122000
H	4.192610000	-1.793049000	4.182395000
C	-7.142398000	-2.339480000	0.282510000
C	-6.654223000	-3.195195000	1.463582000
N	-6.024782000	-1.360407000	0.162667000
N	-2.915067000	1.334253000	-0.345076000
C	-4.831607000	-1.803219000	0.679873000
C	-3.285879000	0.261615000	-0.032996000
B	-3.520168000	-1.119639000	0.563720000
H	-6.986951000	-4.240425000	1.382394000
H	-7.076066000	-2.790693000	2.395969000
C	-5.109246000	-3.069485000	1.502583000
C	-7.293370000	-3.199688000	-0.985955000
H	-8.027965000	-4.000113000	-0.805550000
H	-7.650508000	-2.603635000	-1.834519000

H	-6.340969000	-3.668959000	-1.269447000
C	-8.476888000	-1.650745000	0.569573000
H	-8.760833000	-0.975620000	-0.251019000
H	-9.266118000	-2.410602000	0.676885000
H	-8.438015000	-1.064920000	1.496197000
C	-4.405926000	-4.306664000	0.922092000
H	-4.695226000	-4.494531000	-0.121999000
H	-3.317575000	-4.168903000	0.955096000
H	-4.654764000	-5.204112000	1.512370000
C	-4.646936000	-2.866883000	2.952468000
H	-3.560589000	-2.758968000	3.014528000
H	-5.091047000	-1.957314000	3.381869000
H	-4.946878000	-3.726347000	3.576838000
C	1.850722000	-2.473931000	6.132563000
H	2.720035000	-2.365991000	6.798894000
H	0.965590000	-2.102841000	6.669107000
H	1.715639000	-3.542927000	5.928153000
C	2.408408000	-0.227719000	5.257360000
H	1.569699000	0.205275000	5.816645000
H	3.294315000	-0.214104000	5.909951000
H	2.616100000	0.409459000	4.391500000
C	3.296351000	-3.474728000	1.807044000
H	2.825388000	-4.376288000	2.225618000
H	3.113224000	-3.458519000	0.727130000
H	4.385862000	-3.562066000	1.951281000
C	3.385659000	-0.961647000	1.835532000
H	3.049565000	-0.889309000	0.796131000
H	3.072907000	-0.044425000	2.346557000
H	4.485837000	-0.992843000	1.839320000
C	1.080963000	-6.227295000	-5.041781000
H	1.422016000	-7.050963000	-5.686419000
H	0.164874000	-6.553278000	-4.527774000
H	0.830573000	-5.374401000	-5.684017000
C	2.553393000	-7.148034000	-3.248099000
H	1.673729000	-7.628697000	-2.808073000
H	3.019458000	-7.870629000	-3.934701000
H	3.271219000	-6.930734000	-2.446278000
C	4.448426000	-2.963649000	-4.541833000
H	3.618469000	-2.497994000	-5.094400000
H	4.899420000	-2.198963000	-3.898751000
H	5.203584000	-3.295210000	-5.273355000
C	5.112819000	-4.672454000	-2.828802000

H	5.983124000	-4.950460000	-3.444384000
H	5.417484000	-3.874261000	-2.136707000
H	4.823927000	-5.547026000	-2.228885000
C	8.150772000	3.540897000	0.463223000
H	8.686148000	4.483412000	0.272188000
H	8.109113000	3.389310000	1.551679000
H	8.734857000	2.727358000	0.018207000
C	6.043250000	4.844126000	0.464166000
H	5.981679000	4.739978000	1.555022000
H	6.620965000	5.755041000	0.246668000
H	5.029859000	4.982972000	0.069523000
C	6.083556000	2.102857000	-3.534190000
H	6.966797000	1.467815000	-3.369510000
H	5.269147000	1.458835000	-3.899946000
H	6.320180000	2.836533000	-4.322108000
C	4.404392000	3.650490000	-2.520757000
H	3.579765000	3.001492000	-2.842923000
H	4.062753000	4.196902000	-1.634788000
H	4.600256000	4.386235000	-3.317532000
C	1.354046000	5.447259000	-1.771565000
H	2.232990000	5.519704000	-2.428337000
H	0.947469000	6.460553000	-1.642549000
H	1.686694000	5.076559000	-0.795001000
C	0.044302000	5.047308000	-3.825087000
H	-0.372682000	6.063162000	-3.787245000
H	0.992776000	5.093355000	-4.382931000
H	-0.646383000	4.411081000	-4.389740000
C	-0.025801000	0.900269000	-1.410330000
H	0.381789000	1.133540000	-0.417440000
H	-0.846029000	0.184282000	-1.278498000
H	0.765905000	0.396053000	-1.987910000
C	-1.180656000	1.789107000	-3.454259000
H	-1.996296000	1.083985000	-3.247256000
H	-1.626055000	2.660165000	-3.952389000
H	-0.476462000	1.318284000	-4.158488000
C	0.401405000	-4.469575000	-2.740507000
C	-0.180638000	-5.067648000	-1.603001000
C	-0.282712000	-3.467253000	-3.474835000
C	-1.445961000	-4.623741000	-1.198596000
C	-1.530696000	-3.041710000	-3.007507000
C	-2.109505000	-3.603020000	-1.872217000
H	-1.901766000	-5.062621000	-0.311726000

H	-2.056369000	-2.243692000	-3.532078000
H	-3.063427000	-3.224120000	-1.500420000
C	5.976064000	1.672454000	1.319058000
C	6.983239000	0.686515000	1.527510000
C	5.051281000	1.977766000	2.353010000
C	7.135019000	0.126071000	2.799922000
C	5.289410000	1.416117000	3.620940000
C	6.321406000	0.519929000	3.858610000
H	7.908241000	-0.626417000	2.964957000
H	4.603127000	1.662833000	4.433291000
H	6.466425000	0.098288000	4.856160000
C	-1.643058000	5.582936000	-1.161920000
C	-2.692461000	6.087403000	-1.970440000
C	-1.334284000	6.204366000	0.073140000
C	-3.361683000	7.246902000	-1.561335000
C	-2.026328000	7.366454000	0.435260000
C	-3.024891000	7.894826000	-0.376585000
H	-4.174703000	7.640138000	-2.175793000
H	-1.795900000	7.851907000	1.386204000
H	-3.559975000	8.798024000	-0.072576000
C	-6.203025000	-0.030239000	-0.331128000
C	-6.110387000	0.245447000	-1.713468000
C	-6.446596000	1.009805000	0.602520000
C	-6.350602000	1.554659000	-2.150949000
C	-6.659504000	2.303575000	0.117127000
C	-6.639367000	2.572768000	-1.248062000
H	-6.284426000	1.786201000	-3.216307000
H	-6.807876000	3.126312000	0.816526000
H	-6.811440000	3.589934000	-1.601622000
C	-0.386693000	-1.438422000	4.312280000
C	-1.200350000	-2.476218000	4.830347000
C	-0.873520000	-0.113480000	4.202903000
C	-2.464087000	-2.141946000	5.329834000
C	-2.158036000	0.161609000	4.692178000
C	-2.937967000	-0.833155000	5.272814000
H	-3.102570000	-2.925990000	5.741079000
H	-2.555711000	1.174237000	4.606912000
H	-3.933687000	-0.593654000	5.652927000
C	-0.092902000	1.013336000	3.539863000
H	0.888871000	0.615936000	3.257008000
C	0.117526000	2.209345000	4.482486000
H	0.516789000	1.910567000	5.461652000



H	0.820405000	2.928376000	4.033322000
H	-0.826912000	2.746714000	4.656942000
C	-0.775982000	1.481853000	2.247488000
H	-0.193439000	2.280918000	1.767479000
H	-0.876639000	0.663574000	1.528507000
H	-1.780431000	1.887268000	2.436015000
C	-0.776056000	-3.939651000	4.789847000
H	0.281115000	-3.967478000	4.498249000
C	-1.549039000	-4.711686000	3.707624000
H	-1.169241000	-5.743427000	3.631291000
H	-2.622376000	-4.764228000	3.943025000
H	-1.437774000	-4.232636000	2.726105000
C	-0.921419000	-4.641010000	6.147672000
H	-1.979516000	-4.736397000	6.438541000
H	-0.504202000	-5.659853000	6.100238000
H	-0.404175000	-4.096055000	6.950301000
C	-5.697666000	-0.807088000	-2.731384000
H	-5.573395000	-1.754277000	-2.193673000
C	-6.759477000	-1.002552000	-3.823902000
H	-6.496901000	-1.849953000	-4.478352000
H	-7.755447000	-1.194584000	-3.396673000
H	-6.845012000	-0.106927000	-4.459808000
C	-4.336628000	-0.470040000	-3.359683000
H	-4.050090000	-1.243564000	-4.091887000
H	-4.363517000	0.495940000	-3.887482000
H	-3.556529000	-0.410226000	-2.589538000
C	-6.443463000	0.782798000	2.109162000
H	-6.428056000	-0.301238000	2.283341000
C	-5.179592000	1.370770000	2.761731000
H	-5.091328000	2.449780000	2.563749000
H	-5.210279000	1.215059000	3.853273000
H	-4.275332000	0.882708000	2.375881000
C	-7.704609000	1.347004000	2.781569000
H	-8.625048000	0.977232000	2.303699000
H	-7.731198000	1.062766000	3.846177000
H	-7.725578000	2.446791000	2.735802000
C	-3.177046000	5.371258000	-3.222859000
H	-2.483599000	4.547251000	-3.416892000
C	-4.555343000	4.737925000	-2.987254000
H	-4.527307000	4.058623000	-2.128277000
H	-5.320222000	5.507196000	-2.790842000
H	-4.872137000	4.163199000	-3.873912000

C	-3.204270000	6.281037000	-4.459183000
H	-2.233626000	6.767160000	-4.636426000
H	-3.463252000	5.698692000	-5.358746000
H	-3.960109000	7.076224000	-4.356975000
C	-0.343753000	5.613305000	1.066999000
H	0.089928000	4.718651000	0.599433000
C	0.791421000	6.586658000	1.422903000
H	1.305315000	6.974111000	0.532594000
H	0.407675000	7.451756000	1.987095000
H	1.540769000	6.088363000	2.058792000
C	-1.058759000	5.161330000	2.350704000
H	-1.872209000	4.459802000	2.131635000
H	-0.344659000	4.677038000	3.033904000
H	-1.497138000	6.021779000	2.881315000
C	7.876079000	0.156071000	0.409743000
H	7.728176000	0.786958000	-0.475857000
C	7.451940000	-1.272928000	0.024757000
H	8.050792000	-1.635098000	-0.826654000
H	7.605144000	-1.968221000	0.866134000
H	6.392911000	-1.310876000	-0.264474000
C	9.369798000	0.179573000	0.771311000
H	9.977705000	-0.088960000	-0.107334000
H	9.695882000	1.168118000	1.124790000
H	9.605467000	-0.548873000	1.562836000
C	3.711689000	2.732689000	2.267348000
H	3.040818000	2.072038000	2.843227000
C	3.694995000	4.067742000	3.031402000
H	2.654629000	4.395474000	3.180303000
H	4.164166000	3.977327000	4.022595000
H	4.212877000	4.864852000	2.482396000
C	3.042562000	2.861724000	0.900369000
H	3.530796000	3.603710000	0.261321000
H	3.031656000	1.908983000	0.355173000
H	1.999687000	3.184195000	1.040384000
C	0.508885000	-6.148045000	-0.787093000
H	1.549183000	-6.208301000	-1.130102000
C	0.546587000	-5.828252000	0.712856000
H	-0.459047000	-5.846938000	1.156794000
H	1.153783000	-6.578035000	1.245179000
H	0.970098000	-4.836505000	0.907730000
C	-0.168348000	-7.509616000	-1.020651000
H	0.393491000	-8.319072000	-0.527132000

H	-1.188646000	-7.506649000	-0.605350000
H	-0.256415000	-7.751600000	-2.090607000
C	0.275730000	-2.824813000	-4.739004000
H	1.217851000	-3.326175000	-4.994673000
C	0.589158000	-1.337461000	-4.533957000
H	1.321586000	-1.187716000	-3.729405000
H	0.996523000	-0.896038000	-5.457787000
H	-0.318535000	-0.780155000	-4.267097000
C	-0.683483000	-3.013810000	-5.926046000
H	-0.950726000	-4.071511000	-6.071642000
H	-1.619388000	-2.454069000	-5.774769000
H	-0.222692000	-2.641999000	-6.855186000

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B	-1.242999000	-2.600542000	1.605022000
B	-2.261447000	-0.711777000	-1.839206000
C	-2.378532000	-0.911125000	-3.301230000
N	-2.507982000	-2.112046000	-3.970195000
C	-2.369773000	0.228743000	-4.332852000
C	-2.703810000	-0.500523000	-5.660483000
C	-2.338284000	-1.982511000	-5.454086000
C	-1.933633000	-3.323049000	2.693649000
C	-3.139976000	-4.250725000	2.483320000
C	-3.528576000	-4.629710000	3.928292000
C	-2.272307000	-4.421952000	4.796593000
N	-1.556205000	-3.349769000	4.026156000
C	0.232403000	-2.269762000	1.624308000
N	-2.093635000	0.631804000	-1.266158000
C	-2.082988000	-1.743157000	-0.730379000
H	-2.178551000	-0.061886000	-6.521210000
H	-3.782525000	-0.416525000	-5.863052000
H	-3.922693000	-5.653727000	4.005948000
H	-4.316930000	-3.946301000	4.281037000
H	-3.233370000	4.009921000	3.939786000
N	2.971644000	0.613985000	0.428653000
C	-2.993781000	4.729839000	3.141981000
C	-1.699455000	4.285977000	2.435247000
B	-1.353403000	2.559890000	0.440651000
C	-2.220546000	3.432148000	1.273354000
H	-2.899340000	5.720452000	3.610913000
C	-4.111391000	4.695679000	2.092188000
N	-3.571194000	3.680652000	1.121489000

C	-1.865040000	1.530907000	-0.536215000
N	-1.857695000	-2.254967000	0.309715000
H	4.553325000	-5.865764000	0.756839000
N	4.344509000	-3.491285000	-0.745393000
B	2.644660000	-2.050675000	0.595395000
C	2.959022000	-0.563126000	0.425682000
C	3.268587000	-3.310254000	0.091973000
C	3.839207000	-5.659060000	-0.055449000
N	1.346023000	-2.147088000	1.257173000
C	4.572494000	-4.912454000	-1.171150000
C	2.733202000	-4.715717000	0.466841000
H	3.437109000	-6.625356000	-0.393002000
C	5.344554000	4.947625000	0.090697000
C	6.112362000	3.746060000	-0.466260000
N	3.949108000	4.382027000	0.100920000
N	0.119214000	2.551449000	0.555477000
C	3.927149000	2.995669000	0.187259000
C	1.290537000	2.440523000	0.477730000
B	2.771556000	2.083174000	0.377813000
H	7.176636000	3.750793000	-0.189337000
H	6.055560000	3.772132000	-1.565884000
C	5.373418000	2.490320000	0.038028000
C	5.884473000	5.315342000	1.498967000
H	6.971470000	5.149600000	1.534655000
H	5.719397000	6.373645000	1.740739000
H	5.422395000	4.709294000	2.286808000
C	5.457202000	6.170211000	-0.817986000
H	4.842997000	7.005698000	-0.452270000
H	6.505972000	6.504325000	-0.845057000
H	5.140927000	5.940966000	-1.843425000
C	5.924868000	1.970498000	1.378802000
H	5.880011000	2.727574000	2.171261000
H	5.342190000	1.103186000	1.714474000
H	6.974929000	1.654195000	1.264335000
C	5.540271000	1.395922000	-1.022817000
H	5.187603000	0.415536000	-0.692014000
H	5.011068000	1.652132000	-1.951763000
H	6.607511000	1.290464000	-1.262002000
C	6.053174000	-5.302113000	-1.227817000
H	6.126460000	-6.355551000	-1.538236000
H	6.607638000	-4.696280000	-1.958389000
H	6.542360000	-5.208365000	-0.251646000

C	3.973667000	-5.185039000	-2.560994000
H	4.539616000	-4.649034000	-3.333189000
H	4.034037000	-6.260697000	-2.786728000
H	2.923828000	-4.879298000	-2.631307000
C	2.582597000	-4.926131000	1.978466000
H	3.503977000	-4.643837000	2.504947000
H	1.752999000	-4.345949000	2.395358000
H	2.381817000	-5.991506000	2.181949000
C	1.387280000	-5.031136000	-0.207790000
H	0.597027000	-4.341521000	0.112580000
H	1.462804000	-4.978279000	-1.297280000
H	1.070281000	-6.052719000	0.059582000
C	-2.644977000	-3.970399000	6.209125000
H	-3.236498000	-4.761032000	6.695900000
H	-1.756791000	-3.777384000	6.826288000
H	-3.245776000	-3.050784000	6.190211000
C	-1.432998000	-5.710135000	4.870868000
H	-0.590263000	-5.602134000	5.561784000
H	-2.055233000	-6.545077000	5.229744000
H	-1.029847000	-5.980601000	3.886666000
C	-4.325226000	-3.571757000	1.772980000
H	-4.641587000	-2.661213000	2.300493000
H	-4.082806000	-3.301867000	0.737881000
H	-5.184245000	-4.262845000	1.749047000
C	-2.723652000	-5.472810000	1.638456000
H	-3.564974000	-6.179722000	1.543561000
H	-2.433964000	-5.146953000	0.630975000
H	-1.870211000	-6.008416000	2.074735000
C	-3.245710000	-2.944081000	-6.220998000
H	-3.089312000	-2.810365000	-7.301824000
H	-3.015126000	-3.990730000	-5.972115000
H	-4.306444000	-2.770190000	-6.009441000
C	-0.886259000	-2.214779000	-5.919025000
H	-0.562659000	-3.249336000	-5.767166000
H	-0.817130000	-1.994329000	-6.995326000
H	-0.178371000	-1.558351000	-5.399604000
C	-3.457446000	1.273882000	-4.031643000
H	-4.447968000	0.807864000	-3.939333000
H	-3.258994000	1.811501000	-3.099493000
H	-3.503170000	2.015263000	-4.847271000
C	-1.004671000	0.943112000	-4.371872000
H	-0.798243000	1.427217000	-3.408945000

H	-0.176425000	0.250867000	-4.573405000
H	-0.998967000	1.720474000	-5.153488000
C	-5.434698000	4.274897000	2.729890000
H	-5.724161000	5.027843000	3.479107000
H	-6.238053000	4.220976000	1.983572000
H	-5.351820000	3.306143000	3.237815000
C	-4.339521000	6.058239000	1.418748000
H	-5.085683000	5.971516000	0.616321000
H	-4.723206000	6.774971000	2.160540000
H	-3.421396000	6.474171000	0.991295000
C	-0.796856000	3.527524000	3.420777000
H	-1.301542000	2.644017000	3.830489000
H	0.134149000	3.189078000	2.952441000
H	-0.532730000	4.188829000	4.262367000
C	-0.916397000	5.483086000	1.870282000
H	-0.026501000	5.141022000	1.333534000
H	-1.506711000	6.079202000	1.163717000
H	-0.594212000	6.150276000	2.685830000
C	-0.980908000	-2.226236000	4.716539000
C	0.261527000	-2.326181000	5.387515000
C	-1.735895000	-1.025047000	4.825937000
C	0.676547000	-1.271271000	6.216056000
C	-1.268868000	0.005538000	5.647577000
C	-0.081327000	-0.117234000	6.363572000
H	1.626055000	-1.357184000	6.747761000
H	-1.852496000	0.924874000	5.728133000
H	0.259730000	0.690934000	7.014977000
C	-3.092674000	-3.239746000	-3.299510000
C	-4.502824000	-3.219333000	-3.097090000
C	-2.320273000	-4.302158000	-2.772471000
C	-5.104794000	-4.243215000	-2.359079000
C	-2.981789000	-5.313642000	-2.054418000
C	-4.352199000	-5.289226000	-1.833370000
H	-6.183669000	-4.219625000	-2.192572000
H	-2.384984000	-6.131732000	-1.643943000
H	-4.830715000	-6.078417000	-1.248952000
C	-4.338724000	3.360099000	-0.054100000
C	-4.117825000	4.077412000	-1.264000000
C	-5.372370000	2.387729000	0.006249000
C	-4.984143000	3.863167000	-2.342782000
C	-6.211833000	2.218573000	-1.104345000
C	-6.038491000	2.959053000	-2.266291000

H	-4.820016000	4.415479000	-3.269942000
H	-7.009855000	1.475684000	-1.056331000
H	-6.705021000	2.814067000	-3.119804000
C	2.829101000	5.173040000	-0.304038000
C	2.306649000	6.172874000	0.560704000
C	2.314830000	5.022536000	-1.618301000
C	1.313012000	7.029486000	0.069694000
C	1.312396000	5.899314000	-2.050773000
C	0.817030000	6.901319000	-1.224650000
H	0.903628000	7.804813000	0.715078000
H	0.932389000	5.804542000	-3.069364000
H	0.041838000	7.581511000	-1.585755000
C	5.194860000	-2.478626000	-1.287345000
C	6.430946000	-2.233068000	-0.635803000
C	4.888546000	-1.857878000	-2.522137000
C	7.399956000	-1.480266000	-1.308010000
C	5.894089000	-1.112252000	-3.154797000
C	7.149684000	-0.957139000	-2.575902000
H	8.366778000	-1.300573000	-0.834987000
H	5.684566000	-0.644639000	-4.119083000
H	7.925100000	-0.388962000	-3.095512000
C	3.503460000	-1.925109000	-3.150357000
H	2.915929000	-2.640733000	-2.564124000
C	3.512879000	-2.377916000	-4.617876000
H	4.057107000	-3.320792000	-4.766603000
H	2.480258000	-2.521247000	-4.973885000
H	3.978551000	-1.619355000	-5.267050000
C	2.792314000	-0.565234000	-3.046690000
H	1.760378000	-0.644538000	-3.422350000
H	2.743272000	-0.203597000	-2.014182000
H	3.314511000	0.197033000	-3.646872000
C	6.696160000	-2.741930000	0.775868000
H	6.006044000	-3.575692000	0.957880000
C	6.355093000	-1.658477000	1.811256000
H	6.502356000	-2.043234000	2.833558000
H	6.999349000	-0.775468000	1.682778000
H	5.308281000	-1.339116000	1.717690000
C	8.127270000	-3.252689000	0.984071000
H	8.860611000	-2.430999000	0.960574000
H	8.218017000	-3.736085000	1.969630000
H	8.419722000	-3.983467000	0.214926000
C	2.826133000	6.336489000	1.986167000

H	3.907991000	6.467243000	1.900118000
C	2.314049000	7.586330000	2.709004000
H	2.801186000	7.667578000	3.693198000
H	2.533350000	8.508968000	2.149799000
H	1.228006000	7.546284000	2.886211000
C	2.598085000	5.090551000	2.858571000
H	3.158810000	5.182911000	3.802832000
H	1.536965000	4.982010000	3.113449000
H	2.919194000	4.167107000	2.360748000
C	2.819556000	3.982664000	-2.611579000
H	3.595193000	3.389091000	-2.117144000
C	1.699296000	3.014325000	-3.020766000
H	0.887997000	3.537056000	-3.550756000
H	2.088103000	2.236125000	-3.694675000
H	1.263914000	2.514671000	-2.145526000
C	3.449562000	4.629823000	-3.855133000
H	4.265987000	5.318010000	-3.589641000
H	3.862973000	3.854409000	-4.520359000
H	2.708977000	5.202926000	-4.435555000
C	-2.958559000	5.041562000	-1.486836000
H	-2.406335000	5.140811000	-0.546777000
C	-1.978231000	4.472678000	-2.524432000
H	-1.572801000	3.505868000	-2.202556000
H	-2.465679000	4.334338000	-3.502117000
H	-1.132952000	5.159564000	-2.658006000
C	-3.418490000	6.441245000	-1.925501000
H	-4.168718000	6.866906000	-1.245386000
H	-2.556572000	7.127256000	-1.956071000
H	-3.856944000	6.423779000	-2.935844000
C	-5.577606000	1.440004000	1.180454000
H	-4.864009000	1.725284000	1.962432000
C	-6.999065000	1.474646000	1.765696000
H	-7.326276000	2.485452000	2.039083000
H	-7.731133000	1.071140000	1.048372000
H	-7.050170000	0.845007000	2.668857000
C	-5.264352000	-0.003653000	0.756381000
H	-4.280804000	-0.093825000	0.278277000
H	-5.285912000	-0.673719000	1.627653000
H	-6.015254000	-0.370003000	0.044521000
C	-5.401451000	-2.120103000	-3.649805000
H	-4.795630000	-1.494784000	-4.312441000
C	-5.926293000	-1.205573000	-2.537604000



H	-6.544648000	-0.396594000	-2.958681000
H	-6.547181000	-1.767943000	-1.821496000
H	-5.094559000	-0.748054000	-1.989586000
C	-6.564223000	-2.685229000	-4.480875000
H	-7.109963000	-1.866855000	-4.977717000
H	-6.214880000	-3.384816000	-5.255443000
H	-7.288506000	-3.225591000	-3.851291000
C	-0.818153000	-4.517084000	-2.932586000
H	-0.542058000	-5.136755000	-2.066305000
C	-0.537528000	-5.404168000	-4.160750000
H	0.543616000	-5.590849000	-4.268731000
H	-1.044506000	-6.376008000	-4.058932000
H	-0.898945000	-4.951705000	-5.093940000
C	0.086269000	-3.286098000	-2.850355000
H	-0.152454000	-2.522657000	-3.589564000
H	0.028452000	-2.815771000	-1.861636000
H	1.128827000	-3.593051000	-3.009270000
C	1.211269000	-3.502885000	5.232876000
H	0.781476000	-4.179032000	4.480443000
C	2.581553000	-3.027488000	4.720946000
H	3.056721000	-2.342862000	5.440137000
H	3.259576000	-3.883198000	4.586909000
H	2.496585000	-2.501733000	3.760221000
C	1.392257000	-4.277552000	6.549158000
H	1.984758000	-5.192415000	6.385839000
H	1.925610000	-3.664833000	7.293540000
H	0.431426000	-4.568062000	6.997691000
C	-2.980777000	-0.758215000	4.003071000
H	-3.256768000	-1.684668000	3.494639000
C	-2.623074000	0.273016000	2.922787000
H	-1.635305000	0.075078000	2.488680000
H	-3.342668000	0.263812000	2.103883000
H	-2.606548000	1.288859000	3.339102000
C	-4.196526000	-0.316981000	4.826523000
H	-4.470410000	-1.069620000	5.582908000
H	-4.018335000	0.635208000	5.351184000
H	-5.066958000	-0.167356000	4.166839000

**TS<sub>1-2-dib</sub>** (im. freq.: -38.3 cm<sup>-1</sup>)

N	0.559711000	1.752426000	-2.614779000
C	-0.321139000	1.405288000	-1.920553000
B	-1.493219000	1.084436000	-1.093233000

N	0.391480000	-2.943254000	1.796735000
C	0.718150000	-2.160388000	0.988191000
B	1.171591000	-1.153295000	0.006821000
C	-2.820739000	1.206375000	-0.605290000
N	-3.684959000	0.410016000	0.107990000
C	-5.058409000	0.979839000	0.265962000
C	-5.000456000	2.166587000	-0.714292000
H	-5.618298000	3.013288000	-0.380429000
H	-5.385784000	1.840297000	-1.692262000
C	-3.515635000	2.566890000	-0.876123000
C	-3.343793000	-0.914388000	0.528138000
C	-3.481539000	-1.991781000	-0.381103000
C	-3.217852000	-3.288961000	0.078197000
H	-3.319284000	-4.131625000	-0.609139000
C	-2.822176000	-3.521555000	1.392204000
H	-2.614356000	-4.538436000	1.731750000
C	-2.639433000	-2.449283000	2.260068000
H	-2.263503000	-2.636620000	3.266657000
C	-2.874173000	-1.133473000	1.845579000
C	-3.845834000	-1.785138000	-1.845268000
H	-4.149675000	-0.737738000	-1.968869000
C	-5.008268000	-2.678614000	-2.301450000
H	-5.312494000	-2.418445000	-3.328090000
H	-5.885615000	-2.574124000	-1.646320000
H	-4.722491000	-3.742287000	-2.306015000
C	-2.615966000	-1.996597000	-2.740573000
H	-2.864380000	-1.807189000	-3.797581000
H	-2.236210000	-3.028014000	-2.659785000
H	-1.805845000	-1.311549000	-2.457929000
H	-0.740492000	1.027187000	3.529933000
H	-2.983961000	0.781748000	4.769378000
C	-6.145141000	-0.024210000	-0.136664000
H	-7.135856000	0.433228000	0.006433000
H	-6.097908000	-0.931280000	0.483599000
H	-6.058828000	-0.317976000	-1.189360000
C	-5.350370000	1.421388000	1.709921000
H	-6.353463000	1.871777000	1.761839000
H	-4.628536000	2.159671000	2.078665000
H	-5.336699000	0.557384000	2.387655000
C	-3.073943000	3.602388000	0.176574000
H	-3.712079000	4.499980000	0.124371000
H	-2.033095000	3.907304000	-0.001823000

H	-3.124953000	3.201180000	1.197189000
C	-3.253150000	3.133541000	-2.277246000
H	-3.852556000	4.045475000	-2.431621000
H	-3.520370000	2.405064000	-3.056728000
H	-2.195793000	3.405436000	-2.414957000
C	2.241569000	-0.803406000	-0.898628000
N	3.244713000	0.102064000	-0.753562000
C	4.034432000	0.343876000	-2.011511000
C	3.185022000	-0.420631000	-3.049762000
H	2.500270000	0.286402000	-3.536773000
H	3.811561000	-0.884910000	-3.825603000
C	2.348224000	-1.469342000	-2.282418000
C	3.620000000	0.605705000	0.544611000
C	3.193109000	1.890699000	0.965487000
C	3.612861000	2.359907000	2.218428000
H	3.293112000	3.351202000	2.545646000
C	4.406505000	1.585234000	3.056686000
H	4.721489000	1.970949000	4.029352000
C	4.778267000	0.305431000	2.656534000
H	5.378317000	-0.313620000	3.326402000
C	4.396104000	-0.210907000	1.411882000
C	2.240801000	2.759735000	0.161821000
H	2.036669000	2.253286000	-0.784992000
C	0.895635000	2.902397000	0.889107000
H	0.193152000	3.482882000	0.272823000
H	1.009981000	3.421952000	1.854546000
H	0.436362000	1.924448000	1.079231000
C	2.817965000	4.149226000	-0.146860000
H	2.145818000	4.691738000	-0.830403000
H	3.807822000	4.092344000	-0.620701000
H	2.920503000	4.756169000	0.767343000
C	4.818339000	-1.634963000	1.077569000
H	4.465106000	-1.857144000	0.066811000
C	4.161117000	-2.654783000	2.021602000
H	4.429648000	-3.680097000	1.719635000
H	3.066747000	-2.579040000	2.015133000
H	4.503836000	-2.514278000	3.059362000
C	6.345660000	-1.807847000	1.095320000
H	6.620112000	-2.814421000	0.740631000
H	6.747914000	-1.699270000	2.114952000
H	6.853461000	-1.070918000	0.457625000
C	5.467506000	-0.192331000	-1.887941000

H	6.018964000	0.025575000	-2.814538000
H	5.505923000	-1.274711000	-1.720697000
H	5.993360000	0.304689000	-1.060283000
C	4.115947000	1.831153000	-2.362597000
H	4.670426000	1.944700000	-3.306911000
H	4.660171000	2.389857000	-1.588236000
H	3.118322000	2.265067000	-2.496363000
C	0.999617000	-1.740384000	-2.955958000
H	1.161245000	-2.200855000	-3.943718000
H	0.428375000	-0.816487000	-3.096131000
H	0.392412000	-2.440757000	-2.361787000
C	3.088317000	-2.817292000	-2.136327000
H	3.234759000	-3.266623000	-3.131582000
H	2.502218000	-3.518410000	-1.523585000
H	4.074672000	-2.711076000	-1.668798000
C	-2.524282000	0.014023000	2.782064000
H	-2.879648000	0.939019000	2.314090000
C	-0.999534000	0.143242000	2.924981000
H	-0.525043000	0.250763000	1.939837000
H	-0.563670000	-0.745585000	3.405503000
C	-3.186351000	-0.114038000	4.160426000
H	-2.794691000	-0.981654000	4.714448000
H	-4.277396000	-0.235068000	4.083812000

### 2-dib; B3LYP-D3(BJ)/def2-SVP

N	-0.917687000	3.157993000	1.506649000
C	-0.198524000	2.309272000	1.144151000
B	0.623138000	1.067881000	0.694517000
N	0.354168000	-2.875138000	1.355906000
C	0.157775000	-1.758130000	1.082009000
B	-0.247388000	-0.291287000	0.889149000
C	2.064141000	1.354036000	0.277525000
N	2.946825000	0.527271000	-0.324940000
C	4.173677000	1.214792000	-0.865426000
C	4.208187000	2.457720000	0.028446000
H	4.662300000	3.320669000	-0.478860000
H	4.819499000	2.240651000	0.917956000
C	2.746112000	2.727216000	0.458803000
C	2.801304000	-0.896370000	-0.429893000
C	3.346550000	-1.689461000	0.609132000
C	3.318598000	-3.079155000	0.462217000
H	3.726207000	-3.710525000	1.252680000

C	2.742680000	-3.674373000	-0.656497000
H	2.715834000	-4.762878000	-0.742807000
C	2.171322000	-2.882058000	-1.645864000
H	1.693691000	-3.356714000	-2.505546000
C	2.186895000	-1.483214000	-1.558133000
C	3.907131000	-1.085478000	1.892513000
H	4.105281000	-0.022278000	1.705436000
C	5.229716000	-1.733760000	2.325963000
H	5.671336000	-1.172606000	3.164820000
H	5.963064000	-1.760610000	1.505350000
H	5.080216000	-2.768260000	2.672254000
C	2.877491000	-1.144080000	3.033645000
H	3.307788000	-0.718274000	3.955084000
H	2.569670000	-2.180704000	3.237197000
H	1.977806000	-0.571821000	2.773874000
H	-0.461404000	-0.299018000	-3.486889000
H	1.758168000	-0.256490000	-4.793576000
C	5.437858000	0.363973000	-0.743729000
H	6.283932000	0.929777000	-1.162249000
H	5.346259000	-0.576444000	-1.305595000
H	5.678303000	0.123886000	0.297999000
C	3.986240000	1.583809000	-2.346528000
H	4.824032000	2.219590000	-2.670829000
H	3.052869000	2.133686000	-2.519563000
H	3.981676000	0.688913000	-2.979270000
C	2.098461000	3.833807000	-0.396240000
H	2.677064000	4.765282000	-0.287708000
H	1.069942000	4.032734000	-0.072577000
H	2.075070000	3.572063000	-1.462819000
C	2.718977000	3.152087000	1.939798000
H	3.361654000	4.037560000	2.078591000
H	3.101169000	2.346319000	2.585334000
H	1.705866000	3.409242000	2.272183000
C	-1.715862000	-0.025966000	1.421206000
N	-2.776591000	0.262663000	0.707163000
C	-3.973871000	0.734827000	1.534454000
C	-3.337365000	0.851941000	2.932175000
H	-3.055591000	1.898405000	3.111976000
H	-4.035380000	0.540447000	3.722272000
C	-2.057470000	-0.004880000	2.910379000
C	-2.945102000	-0.013317000	-0.715871000
C	-2.925729000	1.035228000	-1.668068000

C	-3.300669000	0.738793000	-2.985576000
H	-3.292537000	1.540082000	-3.726019000
C	-3.654144000	-0.547864000	-3.373168000
H	-3.948935000	-0.752784000	-4.405033000
C	-3.588726000	-1.579625000	-2.444656000
H	-3.813933000	-2.599698000	-2.759561000
C	-3.227159000	-1.348993000	-1.110463000
C	-2.397449000	2.433289000	-1.390873000
H	-2.233729000	2.542146000	-0.316517000
C	-1.023567000	2.601149000	-2.063229000
H	-0.602903000	3.586186000	-1.814027000
H	-1.106037000	2.528227000	-3.159847000
H	-0.317714000	1.836515000	-1.713349000
C	-3.341210000	3.554152000	-1.849224000
H	-2.953242000	4.525636000	-1.505736000
H	-4.358769000	3.437248000	-1.450245000
H	-3.417280000	3.602032000	-2.947355000
C	-3.096056000	-2.576567000	-0.215297000
H	-2.775728000	-2.253822000	0.780984000
C	-2.006123000	-3.520199000	-0.756678000
H	-1.791668000	-4.311997000	-0.024220000
H	-1.065194000	-2.993078000	-0.944500000
H	-2.332359000	-3.995552000	-1.695632000
C	-4.413843000	-3.354871000	-0.065635000
H	-4.280584000	-4.186366000	0.644436000
H	-4.724757000	-3.793077000	-1.027038000
H	-5.239747000	-2.727177000	0.293072000
C	-5.112261000	-0.283337000	1.462506000
H	-5.957156000	0.088569000	2.060203000
H	-4.823168000	-1.262248000	1.860652000
H	-5.460312000	-0.413412000	0.428229000
C	-4.480592000	2.090210000	1.049996000
H	-5.285075000	2.414915000	1.727507000
H	-4.900484000	2.026204000	0.037690000
H	-3.685923000	2.845855000	1.075173000
C	-0.958062000	0.564254000	3.814228000
H	-1.316951000	0.559619000	4.855658000
H	-0.702526000	1.592319000	3.534552000
H	-0.048323000	-0.049188000	3.763560000
C	-2.326299000	-1.468228000	3.348331000
H	-2.587696000	-1.466118000	4.417718000
H	-1.436849000	-2.095340000	3.205067000

H	-3.157629000	-1.929265000	2.800157000
C	1.522641000	-0.674059000	-2.663233000
H	1.656679000	0.388429000	-2.425929000
C	0.011468000	-0.932379000	-2.721568000
H	-0.460610000	-0.703218000	-1.758783000
H	-0.209014000	-1.981052000	-2.972836000
C	2.152898000	-0.954131000	-4.037450000
H	1.918986000	-1.975529000	-4.377239000
H	3.248853000	-0.860522000	-4.022373000

### 2-dib; PBE0-D3(BJ)/def2-SVP

N	0.917723000	3.158562000	-1.471618000
C	0.201759000	2.306134000	-1.113052000
B	-0.620811000	1.063447000	-0.672768000
N	-0.360180000	-2.869932000	-1.385303000
C	-0.157018000	-1.759299000	-1.094606000
B	0.250487000	-0.294201000	-0.879997000
C	-2.064834000	1.351199000	-0.258603000
N	-2.947336000	0.526673000	0.332401000
C	-4.164224000	1.209853000	0.872685000
C	-4.196561000	2.449691000	-0.015153000
H	-4.655553000	3.311309000	0.490530000
H	-4.803024000	2.232221000	-0.908665000
C	-2.739749000	2.720027000	-0.436586000
C	-2.806200000	-0.891915000	0.425330000
C	-3.354190000	-1.670694000	-0.619329000
C	-3.330286000	-3.058947000	-0.487416000
H	-3.742553000	-3.680121000	-1.284392000
C	-2.757474000	-3.666708000	0.622150000
H	-2.735013000	-4.756057000	0.697470000
C	-2.185134000	-2.888205000	1.617261000
H	-1.709935000	-3.373022000	2.473445000
C	-2.195678000	-1.491439000	1.545280000
C	-3.914310000	-1.054492000	-1.890179000
H	-4.109044000	0.008353000	-1.687664000
C	-5.232238000	-1.692706000	-2.325937000
H	-5.671340000	-1.126258000	-3.161737000
H	-5.967313000	-1.723628000	-1.507335000
H	-5.085911000	-2.725050000	-2.679095000
C	-2.889732000	-1.102146000	-3.025690000
H	-3.315751000	-0.661369000	-3.941333000
H	-2.587387000	-2.137450000	-3.244051000

H	-1.986012000	-0.538999000	-2.756396000
H	0.440253000	-0.347708000	3.496118000
H	-1.774518000	-0.310162000	4.786480000
C	-5.424772000	0.365013000	0.752303000
H	-6.268811000	0.931352000	1.172770000
H	-5.333545000	-0.576165000	1.313526000
H	-5.667630000	0.125671000	-0.289693000
C	-3.973472000	1.573024000	2.347661000
H	-4.813293000	2.202143000	2.678296000
H	-3.042349000	2.127943000	2.519396000
H	-3.960638000	0.675290000	2.977255000
C	-2.093922000	3.819447000	0.415857000
H	-2.666714000	4.753230000	0.301157000
H	-1.062614000	4.012687000	0.094832000
H	-2.075572000	3.562905000	1.483770000
C	-2.704427000	3.141680000	-1.910952000
H	-3.341422000	4.030181000	-2.052577000
H	-3.086898000	2.338184000	-2.558913000
H	-1.687827000	3.394284000	-2.238312000
C	1.714332000	-0.016746000	-1.416294000
N	2.775932000	0.266960000	-0.706804000
C	3.958941000	0.743560000	-1.527761000
C	3.317121000	0.880816000	-2.913885000
H	3.026941000	1.929578000	-3.071119000
H	4.012202000	0.590107000	-3.714689000
C	2.047221000	0.022647000	-2.900387000
C	2.950270000	-0.019157000	0.705696000
C	2.931781000	1.017958000	1.666477000
C	3.309581000	0.710185000	2.977221000
H	3.302517000	1.506617000	3.724014000
C	3.666164000	-0.575800000	3.352173000
H	3.964810000	-0.789349000	4.381130000
C	3.601051000	-1.595881000	2.415796000
H	3.830572000	-2.619392000	2.718906000
C	3.236782000	-1.354500000	1.087559000
C	2.408637000	2.415709000	1.408115000
H	2.238196000	2.535207000	0.333259000
C	1.045510000	2.577521000	2.085681000
H	0.629429000	3.569656000	1.857130000
H	1.130925000	2.484304000	3.180486000
H	0.333473000	1.822690000	1.723122000
C	3.354066000	3.522443000	1.872523000



H	2.965681000	4.499297000	1.546864000
H	4.368652000	3.411440000	1.464924000
H	3.438419000	3.555360000	2.970318000
C	3.113279000	-2.571374000	0.186491000
H	2.791501000	-2.240073000	-0.808966000
C	2.031462000	-3.517312000	0.717577000
H	1.825723000	-4.310303000	-0.015916000
H	1.084753000	-2.997121000	0.900883000
H	2.354818000	-3.992409000	1.657421000
C	4.428118000	-3.339503000	0.035827000
H	4.300021000	-4.167933000	-0.677898000
H	4.738114000	-3.782423000	0.995121000
H	5.253946000	-2.708385000	-0.316971000
C	5.093892000	-0.270766000	-1.474031000
H	5.935277000	0.108560000	-2.071196000
H	4.805261000	-1.246731000	-1.881079000
H	5.447620000	-0.410373000	-0.442384000
C	4.470291000	2.086841000	-1.033468000
H	5.275864000	2.413584000	-1.707873000
H	4.890712000	2.011490000	-0.021522000
H	3.679026000	2.847459000	-1.052441000
C	0.946722000	0.594439000	-3.789086000
H	1.299303000	0.599026000	-4.832178000
H	0.689867000	1.620174000	-3.499313000
H	0.038479000	-0.021727000	-3.738055000
C	2.315599000	-1.428587000	-3.350120000
H	2.569201000	-1.415693000	-4.421074000
H	1.428079000	-2.059992000	-3.208600000
H	3.151961000	-1.894787000	-2.813432000
C	-1.534980000	-0.701171000	2.658238000
H	-1.662649000	0.365627000	2.428325000
C	-0.033024000	-0.968908000	2.720882000
H	0.447017000	-0.731662000	1.762045000
H	0.179047000	-2.021857000	2.962494000
C	-2.171969000	-0.992255000	4.018610000
H	-1.949009000	-2.020080000	4.345286000
H	-3.267006000	-0.889767000	4.002044000

### 2-dib; ωB97XD/def2-SVP

N	0.882189000	3.230505000	-1.413272000
C	0.179131000	2.359893000	-1.081132000
B	-0.632076000	1.086639000	-0.674238000

N	-0.308403000	-2.831599000	-1.487100000
C	-0.130742000	-1.730009000	-1.158823000
B	0.246941000	-0.250934000	-0.910791000
C	-2.073867000	1.350668000	-0.235753000
N	-2.941292000	0.502316000	0.345915000
C	-4.163168000	1.155504000	0.915441000
C	-4.221828000	2.420153000	0.059581000
H	-4.682298000	3.262806000	0.594882000
H	-4.839983000	2.221152000	-0.830078000
C	-2.771060000	2.718400000	-0.374584000
C	-2.786910000	-0.920847000	0.396789000
C	-3.331822000	-1.672921000	-0.668190000
C	-3.299239000	-3.063818000	-0.574918000
H	-3.707089000	-3.667158000	-1.387486000
C	-2.719692000	-3.698526000	0.516014000
H	-2.690406000	-4.788912000	0.561052000
C	-2.148325000	-2.944550000	1.530264000
H	-1.667073000	-3.451731000	2.369887000
C	-2.167719000	-1.546569000	1.496581000
C	-3.898311000	-1.023821000	-1.925833000
H	-4.098926000	0.032334000	-1.699842000
C	-5.218452000	-1.657241000	-2.377399000
H	-5.671598000	-1.057007000	-3.181247000
H	-5.943600000	-1.731686000	-1.552854000
H	-5.066374000	-2.670888000	-2.778921000
C	-2.873002000	-1.038021000	-3.066798000
H	-3.305900000	-0.583608000	-3.972250000
H	-2.561025000	-2.065986000	-3.306035000
H	-1.975943000	-0.469103000	-2.787857000
H	0.476552000	-0.434107000	3.466338000
H	-1.754267000	-0.431865000	4.767976000
C	-5.420381000	0.298987000	0.783043000
H	-6.267076000	0.849892000	1.218342000
H	-5.319575000	-0.653156000	1.323672000
H	-5.666472000	0.080210000	-0.262552000
C	-3.965997000	1.483516000	2.402222000
H	-4.804755000	2.102509000	2.753543000
H	-3.034393000	2.034045000	2.584639000
H	-3.948928000	0.569795000	3.007705000
C	-2.131741000	3.810182000	0.499767000
H	-2.721784000	4.736248000	0.415986000
H	-1.107453000	4.030439000	0.174788000

H	-2.097949000	3.525678000	1.560228000
C	-2.763199000	3.173309000	-1.843796000
H	-3.425185000	4.046976000	-1.959070000
H	-3.132726000	2.373001000	-2.503403000
H	-1.758625000	3.459664000	-2.179427000
C	1.725779000	0.043270000	-1.423111000
N	2.779263000	0.296962000	-0.692990000
C	3.972204000	0.805057000	-1.483294000
C	3.346461000	0.990456000	-2.875015000
H	3.058971000	2.043866000	-3.003144000
H	4.051624000	0.725444000	-3.675764000
C	2.075674000	0.129670000	-2.904828000
C	2.938534000	-0.029218000	0.718504000
C	2.886355000	0.978232000	1.708205000
C	3.254768000	0.639335000	3.013537000
H	3.223288000	1.410685000	3.785394000
C	3.631134000	-0.650277000	3.354380000
H	3.921678000	-0.888544000	4.379661000
C	3.592940000	-1.644122000	2.388901000
H	3.834696000	-2.671189000	2.668880000
C	3.238302000	-1.370260000	1.064601000
C	2.336484000	2.375758000	1.482322000
H	2.170999000	2.518977000	0.411215000
C	0.963696000	2.498369000	2.157850000
H	0.523809000	3.480674000	1.931672000
H	1.047727000	2.402505000	3.252767000
H	0.272433000	1.728227000	1.788789000
C	3.261044000	3.493384000	1.975872000
H	2.859996000	4.467567000	1.658469000
H	4.281331000	3.404346000	1.578126000
H	3.331911000	3.511508000	3.074950000
C	3.125310000	-2.566974000	0.127754000
H	2.808143000	-2.213667000	-0.860561000
C	2.038408000	-3.530060000	0.629056000
H	1.826055000	-4.293877000	-0.132648000
H	1.095620000	-3.010753000	0.835355000
H	2.361690000	-4.040694000	1.550182000
C	4.445834000	-3.329594000	-0.039403000
H	4.324754000	-4.128997000	-0.786300000
H	4.748137000	-3.809173000	0.904547000
H	5.273395000	-2.684097000	-0.360134000
C	5.113659000	-0.209254000	-1.454917000

H	5.956115000	0.189860000	-2.037152000
H	4.828407000	-1.172557000	-1.893145000
H	5.463811000	-0.379951000	-0.426697000
C	4.474491000	2.135067000	-0.933716000
H	5.280530000	2.493491000	-1.590862000
H	4.889966000	2.022192000	0.076888000
H	3.679050000	2.891551000	-0.926366000
C	0.983344000	0.725354000	-3.795412000
H	1.351921000	0.758921000	-4.832260000
H	0.718601000	1.742455000	-3.484460000
H	0.076124000	0.105756000	-3.774593000
C	2.356080000	-1.309731000	-3.398653000
H	2.637126000	-1.260327000	-4.461264000
H	1.465686000	-1.945141000	-3.302746000
H	3.177940000	-1.796535000	-2.858351000
C	-1.503510000	-0.781429000	2.630976000
H	-1.634754000	0.290603000	2.433469000
C	0.003791000	-1.042220000	2.680350000
H	0.477075000	-0.779485000	1.725387000
H	0.224864000	-2.099043000	2.897273000
C	-2.133975000	-1.112274000	3.990036000
H	-1.884362000	-2.139129000	4.300139000
H	-3.231021000	-1.037805000	3.973731000

### 2-dib; M06-D3/def2-SVP

N	0.964629000	3.145035000	-1.504435000
C	0.236450000	2.301614000	-1.144849000
B	-0.603576000	1.066667000	-0.700456000
N	-0.365411000	-2.877473000	-1.433194000
C	-0.162577000	-1.765741000	-1.141152000
B	0.254143000	-0.299994000	-0.915272000
C	-2.039606000	1.366793000	-0.284367000
N	-2.931674000	0.550548000	0.322629000
C	-4.136309000	1.262448000	0.865907000
C	-4.162204000	2.484311000	-0.043329000
H	-4.613042000	3.362000000	0.450324000
H	-4.781239000	2.258478000	-0.930368000
C	-2.707162000	2.736077000	-0.477991000
C	-2.800291000	-0.871746000	0.421663000
C	-3.343909000	-1.657265000	-0.620288000
C	-3.311002000	-3.044904000	-0.486969000
H	-3.717898000	-3.670180000	-1.287440000

C	-2.738797000	-3.648808000	0.624338000
H	-2.711302000	-4.739239000	0.701486000
C	-2.182212000	-2.865463000	1.624167000
H	-1.715366000	-3.347034000	2.490352000
C	-2.199383000	-1.469184000	1.548486000
C	-3.924608000	-1.054085000	-1.886539000
H	-4.101214000	0.019181000	-1.698828000
C	-5.258547000	-1.681734000	-2.276886000
H	-5.722539000	-1.116768000	-3.102257000
H	-5.971105000	-1.707988000	-1.435592000
H	-5.131428000	-2.718128000	-2.632445000
C	-2.940543000	-1.140878000	-3.050969000
H	-3.384600000	-0.702777000	-3.961116000
H	-2.672207000	-2.188746000	-3.268333000
H	-2.009175000	-0.597040000	-2.826349000
H	0.367279000	-0.317346000	3.592774000
H	-1.898460000	-0.277605000	4.793439000
C	-5.405954000	0.434449000	0.774681000
H	-6.242262000	1.022409000	1.186375000
H	-5.328756000	-0.495265000	1.362933000
H	-5.663990000	0.171001000	-0.260840000
C	-3.931915000	1.656162000	2.328523000
H	-4.759181000	2.310830000	2.648497000
H	-2.988360000	2.199175000	2.489571000
H	-3.936097000	0.775532000	2.986896000
C	-2.061795000	3.851256000	0.349124000
H	-2.623396000	4.789038000	0.196943000
H	-1.020606000	4.032383000	0.043989000
H	-2.065593000	3.632017000	1.428362000
C	-2.680056000	3.133954000	-1.956360000
H	-3.329154000	4.014023000	-2.112193000
H	-3.056668000	2.315552000	-2.593865000
H	-1.667373000	3.395406000	-2.297146000
C	1.730930000	-0.037767000	-1.429096000
N	2.781245000	0.246284000	-0.696974000
C	3.990670000	0.701673000	-1.509783000
C	3.374709000	0.819960000	-2.906466000
H	3.102947000	1.872618000	-3.093475000
H	4.081632000	0.504160000	-3.692357000
C	2.094962000	-0.020534000	-2.903877000
C	2.929789000	-0.033271000	0.723936000
C	2.944454000	1.015562000	1.671772000

C	3.321714000	0.714055000	2.983628000
H	3.341011000	1.520438000	3.723169000
C	3.647463000	-0.576779000	3.370112000
H	3.952665000	-0.785966000	4.399317000
C	3.540387000	-1.607359000	2.449084000
H	3.740872000	-2.635427000	2.766104000
C	3.168117000	-1.372890000	1.122102000
C	2.449822000	2.418981000	1.395810000
H	2.288006000	2.531492000	0.315171000
C	1.086292000	2.613435000	2.058019000
H	0.674496000	3.600957000	1.790331000
H	1.163340000	2.562621000	3.158740000
H	0.364843000	1.848249000	1.724379000
C	3.403577000	3.515638000	1.855285000
H	3.039569000	4.494645000	1.502927000
H	4.427573000	3.381982000	1.472382000
H	3.466655000	3.573596000	2.955535000
C	2.984525000	-2.595757000	0.241080000
H	2.643418000	-2.268494000	-0.754156000
C	1.889449000	-3.501499000	0.804974000
H	1.655447000	-4.307508000	0.091401000
H	0.952061000	-2.955790000	0.986875000
H	2.207894000	-3.966007000	1.754273000
C	4.267511000	-3.403079000	0.062274000
H	4.097854000	-4.232859000	-0.643780000
H	4.591081000	-3.852634000	1.016383000
H	5.106802000	-2.800220000	-0.315385000
C	5.113099000	-0.319098000	-1.419781000
H	5.966509000	0.039962000	-2.016296000
H	4.826162000	-1.305731000	-1.810441000
H	5.460935000	-0.440061000	-0.380574000
C	4.509275000	2.045714000	-1.034749000
H	5.319370000	2.355597000	-1.715067000
H	4.934272000	1.985873000	-0.020513000
H	3.727537000	2.819880000	-1.066986000
C	1.023306000	0.551548000	-3.822536000
H	1.412520000	0.568334000	-4.854510000
H	0.747798000	1.576952000	-3.538737000
H	0.115363000	-0.072131000	-3.815770000
C	2.357689000	-1.475391000	-3.336282000
H	2.633187000	-1.472423000	-4.403925000
H	1.460248000	-2.101113000	-3.213142000

H	3.179959000	-1.952815000	-2.782122000
C	-1.571133000	-0.677443000	2.676782000
H	-1.699731000	0.393224000	2.446906000
C	-0.072656000	-0.930415000	2.787539000
H	0.448075000	-0.674334000	1.848893000
H	0.146742000	-1.986728000	3.023246000
C	-2.246157000	-0.975794000	4.013453000
H	-2.006664000	-1.995951000	4.359221000
H	-3.345313000	-0.907903000	3.956449000

### 3-dib

B	1.487131000	-0.851951000	0.416517000
B	-2.536751000	-0.216793000	0.302282000
B	2.194081000	0.578346000	0.047122000
C	-0.001326000	-0.819277000	0.456597000
C	-2.603028000	1.173040000	-0.373948000
C	3.387298000	0.820643000	0.992794000
N	-1.175250000	-0.671217000	0.452720000
N	-2.533356000	2.224215000	-0.876274000
N	4.284724000	0.820359000	1.743265000
N	3.188250000	-2.707329000	0.773023000
C	2.244742000	-1.928327000	1.261575000
N	-5.022700000	-0.720922000	0.519720000
C	3.840086000	-3.619629000	1.805972000
C	5.361771000	-3.556642000	1.750257000
H	5.761589000	-4.174847000	2.568327000
H	5.731014000	-2.533116000	1.885027000
H	5.746164000	-3.960397000	0.805017000
C	3.400615000	-5.069737000	1.584988000
H	3.878443000	-5.703856000	2.345789000
H	3.718658000	-5.428609000	0.596628000
H	2.315884000	-5.198699000	1.671457000
C	3.301497000	-3.011998000	3.110848000
H	4.047930000	-2.315778000	3.519126000
H	3.109766000	-3.783652000	3.869790000
C	2.032484000	-2.218327000	2.741993000
C	0.744901000	-3.057434000	2.898449000
H	0.592724000	-3.283245000	3.965234000
H	0.783476000	-4.009581000	2.352495000
H	-0.129863000	-2.498186000	2.544740000
C	1.897940000	-0.946836000	3.588787000
H	1.877815000	-1.225010000	4.654618000

H	0.965738000	-0.417061000	3.357270000
H	2.736351000	-0.259753000	3.414512000
C	3.431630000	-2.918486000	-0.647485000
C	4.593783000	-2.398802000	-1.267062000
C	5.530372000	-1.374400000	-0.638823000
H	5.206167000	-1.179889000	0.390306000
C	5.417112000	-0.041255000	-1.394127000
H	6.047391000	0.717216000	-0.912771000
H	4.384741000	0.326192000	-1.389019000
H	5.742563000	-0.147293000	-2.441062000
C	7.002040000	-1.819524000	-0.628252000
H	7.606789000	-1.088003000	-0.069997000
H	7.410815000	-1.867515000	-1.650070000
H	7.151168000	-2.805143000	-0.167696000
C	4.852584000	-2.768071000	-2.595057000
H	5.746615000	-2.377985000	-3.083808000
C	3.990013000	-3.591489000	-3.308009000
H	4.215140000	-3.863988000	-4.341704000
C	2.823285000	-4.043364000	-2.701796000
H	2.127885000	-4.660980000	-3.272531000
C	2.512934000	-3.723555000	-1.373743000
C	1.181816000	-4.242484000	-0.836870000
H	1.083908000	-3.943000000	0.213005000
C	0.002514000	-3.616141000	-1.599818000
H	-0.951502000	-3.986186000	-1.199004000
H	0.039883000	-3.876275000	-2.668854000
H	0.001124000	-2.523930000	-1.515426000
C	1.076846000	-5.775958000	-0.901410000
H	0.154561000	-6.112103000	-0.401397000
H	1.928385000	-6.277734000	-0.422838000
H	1.028549000	-6.126697000	-1.944007000
C	-3.698207000	-1.022099000	0.754310000
C	-5.976301000	-1.579544000	1.283672000
C	-6.441656000	-0.914313000	2.592915000
H	-6.971171000	-1.653436000	3.214257000
H	-7.132051000	-0.085773000	2.401159000
H	-5.593528000	-0.526221000	3.172168000
C	-7.204275000	-1.940398000	0.447915000
H	-7.862321000	-2.604373000	1.028987000
H	-6.924090000	-2.459298000	-0.477672000
H	-7.778490000	-1.042892000	0.175370000
C	-5.091320000	-2.805168000	1.583112000



H	-5.225053000	-3.544930000	0.778767000
H	-5.367845000	-3.296911000	2.527207000
C	-3.623660000	-2.310948000	1.582334000
C	-2.725239000	-3.377112000	0.931619000
H	-2.801589000	-4.325623000	1.489733000
H	-1.673034000	-3.071935000	0.921568000
H	-3.029727000	-3.565688000	-0.108250000
C	-3.100049000	-2.019913000	3.002577000
H	-3.060195000	-2.945975000	3.600406000
H	-3.734966000	-1.297179000	3.532255000
H	-2.089081000	-1.591243000	2.956912000
C	-5.410928000	0.112406000	-0.580034000
C	-5.260078000	-0.393649000	-1.898432000
C	-4.711358000	-1.783689000	-2.195772000
H	-4.591414000	-2.305761000	-1.239118000
C	-3.322827000	-1.712857000	-2.851655000
H	-2.912164000	-2.725276000	-3.000138000
H	-2.620607000	-1.148603000	-2.224446000
H	-3.373637000	-1.222098000	-3.836912000
C	-5.674510000	-2.615283000	-3.057309000
H	-5.298270000	-3.645348000	-3.168475000
H	-5.780335000	-2.193805000	-4.069326000
H	-6.680821000	-2.664010000	-2.613947000
C	-5.617943000	0.425226000	-2.974441000
H	-5.500948000	0.049733000	-3.993402000
C	-6.121368000	1.708322000	-2.771861000
H	-6.396746000	2.331506000	-3.626171000
C	-6.254953000	2.196803000	-1.477201000
H	-6.624386000	3.212431000	-1.321552000
C	-5.891078000	1.423701000	-0.366599000
C	-5.982338000	2.047945000	1.016226000
H	-5.538907000	1.333995000	1.721637000
C	-7.443981000	2.299547000	1.420717000
H	-7.509327000	2.643117000	2.466045000
H	-8.064109000	1.396375000	1.316029000
H	-7.895767000	3.078175000	0.785129000
C	-5.169651000	3.348634000	1.115896000
H	-5.141132000	3.701653000	2.159670000
H	-5.618794000	4.151563000	0.509376000
H	-4.141823000	3.202233000	0.760663000
N	1.748247000	3.005058000	-0.735506000
C	1.661062000	1.670756000	-0.897602000

C	1.135522000	3.819354000	-1.860144000
C	0.123518000	4.835520000	-1.326674000
H	-0.257347000	5.425074000	-2.174387000
H	0.585820000	5.530553000	-0.610578000
H	-0.735016000	4.340829000	-0.859420000
C	2.190376000	4.569542000	-2.680750000
H	1.694472000	5.031019000	-3.547667000
H	2.983640000	3.912060000	-3.056523000
H	2.648172000	5.373952000	-2.096037000
C	0.443515000	2.718258000	-2.679586000
H	0.481390000	2.927184000	-3.758356000
H	-0.612628000	2.653820000	-2.382428000
C	1.142200000	1.397084000	-2.315709000
C	2.379360000	1.118485000	-3.206089000
H	2.077880000	1.127430000	-4.265917000
H	2.797384000	0.129573000	-2.973001000
H	3.179149000	1.858735000	-3.068959000
C	0.187480000	0.217341000	-2.488947000
H	-0.098652000	0.145699000	-3.550497000
H	-0.728829000	0.346528000	-1.906372000
H	0.669929000	-0.725268000	-2.203680000
C	2.177884000	3.623888000	0.499937000
C	3.489781000	4.141584000	0.634935000
C	4.569384000	4.054925000	-0.437451000
H	4.159225000	3.487959000	-1.283289000
C	5.817707000	3.307167000	0.063089000
H	6.521425000	3.150206000	-0.770585000
H	5.562104000	2.339793000	0.509182000
H	6.346570000	3.896025000	0.829247000
C	4.997320000	5.450429000	-0.928931000
H	5.654113000	5.366517000	-1.809884000
H	5.563775000	5.976617000	-0.144399000
H	4.146286000	6.091345000	-1.195486000
C	3.842753000	4.750100000	1.847013000
H	4.851580000	5.149345000	1.964664000
C	2.948361000	4.834828000	2.906934000
H	3.249644000	5.306884000	3.845244000
C	1.671316000	4.302992000	2.767427000
H	0.971533000	4.359280000	3.603212000
C	1.256435000	3.693979000	1.576421000
C	-0.158693000	3.133169000	1.529064000
H	-0.360319000	2.758180000	0.519953000

C	-1.217371000	4.199249000	1.850497000
H	-2.222054000	3.786997000	1.681739000
H	-1.108036000	5.093939000	1.221777000
H	-1.157575000	4.520333000	2.902706000
C	-0.307886000	1.942090000	2.484713000
H	-1.313832000	1.504256000	2.393879000
H	-0.157957000	2.247040000	3.533048000
H	0.427623000	1.167840000	2.241504000

#### 4-dib

B	0.733960000	-0.297831000	0.097506000
B	-0.286529000	0.958629000	0.408118000
C	0.198833000	2.315506000	1.063788000
C	1.439002000	2.505629000	1.979796000
N	-0.398489000	3.513206000	0.957287000
C	0.435573000	4.669572000	1.503355000
C	1.169456000	3.897706000	2.596404000
C	0.341700000	-1.716259000	-0.536202000
C	-0.054630000	-1.995954000	-1.983951000
C	-0.149696000	-3.543492000	-2.033952000
C	-0.271561000	-4.012726000	-0.576548000
N	0.390556000	-2.840255000	0.147449000
C	2.237383000	-0.295410000	0.416248000
N	3.390367000	-0.307328000	0.647743000
C	-1.769254000	0.794665000	-0.066305000
N	-2.847022000	0.579373000	-0.498792000
C	-1.362862000	-1.314620000	-2.388278000
C	1.038837000	-1.459353000	-2.927984000
C	1.477507000	1.440867000	3.089318000
H	1.658111000	0.433200000	2.702655000
H	0.529528000	1.418828000	3.645960000
H	2.290749000	1.669586000	3.794528000
H	0.500099000	3.800842000	3.465405000
H	2.091635000	4.389624000	2.933783000
H	0.753437000	-3.964249000	-2.496781000
H	-1.009137000	-3.877177000	-2.629585000
H	2.029029000	-1.876489000	-2.721293000
H	1.106184000	-0.366872000	-2.859030000
H	0.764999000	-1.718234000	-3.962722000
H	-1.243885000	-0.228270000	-2.412807000
H	-2.194896000	-1.555647000	-1.721114000
H	-1.633696000	-1.631472000	-3.405221000

C	2.790114000	2.556846000	1.207114000
H	3.535412000	1.907607000	1.677515000
H	3.211170000	3.568456000	1.211588000
H	2.696834000	2.244227000	0.164342000
B	-3.967774000	0.551141000	-1.504443000
C	-3.448562000	1.079059000	-2.865498000
C	-5.395684000	0.171590000	-1.467933000
C	-6.387773000	0.564911000	-2.620525000
C	-6.093928000	-0.078391000	-3.994007000
C	-6.462091000	2.090023000	-2.841106000
C	-7.744888000	0.029170000	-2.102972000
C	-7.606904000	-0.125430000	-0.579811000
N	-6.156924000	-0.465998000	-0.464760000
H	-6.935960000	0.130608000	-4.675903000
H	-5.988401000	-1.168531000	-3.924674000
H	-5.183293000	0.321961000	-4.451742000
H	-5.499657000	2.484024000	-3.189535000
H	-6.741344000	2.623753000	-1.924038000
H	-7.219581000	2.320937000	-3.608372000
H	-8.582339000	0.684684000	-2.383811000
H	-7.950479000	-0.959836000	-2.540354000
N	-3.090708000	1.441987000	-3.914851000
N	4.451338000	-0.501183000	3.994118000
C	4.567469000	-0.380349000	2.838854000
B	4.694560000	-0.180601000	1.309382000
C	5.936492000	0.364616000	0.727034000
N	6.227169000	0.660985000	-0.602570000
C	7.371531000	1.613858000	-0.736278000
H	8.750512000	2.157441000	0.894113000
C	8.165977000	1.295265000	0.542196000
H	8.881467000	0.487096000	0.325460000
C	7.137236000	0.814915000	1.595074000
H	6.319688000	2.810380000	2.045145000
C	6.762251000	1.951724000	2.568286000
H	6.040038000	1.604034000	3.317878000
H	7.041836000	-0.698096000	3.185000000
C	7.736456000	-0.346599000	2.411684000
H	7.990145000	-1.198061000	1.764165000
H	7.662030000	2.304142000	3.099370000
H	8.661605000	-0.012193000	2.911284000
C	-1.695117000	3.715534000	0.369132000
C	-2.813858000	3.726839000	1.242455000

C	-1.817480000	3.888837000	-1.023260000
C	-4.075476000	3.874523000	0.659601000
C	-3.109162000	4.021577000	-1.551020000
C	-4.223186000	4.004428000	-0.721240000
H	-4.962908000	3.890286000	1.290389000
H	-3.237862000	4.122731000	-2.628924000
H	-5.219964000	4.094713000	-1.152536000
C	5.718596000	-0.106204000	-1.695443000
C	4.730061000	0.420897000	-2.560483000
C	6.255234000	-1.400967000	-1.933514000
C	4.267406000	-0.367529000	-3.623714000
C	5.755984000	-2.152094000	-3.003584000
C	4.763882000	-1.648498000	-3.842216000
H	3.505466000	0.033641000	-4.294813000
H	6.163718000	-3.147222000	-3.194100000
H	4.387749000	-2.249767000	-4.673537000
C	0.983229000	-2.922701000	1.481143000
C	0.199241000	-2.584950000	2.610451000
C	2.362157000	-3.235935000	1.623737000
C	0.820342000	-2.498796000	3.862737000
C	2.911207000	-3.144978000	2.911809000
C	2.172360000	-2.759839000	4.019281000
H	0.223399000	-2.210128000	4.728692000
H	3.979907000	-3.324831000	3.031893000
H	2.662773000	-2.635448000	4.985259000
C	-5.718164000	-1.611274000	0.262683000
C	-5.487334000	-2.836132000	-0.420746000
C	-5.624570000	-1.570140000	1.681337000
C	-5.107567000	-3.969129000	0.309881000
C	-5.280822000	-2.741949000	2.366970000
H	-4.932670000	-4.909517000	-0.217664000
H	-5.222740000	-2.730763000	3.453995000
C	-0.611368000	4.013127000	-1.942958000
H	0.283236000	3.888113000	-1.327365000
C	-0.566671000	5.418813000	-2.566899000
H	0.383115000	5.573148000	-3.103981000
H	-1.384299000	5.550798000	-3.292668000
H	-0.668876000	6.211671000	-1.809723000
C	-0.540584000	2.947148000	-3.038434000
H	-1.419281000	2.955290000	-3.693478000
H	0.353145000	3.115663000	-3.657459000
H	-0.468818000	1.939931000	-2.605408000

C	7.394576000	-1.977014000	-1.102711000
H	7.784523000	-1.163739000	-0.482483000
C	6.924763000	-3.077465000	-0.143610000
H	6.484170000	-3.925242000	-0.692294000
H	7.771665000	-3.463992000	0.445670000
H	6.177331000	-2.682263000	0.555974000
C	8.551386000	-2.481378000	-1.979378000
H	9.416359000	-2.747365000	-1.350892000
H	8.271904000	-3.382676000	-2.547611000
H	8.876080000	-1.720091000	-2.705053000
C	4.205505000	1.839226000	-2.415715000
H	4.551787000	2.209321000	-1.442151000
C	4.777769000	2.741850000	-3.523483000
H	5.873463000	2.684994000	-3.582226000
H	4.381995000	2.442009000	-4.507176000
H	4.496583000	3.794359000	-3.355724000
C	2.678011000	1.929679000	-2.435442000
H	2.266124000	1.654072000	-3.417266000
H	2.207059000	1.285326000	-1.683362000
H	2.357842000	2.963034000	-2.234410000
C	-2.640038000	3.692722000	2.763332000
H	-1.748129000	4.286666000	2.961011000
C	-1.304392000	-2.378001000	2.590567000
H	-1.659229000	-2.395488000	1.555753000
C	-1.725190000	-1.025228000	3.167140000
H	-1.518729000	-0.946751000	4.245775000
H	-1.193168000	-0.215812000	2.655620000
H	-2.803508000	-0.876402000	3.018745000
C	-1.969970000	-3.528747000	3.363843000
H	-3.059609000	-3.430341000	3.333820000
H	-1.698101000	-4.512986000	2.951846000
H	-1.652749000	-3.519870000	4.417675000
C	-3.780825000	4.382115000	3.519059000
H	-3.526335000	4.459948000	4.587866000
H	-3.970650000	5.396913000	3.136930000
H	-4.721181000	3.813634000	3.453211000
C	-2.335557000	2.322946000	3.385836000
H	-1.634826000	1.746032000	2.775617000
H	-1.880370000	2.460796000	4.379669000
H	-3.238583000	1.719655000	3.517165000
C	3.412371000	-3.655005000	0.585114000
H	4.291062000	-3.066420000	0.884164000

C	-7.943769000	1.208616000	0.121743000
H	-8.916444000	1.583947000	-0.231963000
H	-8.009720000	1.096055000	1.211449000
H	-7.185389000	1.971964000	-0.090711000
C	-8.519060000	-1.225114000	-0.038853000
H	-8.388196000	-1.374572000	1.042410000
H	-9.568231000	-0.944112000	-0.217676000
H	-8.332912000	-2.185604000	-0.535929000
C	-0.366392000	5.873982000	2.011224000
H	-1.192861000	6.120875000	1.329133000
H	-0.767809000	5.742074000	3.022192000
H	0.304642000	6.743988000	2.046992000
C	1.363884000	5.217841000	0.398995000
H	1.855628000	4.433251000	-0.181453000
H	0.801533000	5.856535000	-0.292707000
H	2.142762000	5.837626000	0.867778000
C	6.891597000	3.080021000	-0.720238000
H	6.434272000	3.368618000	-1.672890000
H	6.155246000	3.246409000	0.076656000
H	7.745579000	3.752552000	-0.544293000
C	8.193347000	1.369052000	-2.001048000
H	8.617735000	0.357779000	-2.023293000
H	7.590039000	1.503311000	-2.909983000
H	9.025852000	2.088016000	-2.037282000
C	0.401624000	-5.344710000	-0.276337000
H	1.423075000	-5.397545000	-0.662867000
H	0.424276000	-5.540680000	0.805532000
H	-0.181055000	-6.145976000	-0.753644000
C	-1.747933000	-4.112523000	-0.168325000
H	-1.868409000	-4.437207000	0.870262000
H	-2.291071000	-3.169826000	-0.303711000
H	-2.229635000	-4.864797000	-0.808117000
C	3.226534000	-3.325862000	-0.890125000
H	4.146178000	-3.591390000	-1.426702000
H	2.410652000	-3.874589000	-1.368299000
H	3.076329000	-2.254645000	-1.051034000
C	3.812955000	-5.131167000	0.778661000
H	4.670518000	-5.375635000	0.132698000
H	4.105310000	-5.334893000	1.818603000
H	2.994968000	-5.820672000	0.527977000
C	-5.010020000	-3.932023000	1.694126000
H	-4.737877000	-4.829936000	2.253507000

C	-5.757487000	-3.010862000	-1.905855000
H	-6.176981000	-2.070460000	-2.262938000
C	-4.486217000	-3.270505000	-2.719614000
H	-3.786117000	-2.434522000	-2.615292000
H	-3.982602000	-4.197153000	-2.398423000
H	-4.726791000	-3.376322000	-3.789722000
C	-6.804654000	-4.104602000	-2.170140000
H	-7.718740000	-3.944102000	-1.578782000
H	-7.085659000	-4.111611000	-3.235813000
H	-6.422408000	-5.107999000	-1.923154000
C	-5.941785000	-0.296854000	2.459077000
H	-7.001185000	-0.069527000	2.265797000
C	-5.117001000	0.898336000	1.973569000
H	-4.046692000	0.681147000	2.056274000
H	-5.307213000	1.147854000	0.928420000
H	-5.338657000	1.784085000	2.586474000
C	-5.812870000	-0.438339000	3.980073000
H	-4.778161000	-0.663407000	4.285070000
H	-6.097919000	0.508976000	4.463116000
H	-6.465578000	-1.225626000	4.386560000

### Ph<sub>2</sub>S<sub>2</sub>

S	0.656169000	-1.890095000	-0.836140000
S	-0.656068000	-1.890005000	0.836184000
C	1.649101000	-0.452105000	-0.463574000
C	1.320088000	0.777440000	-1.051967000
C	2.077879000	1.914646000	-0.758608000
C	3.157564000	1.828210000	0.123647000
C	3.484324000	0.601049000	0.713436000
C	2.734919000	-0.538516000	0.420716000
C	-1.649009000	-0.452068000	0.463570000
C	-2.734885000	-0.538608000	-0.420640000
C	-3.484440000	0.600872000	-0.713357000
C	-3.157742000	1.828076000	-0.123657000
C	-2.077952000	1.914659000	0.758477000
C	-1.320052000	0.777545000	1.051855000
H	2.976438000	-1.500052000	0.877747000
H	4.329741000	0.532858000	1.402372000
H	3.747843000	2.718352000	0.354203000
H	1.818384000	2.871872000	-1.217083000
H	0.465934000	0.834328000	-1.728718000
H	-2.976369000	-1.500182000	-0.877606000



H	-4.329897000	0.532530000	-1.402228000
H	-3.748101000	2.718183000	-0.354148000
H	-1.818530000	2.871950000	1.216857000
H	-0.465827000	0.834549000	1.728508000

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N	-0.190734000	-3.376599000	0.731169000
C	0.356318000	-2.373545000	0.500987000
B	0.922271000	-0.972788000	0.082561000
N	-1.460563000	1.743764000	1.439158000
C	-1.117291000	0.947404000	0.664274000
B	-0.663137000	-0.048075000	-0.449497000
C	2.162663000	-0.477572000	1.060024000
N	2.851003000	0.661296000	1.089569000
C	4.288198000	0.454048000	1.588674000
C	4.051716000	-0.668829000	2.590004000
H	3.790380000	-0.240851000	3.569021000
H	4.946379000	-1.289262000	2.730582000
C	2.863269000	-1.479956000	2.025781000
C	2.363305000	1.999449000	0.792767000
C	2.612364000	2.640378000	-0.446955000
C	2.112059000	3.936630000	-0.622316000
H	2.273199000	4.439156000	-1.576691000
C	1.414884000	4.594362000	0.385284000
H	1.015868000	5.595828000	0.209660000
C	1.240048000	3.976930000	1.617229000
H	0.724868000	4.507308000	2.419394000
C	1.737154000	2.690667000	1.862936000
C	3.532719000	2.087452000	-1.529226000
H	3.703862000	1.028565000	-1.312159000
C	4.876934000	2.841731000	-1.484991000
H	5.607360000	2.369697000	-2.162039000
H	5.315957000	2.873477000	-0.477953000
H	4.744358000	3.885191000	-1.812172000
C	2.974210000	2.158713000	-2.955706000
H	3.710962000	1.736564000	-3.657973000
H	2.780851000	3.196853000	-3.269800000
H	2.042074000	1.591595000	-3.044965000
H	0.437664000	1.582903000	4.940146000
H	2.618786000	2.775901000	5.215991000
C	5.181855000	-0.038431000	0.435739000
H	6.086222000	-0.493870000	0.865707000

H	5.500658000	0.780119000	-0.215023000
H	4.672234000	-0.789157000	-0.178971000
C	4.899585000	1.698374000	2.217233000
H	5.952682000	1.482734000	2.451774000
H	4.401324000	1.981257000	3.148933000
H	4.874612000	2.558310000	1.535584000
C	1.882809000	-1.790883000	3.173215000
H	2.441624000	-2.298659000	3.975761000
H	1.073423000	-2.451723000	2.850223000
H	1.444987000	-0.875421000	3.593725000
C	3.345926000	-2.805667000	1.422345000
H	3.819233000	-3.393672000	2.223940000
H	4.083459000	-2.663228000	0.625155000
H	2.521369000	-3.400261000	1.020880000
C	-1.839756000	-1.128386000	-0.839146000
N	-2.908406000	-1.461511000	-0.129126000
C	-3.649924000	-2.715088000	-0.637817000
C	-2.707045000	-3.173497000	-1.746956000
H	-2.027188000	-3.941914000	-1.353530000
H	-3.252625000	-3.600988000	-2.599843000
C	-1.880585000	-1.946698000	-2.149526000
C	-3.591072000	-0.725219000	0.932048000
C	-3.562088000	-1.200905000	2.264306000
C	-4.468308000	-0.659277000	3.185554000
H	-4.450638000	-1.018271000	4.215541000
C	-5.375489000	0.326793000	2.819734000
H	-6.089038000	0.720090000	3.547607000
C	-5.333269000	0.840712000	1.529767000
H	-6.000463000	1.660040000	1.259058000
C	-4.437001000	0.356572000	0.567811000
C	-2.515953000	-2.164668000	2.801139000
H	-2.000353000	-2.636379000	1.960737000
C	-1.459655000	-1.361286000	3.569467000
H	-0.732372000	-2.038037000	4.039041000
H	-1.919863000	-0.750042000	4.361311000
H	-0.924900000	-0.683235000	2.895457000
C	-3.079982000	-3.271053000	3.704519000
H	-2.293375000	-4.012699000	3.913998000
H	-3.928966000	-3.799542000	3.249067000
H	-3.416867000	-2.873066000	4.674951000
C	-4.384394000	1.115746000	-0.754878000
H	-3.536631000	0.741401000	-1.342078000

C	-4.123543000	2.608592000	-0.490713000
H	-3.926388000	3.123278000	-1.439628000
H	-3.266890000	2.754270000	0.175416000
H	-5.004564000	3.084912000	-0.032075000
C	-5.661488000	0.998279000	-1.602855000
H	-5.541941000	1.579278000	-2.530747000
H	-6.526105000	1.415192000	-1.061936000
H	-5.913282000	-0.031671000	-1.877646000
C	-5.056471000	-2.383422000	-1.137310000
H	-5.550536000	-3.323566000	-1.422359000
H	-5.043461000	-1.736837000	-2.018963000
H	-5.660864000	-1.906973000	-0.353756000
C	-3.767825000	-3.789845000	0.440566000
H	-4.201411000	-4.682884000	-0.035187000
H	-4.441103000	-3.484940000	1.250674000
H	-2.788562000	-4.064730000	0.847392000
C	-0.571570000	-2.397417000	-2.789025000
H	-0.820330000	-3.016822000	-3.665950000
H	0.020133000	-3.013811000	-2.108881000
H	0.039172000	-1.554043000	-3.123871000
C	-2.628369000	-1.086292000	-3.202391000
H	-2.820034000	-1.714898000	-4.085800000
H	-2.000103000	-0.239714000	-3.497452000
H	-3.586894000	-0.693608000	-2.847399000
C	1.725122000	2.196549000	3.310443000
H	2.312243000	1.272163000	3.351787000
C	0.341547000	1.871690000	3.880488000
H	-0.144574000	1.059927000	3.336854000
H	-0.334935000	2.736088000	3.815734000
C	2.413823000	3.225420000	4.231051000
H	1.764333000	4.098019000	4.399610000
H	3.360593000	3.598938000	3.816030000
S	2.136669000	-1.117747000	-1.499077000
S	-0.139628000	0.955698000	-2.044503000
C	2.925841000	-2.690927000	-1.774920000
C	2.375194000	-3.957615000	-1.521093000
C	3.090093000	-5.112305000	-1.846026000
C	4.350909000	-5.032261000	-2.443259000
C	4.897326000	-3.774431000	-2.714656000
C	4.195813000	-2.615884000	-2.380165000
C	-1.124101000	2.428284000	-2.278923000
C	-1.785648000	2.610073000	-3.505993000

C	-2.399307000	3.828329000	-3.810520000
C	-2.358758000	4.885145000	-2.896188000
C	-1.709461000	4.706003000	-1.671364000
C	-1.100466000	3.489656000	-1.362257000
H	4.627427000	-1.634385000	-2.589168000
H	5.880774000	-3.691355000	-3.184362000
H	4.901731000	-5.940922000	-2.696609000
H	2.648551000	-6.088312000	-1.628766000
H	1.402962000	-4.052920000	-1.044482000
H	-1.798933000	1.797700000	-4.234999000
H	-2.904769000	3.952683000	-4.771788000
H	-2.832614000	5.839956000	-3.136544000
H	-1.678242000	5.519866000	-0.942204000
H	-0.607131000	3.356145000	-0.405667000

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B	1.035527000	-1.097723000	-2.108773000
B	2.007804000	0.422065000	1.396253000
B	-1.444715000	2.337689000	0.452347000
C	1.850331000	-0.366517000	-1.063531000
C	0.786204000	1.313411000	1.364720000
N	2.182826000	-0.104065000	0.043683000
N	-0.152553000	1.946806000	1.022477000
N	2.319091000	-0.979954000	-4.338622000
N	-1.136717000	4.864636000	0.335169000
C	1.409038000	-1.541498000	-3.478088000
C	2.437238000	-1.696516000	-5.653148000
C	1.666951000	-0.961231000	-6.760609000
H	1.742403000	-1.528142000	-7.700857000
H	2.092835000	0.036558000	-6.933567000
H	0.603473000	-0.845944000	-6.517472000
C	3.887205000	-1.857733000	-6.108172000
H	3.907709000	-2.423390000	-7.052527000
H	4.478031000	-2.411539000	-5.368708000
H	4.365216000	-0.884284000	-6.287310000
C	1.810295000	-3.054584000	-5.313922000
H	2.608758000	-3.754611000	-5.027322000
H	1.288822000	-3.490596000	-6.178598000
C	0.872129000	-2.839903000	-4.104227000
C	1.001431000	-4.029705000	-3.137939000
H	0.707759000	-4.961541000	-3.650478000
H	0.384736000	-3.921771000	-2.237570000

H	2.039741000	-4.137123000	-2.794596000
C	-0.595847000	-2.711144000	-4.546914000
H	-0.924692000	-3.643432000	-5.034883000
H	-0.742845000	-1.887042000	-5.259105000
H	-1.245166000	-2.535840000	-3.680942000
C	2.889080000	0.333420000	-4.214504000
C	4.250552000	0.470432000	-3.846668000
C	5.060629000	-0.666128000	-3.241911000
H	4.446868000	-1.576954000	-3.289168000
C	5.337281000	-0.365326000	-1.762494000
H	5.827994000	-1.218763000	-1.280586000
H	4.417106000	-0.151792000	-1.209835000
H	6.001545000	0.506151000	-1.656290000
C	6.393996000	-0.927019000	-3.960083000
H	6.886896000	-1.811519000	-3.526140000
H	7.084714000	-0.078252000	-3.832533000
H	6.272804000	-1.096853000	-5.038220000
C	4.857456000	1.730116000	-3.956159000
H	5.908761000	1.838767000	-3.683022000
C	4.145438000	2.839574000	-4.397126000
H	4.638056000	3.810171000	-4.492982000
C	2.785983000	2.713143000	-4.669762000
H	2.213266000	3.597538000	-4.956310000
C	2.127991000	1.480981000	-4.563370000
C	0.615168000	1.469048000	-4.740075000
H	0.278864000	0.425571000	-4.716805000
C	0.144966000	2.101176000	-6.058748000
H	-0.941515000	1.959816000	-6.178312000
H	0.643213000	1.662772000	-6.934308000
H	0.334030000	3.186288000	-6.075720000
C	-0.048718000	2.188484000	-3.553944000
H	-1.136224000	2.231310000	-3.694444000
H	0.314001000	3.223774000	-3.466803000
H	0.154488000	1.674513000	-2.605555000
C	-1.847907000	3.720661000	0.090551000
C	-1.766901000	6.122003000	-0.181296000
C	-0.778456000	6.977715000	-0.978146000
H	-1.296207000	7.873137000	-1.354688000
H	-0.373607000	6.432676000	-1.839414000
H	0.058167000	7.311249000	-0.347891000
C	-2.328718000	6.995967000	0.951738000
H	-2.767640000	7.910303000	0.524713000

H	-1.527058000	7.297558000	1.640107000
H	-3.108505000	6.487525000	1.530494000
C	-2.866469000	5.546009000	-1.089568000
H	-2.487835000	5.497825000	-2.121997000
H	-3.767115000	6.177233000	-1.098848000
C	-3.158280000	4.111234000	-0.595704000
C	-3.516002000	3.204430000	-1.775532000
H	-4.399056000	3.598927000	-2.303147000
H	-3.764893000	2.188202000	-1.447721000
H	-2.682657000	3.139793000	-2.487866000
C	-4.317162000	4.079552000	0.421561000
H	-5.246056000	4.446566000	-0.046111000
H	-4.112194000	4.699547000	1.304828000
H	-4.487965000	3.054114000	0.769563000
C	0.035729000	4.903472000	1.163062000
C	-0.110777000	4.941232000	2.572677000
C	-1.458788000	4.803513000	3.268638000
H	-2.237311000	4.848326000	2.500594000
C	-1.588266000	3.429413000	3.943203000
H	-2.581269000	3.322948000	4.408697000
H	-0.827081000	3.290760000	4.727055000
H	-1.472692000	2.626189000	3.205993000
C	-1.724541000	5.926869000	4.280960000
H	-2.748872000	5.848081000	4.679603000
H	-1.610127000	6.923131000	3.829614000
H	-1.035878000	5.868754000	5.138598000
C	1.041277000	5.041652000	3.362017000
H	0.943778000	5.068813000	4.449136000
C	2.308728000	5.090502000	2.787040000
H	3.196286000	5.170909000	3.419081000
C	2.440225000	4.996986000	1.405644000
H	3.436594000	4.989116000	0.961134000
C	1.320297000	4.883163000	0.570728000
C	1.552270000	4.643328000	-0.915249000
H	0.570565000	4.617202000	-1.406644000
C	2.402691000	5.741170000	-1.573161000
H	2.457213000	5.575431000	-2.661079000
H	3.436295000	5.721869000	-1.192636000
H	2.001505000	6.749328000	-1.397748000
C	2.214273000	3.276629000	-1.140255000
H	2.410276000	3.111533000	-2.205916000
H	1.581193000	2.461524000	-0.780383000

H	3.175355000	3.212192000	-0.613561000
N	3.749051000	-0.811663000	2.864502000
C	2.635687000	-0.050147000	2.667446000
C	3.973035000	-1.227295000	4.300698000
C	4.170756000	-2.737010000	4.426817000
H	4.200674000	-3.004399000	5.494794000
H	5.117610000	-3.058842000	3.972672000
H	3.342573000	-3.286523000	3.964053000
C	5.187412000	-0.522140000	4.923002000
H	5.302099000	-0.863925000	5.962627000
H	5.076508000	0.568472000	4.938890000
H	6.111435000	-0.770771000	4.383255000
C	2.653496000	-0.795709000	4.950153000
H	2.800071000	-0.438840000	5.980136000
H	1.975898000	-1.659600000	4.993855000
C	2.030412000	0.282754000	4.044718000
C	2.437177000	1.708784000	4.472582000
H	2.031619000	1.927692000	5.474710000
H	2.037664000	2.451601000	3.769221000
H	3.526303000	1.842857000	4.516979000
C	0.503295000	0.178212000	4.113561000
H	0.178909000	0.175324000	5.167277000
H	0.135149000	-0.735683000	3.630381000
H	0.021066000	1.032593000	3.627141000
C	4.851894000	-1.037585000	1.963808000
C	5.840815000	-0.025286000	1.839098000
C	5.578587000	1.421382000	2.231323000
H	4.685114000	1.442042000	2.863413000
C	5.247255000	2.240205000	0.974710000
H	4.985617000	3.274721000	1.246683000
H	4.395257000	1.802661000	0.439571000
H	6.106318000	2.272636000	0.285251000
C	6.724872000	2.075194000	3.013628000
H	6.417679000	3.071145000	3.371945000
H	7.618022000	2.220302000	2.385542000
H	7.023195000	1.475662000	3.885717000
C	7.080427000	-0.359272000	1.281476000
H	7.851437000	0.408385000	1.194062000
C	7.350878000	-1.657483000	0.854323000
H	8.337572000	-1.912518000	0.459521000
C	6.336388000	-2.607995000	0.876200000
H	6.520223000	-3.602351000	0.464678000

C	5.061205000	-2.313789000	1.385319000
C	3.944278000	-3.318340000	1.146571000
H	3.023925000	-2.947287000	1.618204000
C	4.218111000	-4.738826000	1.659526000
H	3.317256000	-5.352606000	1.512103000
H	4.469957000	-4.767558000	2.727178000
H	5.044379000	-5.214408000	1.105058000
C	3.675461000	-3.382927000	-0.369313000
H	2.805258000	-4.027309000	-0.550904000
H	4.551580000	-3.783055000	-0.907479000
H	3.443897000	-2.393941000	-0.779641000
S	0.418089000	-3.752066000	0.629782000
C	0.489269000	-4.578273000	2.173633000
C	0.376297000	-5.985150000	2.278411000
C	0.452304000	-6.630728000	3.513313000
C	0.635133000	-5.899291000	4.693004000
C	0.740174000	-4.505465000	4.611467000
C	0.669440000	-3.858174000	3.378792000
H	0.754154000	-2.773173000	3.315400000
H	0.880747000	-3.915198000	5.522647000
H	0.693538000	-6.406773000	5.659096000
H	0.368757000	-7.721133000	3.556559000
H	0.237333000	-6.561395000	1.360261000
C	-2.248010000	1.080033000	0.199276000
C	-1.081908000	-1.794066000	-0.711925000
B	-2.406283000	-1.537133000	0.151447000
N	-2.644703000	-0.031740000	0.117016000
N	-0.204680000	-1.560402000	-1.455880000
C	-3.622856000	-2.502634000	-0.327517000
N	-4.787532000	-2.114583000	-0.799164000
C	-5.745527000	-3.263417000	-1.151041000
C	-7.122982000	-3.058460000	-0.532288000
H	-7.730679000	-3.949372000	-0.750881000
H	-7.639036000	-2.185252000	-0.952513000
H	-7.061928000	-2.952072000	0.557364000
C	-5.889675000	-3.397134000	-2.668290000
H	-6.554352000	-4.248317000	-2.875303000
H	-4.930409000	-3.593270000	-3.160208000
H	-6.342157000	-2.500248000	-3.110177000
C	-5.015096000	-4.446494000	-0.525325000
H	-5.118830000	-5.358870000	-1.127684000
H	-5.441035000	-4.657119000	0.466934000



C	-3.539858000	-4.038092000	-0.350328000
C	-2.659605000	-4.422906000	-1.570128000
H	-2.804097000	-5.494163000	-1.776548000
H	-1.600925000	-4.268473000	-1.320168000
H	-2.903357000	-3.864071000	-2.484434000
C	-2.963068000	-4.772924000	0.867410000
H	-3.098399000	-5.852529000	0.689067000
H	-3.487123000	-4.510920000	1.794476000
H	-1.892607000	-4.572303000	0.990759000
C	-5.218132000	-0.787705000	-1.221273000
C	-4.891203000	-0.359779000	-2.531981000
C	-3.764874000	-0.951766000	-3.368961000
H	-3.405532000	-1.866504000	-2.881536000
C	-2.600889000	0.049548000	-3.399571000
H	-1.742242000	-0.362408000	-3.941203000
H	-2.261598000	0.317675000	-2.394514000
H	-2.913298000	0.973323000	-3.907397000
C	-4.172276000	-1.307445000	-4.806881000
H	-3.340152000	-1.819555000	-5.313013000
H	-4.398535000	-0.402561000	-5.391911000
H	-5.053060000	-1.961762000	-4.850916000
C	-5.575228000	0.747215000	-3.050091000
H	-5.343563000	1.085539000	-4.060927000
C	-6.518622000	1.437267000	-2.296669000
H	-7.045472000	2.292615000	-2.725479000
C	-6.745761000	1.064394000	-0.977120000
H	-7.434454000	1.647270000	-0.363848000
C	-6.105941000	-0.046112000	-0.408761000
C	-6.318049000	-0.309133000	1.073804000
H	-5.815911000	-1.248935000	1.338700000
C	-7.792867000	-0.406970000	1.493028000
H	-7.853802000	-0.698598000	2.553027000
H	-8.361994000	-1.137752000	0.903609000
H	-8.299549000	0.565989000	1.395644000
C	-5.643888000	0.811988000	1.878679000
H	-5.739350000	0.616426000	2.953094000
H	-6.122619000	1.779625000	1.664234000
H	-4.577674000	0.892738000	1.642517000
S	-1.898810000	-1.991828000	1.981602000
C	-3.177935000	-1.318869000	3.051315000
C	-4.304006000	-2.082932000	3.402242000
C	-5.152844000	-1.671151000	4.432607000

C	-4.880688000	-0.495482000	5.140774000
C	-3.771821000	0.279307000	4.788941000
C	-2.934914000	-0.123310000	3.745826000
H	-2.069570000	0.477041000	3.473456000
H	-3.552752000	1.203501000	5.329011000
H	-5.531791000	-0.185524000	5.961632000
H	-6.017952000	-2.283798000	4.699458000
H	-4.492794000	-3.025801000	2.885922000

## Int-2

N	2.619117000	-3.135184000	0.132551000
C	1.866010000	-2.249502000	0.068477000
B	0.873427000	-1.073021000	0.015019000
C	-0.608722000	-1.347811000	0.181473000
N	-1.605721000	-0.421571000	0.273527000
C	-2.942421000	-1.004654000	0.639527000
C	-2.741374000	-2.465514000	0.209873000
H	-3.086513000	-2.582398000	-0.828792000
H	-3.325507000	-3.161451000	0.828338000
C	-1.220221000	-2.754249000	0.277611000
C	-1.437830000	0.953090000	-0.110458000
C	-1.187844000	1.951179000	0.858541000
C	-1.022960000	3.271810000	0.421549000
H	-0.825006000	4.055244000	1.155738000
C	-1.075886000	3.597801000	-0.929986000
H	-0.932705000	4.632643000	-1.250004000
C	-1.297649000	2.599487000	-1.875099000
H	-1.320805000	2.859280000	-2.935196000
C	-1.483849000	1.266369000	-1.492209000
C	-1.038064000	1.649929000	2.342282000
H	-1.147372000	0.566652000	2.471539000
C	-2.127367000	2.353484000	3.168166000
H	-2.091293000	2.026538000	4.219692000
H	-3.136988000	2.151619000	2.779507000
H	-1.986846000	3.446051000	3.155206000
C	0.356090000	2.025230000	2.871244000
H	0.450819000	1.733382000	3.929622000
H	0.530915000	3.111236000	2.809587000
H	1.146260000	1.525335000	2.295476000
H	-0.576066000	-0.825257000	-4.131353000
H	-3.061307000	-0.251811000	-4.207874000
C	-3.210546000	-0.900010000	2.150332000

H	-4.111736000	-1.481955000	2.395936000
H	-3.390295000	0.136788000	2.456431000
H	-2.377116000	-1.298537000	2.742755000
C	-4.087449000	-0.321811000	-0.107173000
H	-5.037882000	-0.790629000	0.188662000
H	-3.985562000	-0.422679000	-1.194010000
H	-4.144969000	0.748548000	0.138989000
C	-0.817736000	-3.637432000	-0.919436000
H	-1.412735000	-4.565629000	-0.906671000
H	0.243080000	-3.914584000	-0.888339000
H	-1.012210000	-3.120896000	-1.872207000
C	-0.817514000	-3.464172000	1.585730000
H	-1.329040000	-4.437666000	1.657048000
H	-1.084343000	-2.873744000	2.473478000
H	0.265036000	-3.647239000	1.613124000
C	-1.694504000	0.214858000	-2.575717000
H	-1.952804000	-0.730361000	-2.081484000
C	-0.409067000	-0.035567000	-3.381177000
H	0.419837000	-0.342224000	-2.730479000
H	-0.094909000	0.875869000	-3.914989000
C	-2.853297000	0.580541000	-3.516852000
H	-2.611280000	1.462099000	-4.130808000
H	-3.776952000	0.807405000	-2.963459000
S	1.582080000	0.598003000	-0.268194000
C	3.352883000	0.375038000	-0.128611000
C	4.160808000	0.755550000	-1.208190000
C	5.550779000	0.658860000	-1.108778000
C	6.140176000	0.180741000	0.064467000
C	5.333305000	-0.195403000	1.142443000
C	3.944604000	-0.093324000	1.052520000
H	3.316526000	-0.384546000	1.895850000
H	5.787216000	-0.571632000	2.062322000
H	7.227108000	0.099911000	0.138991000
H	6.174833000	0.952262000	-1.956504000
H	3.694292000	1.119613000	-2.125933000

## VIII

S	-0.126143000	1.868915000	-0.413108000
S	-1.342072000	-0.701224000	1.093884000
N	1.849801000	-0.875168000	0.052276000
N	-2.231408000	-0.329916000	-2.703849000
C	0.717505000	-1.029232000	-0.607109000

C	2.593656000	-2.186162000	0.277550000
C	4.104882000	-1.993936000	0.287318000
H	4.583297000	-2.974389000	0.430035000
H	4.472605000	-1.571224000	-0.655712000
C	2.129141000	-2.814308000	1.599434000
H	2.499297000	-3.849245000	1.648176000
H	1.032972000	-2.830404000	1.670459000
H	2.524452000	-2.276973000	2.467541000
H	2.016644000	-4.068408000	-0.680128000
C	0.703602000	-2.400808000	-1.301912000
C	0.655676000	-2.196728000	-2.835904000
H	0.894288000	-3.160296000	-3.313494000
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H	-0.331464000	-1.872329000	-3.179974000
C	-0.466995000	-3.306786000	-0.892545000
H	-0.390632000	-4.256531000	-1.444594000
H	-1.433348000	-2.848672000	-1.136538000
H	-0.458408000	-3.524598000	0.182673000
C	2.449131000	0.400447000	0.400295000
C	3.148028000	1.069774000	-0.634185000
C	3.275637000	0.524487000	-2.052035000
H	2.955489000	-0.524137000	-2.041377000
C	2.356835000	1.270093000	-3.033157000
H	2.440321000	0.835539000	-4.042348000
H	2.637514000	2.333447000	-3.096749000
H	1.306283000	1.233465000	-2.715382000
C	4.728579000	0.538618000	-2.552069000
H	4.801110000	0.015885000	-3.518865000
H	5.412290000	0.046892000	-1.842933000
H	5.095356000	1.564580000	-2.709041000
C	3.740117000	2.301968000	-0.335300000
H	4.266532000	2.844874000	-1.121852000
C	3.667411000	2.846171000	0.943250000
H	4.136116000	3.809785000	1.155898000
C	2.990841000	2.162376000	1.947447000
H	2.925459000	2.599842000	2.945033000
C	2.360639000	0.935853000	1.701084000
C	1.581698000	0.286400000	2.832105000
H	1.074495000	-0.598418000	2.429659000
C	2.512377000	-0.156251000	3.972462000
H	1.950710000	-0.722320000	4.732535000
H	2.964418000	0.715143000	4.472175000

H	3.339439000	-0.788330000	3.614269000
C	0.484852000	1.221536000	3.363146000
H	-0.168135000	0.681589000	4.066053000
H	-0.131201000	1.594888000	2.536284000
H	0.915214000	2.085343000	3.894370000
C	-1.510629000	-0.222375000	-1.798970000
C	-1.803739000	2.497660000	-0.360712000
C	-2.485836000	2.808421000	-1.545832000
H	-1.988049000	2.658320000	-2.504291000
C	-3.801000000	3.276317000	-1.497390000
H	-4.327310000	3.502970000	-2.427804000
C	-4.443697000	3.446530000	-0.267346000
H	-5.473645000	3.809923000	-0.231922000
C	-3.762990000	3.149391000	0.916665000
H	-4.258776000	3.276696000	1.882134000
C	-2.449221000	2.676472000	0.872061000
H	-1.924450000	2.425683000	1.793365000
C	-2.958210000	-1.349595000	0.714447000
C	-3.939289000	-0.561348000	0.091566000
H	-3.706749000	0.455278000	-0.218534000
C	-5.215729000	-1.081683000	-0.124467000
H	-5.967262000	-0.460984000	-0.617911000
C	-5.533995000	-2.378914000	0.288037000
H	-6.536084000	-2.779622000	0.117365000
C	-4.563823000	-3.160451000	0.922244000
H	-4.803952000	-4.174532000	1.251735000
C	-3.280609000	-2.651371000	1.130687000
H	-2.518483000	-3.260477000	1.620661000
B	-0.537024000	-0.010376000	-0.588489000
H	4.421886000	-1.336579000	1.109091000
C	2.084367000	-2.998341000	-0.917092000
H	2.785287000	-2.891978000	-1.758248000

### 1 (T<sub>1</sub>)

N	-0.272084000	0.088046000	-0.539152000
C	-1.360496000	0.135257000	0.259303000
B	-1.315021000	0.030404000	1.747341000
N	-3.169442000	0.001449000	3.660118000
C	-0.565283000	0.161102000	-2.009846000
C	0.345412000	1.164940000	-2.721295000
H	0.092408000	1.180221000	-3.791960000
H	1.404471000	0.884438000	-2.625982000

H	0.215754000	2.181601000	-2.330802000
C	-0.384949000	-1.211046000	-2.675045000
H	-0.627220000	-1.127598000	-3.744955000
H	-1.041032000	-1.973957000	-2.237789000
H	0.655207000	-1.553992000	-2.590027000
C	-2.037781000	0.621609000	-1.994181000
H	-2.613377000	0.168119000	-2.813804000
H	-2.073678000	1.712450000	-2.134347000
C	-2.616680000	0.269110000	-0.601226000
C	-3.379978000	-1.070686000	-0.600168000
H	-4.262406000	-1.005035000	-1.257030000
H	-3.723573000	-1.315011000	0.415708000
H	-2.752235000	-1.902010000	-0.952770000
C	1.062608000	-0.060739000	-0.023617000
C	-3.544435000	1.379871000	-0.087539000
H	-4.392617000	1.511640000	-0.778941000
H	-3.009067000	2.339144000	-0.013380000
H	-3.945626000	1.136496000	0.906235000
C	1.812905000	1.102166000	0.263800000
C	1.195097000	2.493508000	0.248575000
H	0.218075000	2.423258000	-0.246931000
C	0.927618000	2.960234000	1.690080000
H	0.420229000	3.938404000	1.692895000
H	1.869195000	3.062883000	2.253123000
H	0.291659000	2.238033000	2.224613000
C	2.039709000	3.520127000	-0.517300000
H	1.507362000	4.482413000	-0.580053000
H	2.262544000	3.183850000	-1.541091000
H	2.999710000	3.712681000	-0.013143000
C	3.140115000	0.944032000	0.681508000
H	3.739759000	1.828250000	0.905654000
C	3.699783000	-0.322125000	0.837628000
H	4.739054000	-0.425193000	1.158618000
C	2.920725000	-1.455881000	0.622172000
H	3.349044000	-2.444038000	0.800872000
C	1.586677000	-1.352694000	0.205268000
C	0.732458000	-2.611020000	0.137718000
H	-0.232618000	-2.341106000	-0.306110000
C	1.355436000	-3.717995000	-0.723023000
H	0.663519000	-4.570795000	-0.808411000
H	2.288654000	-4.098951000	-0.279242000
H	1.590018000	-3.366439000	-1.739022000

C	0.438631000	-3.119893000	1.559783000
H	-0.239339000	-3.987889000	1.526956000
H	-0.035327000	-2.333486000	2.166950000
H	1.364728000	-3.430588000	2.069486000
C	-2.377153000	0.022409000	2.794275000

#### NHC1 (T<sub>0</sub>)

N	-0.963363000	0.000077000	-0.825898000
C	0.095239000	0.000032000	0.066196000
B	0.040506000	-0.000033000	1.557676000
N	-1.973933000	-0.000049000	3.297311000
C	-0.501582000	0.000106000	-2.129738000
C	0.860233000	0.000083000	-2.076631000
H	1.606750000	0.000083000	-2.864565000
C	-2.339308000	0.000082000	-0.426643000
C	-2.977289000	-1.235730000	-0.215794000
C	-2.239703000	-2.557220000	-0.365799000
H	-1.197018000	-2.330944000	-0.631138000
C	-2.208279000	-3.327623000	0.963163000
H	-1.578435000	-4.227068000	0.870195000
H	-3.217298000	-3.655108000	1.260931000
H	-1.807522000	-2.701428000	1.773019000
C	-2.827125000	-3.405380000	-1.503173000
H	-2.256440000	-4.340087000	-1.624969000
H	-2.803679000	-2.862442000	-2.461307000
H	-3.875144000	-3.678079000	-1.299528000
C	-4.320204000	-1.209453000	0.178395000
H	-4.846805000	-2.149456000	0.355653000
C	-4.986654000	0.000089000	0.368212000
H	-6.032309000	0.000087000	0.684723000
C	-4.320147000	1.209621000	0.178580000
H	-4.846696000	2.149627000	0.355976000
C	-2.977227000	1.235887000	-0.215607000
C	-2.239583000	2.557364000	-0.365408000
H	-1.196874000	2.331076000	-0.630641000
C	-2.826850000	3.405648000	-1.502766000
H	-2.256128000	4.340355000	-1.624401000
H	-3.874887000	3.678359000	-1.299222000
H	-2.803305000	2.862811000	-2.460954000
C	-2.208298000	3.327634000	0.963633000
H	-1.578417000	4.227068000	0.870824000
H	-1.807649000	2.701344000	1.773469000

H	-3.217345000	3.655116000	1.261313000
C	-1.103179000	-0.000057000	2.507550000
H	-1.183838000	0.000142000	-2.974237000
N	1.218911000	0.000025000	-0.738729000
C	2.561010000	-0.000052000	-0.238147000
C	3.187972000	-1.237278000	0.004562000
C	3.188206000	1.237099000	0.004353000
C	4.494476000	-1.210432000	0.508662000
C	4.494708000	1.210092000	0.508445000
C	5.140886000	-0.000210000	0.758028000
H	5.010626000	-2.149799000	0.715750000
H	5.011042000	2.149395000	0.715364000
H	6.158927000	-0.000272000	1.154897000
C	2.463417000	2.556473000	-0.218651000
H	1.558367000	2.344453000	-0.806809000
C	3.302262000	3.557868000	-1.023535000
H	3.633698000	3.128061000	-1.981828000
H	2.712318000	4.462689000	-1.239092000
H	4.199470000	3.877784000	-0.470264000
C	2.002784000	3.152432000	1.121805000
H	1.370655000	2.438302000	1.671504000
H	2.866429000	3.403071000	1.758959000
H	1.421076000	4.073752000	0.956942000
C	2.462972000	-2.556561000	-0.218274000
H	1.557735000	-2.344411000	-0.806094000
C	2.002755000	-3.152600000	1.122287000
H	2.866593000	-3.403390000	1.759120000
H	1.370881000	-2.438458000	1.672263000
H	1.420900000	-4.073846000	0.957538000
C	3.301456000	-3.557953000	-1.023547000
H	2.711394000	-4.462742000	-1.238913000
H	3.632523000	-3.128108000	-1.981950000
H	4.198877000	-3.877917000	-0.470649000

#### NHC1 (S<sub>1</sub>)

N	0.252527000	-0.774626000	1.094430000
C	0.204255000	0.057053000	0.000000000
B	0.218800000	1.550295000	0.000000000
N	-1.731868000	3.356263000	0.000000000
C	0.338761000	-2.106493000	0.677955000
C	0.338761000	-2.106493000	-0.677955000
H	0.397476000	-2.918059000	-1.396179000



C	0.110385000	-0.283097000	2.430205000
C	1.271337000	0.026229000	3.166043000
C	2.662969000	-0.147862000	2.578219000
H	2.549356000	-0.610584000	1.587356000
C	3.342822000	1.213755000	2.365118000
H	4.328752000	1.080979000	1.891038000
H	3.496819000	1.738739000	3.322019000
H	2.730273000	1.852891000	1.710986000
C	3.525705000	-1.089697000	3.430432000
H	4.504989000	-1.251842000	2.952624000
H	3.041642000	-2.070468000	3.560821000
H	3.712142000	-0.672783000	4.433187000
C	1.100895000	0.530094000	4.462276000
H	1.979110000	0.781930000	5.060465000
C	-0.173469000	0.724085000	4.993132000
H	-0.285451000	1.120631000	6.005155000
C	-1.307147000	0.424678000	4.237468000
H	-2.298564000	0.589073000	4.663623000
C	-1.190732000	-0.079465000	2.936380000
C	-2.426577000	-0.433050000	2.122117000
H	-2.104864000	-0.592092000	1.083924000
C	-3.032903000	-1.756123000	2.617350000
H	-3.897456000	-2.043278000	1.997498000
H	-3.377973000	-1.667373000	3.660332000
H	-2.296736000	-2.574202000	2.576805000
C	-3.466540000	0.694383000	2.099294000
H	-4.304295000	0.418043000	1.439383000
H	-3.035088000	1.631459000	1.719292000
H	-3.887249000	0.884263000	3.099739000
C	-0.883948000	2.542207000	0.000000000
H	0.397476000	-2.918059000	1.396179000
N	0.252527000	-0.774626000	-1.094430000
C	0.110385000	-0.283097000	-2.430205000
C	1.271337000	0.026229000	-3.166043000
C	-1.190732000	-0.079465000	-2.936380000
C	1.100895000	0.530094000	-4.462276000
C	-1.307147000	0.424678000	-4.237468000
C	-0.173469000	0.724085000	-4.993132000
H	1.979110000	0.781930000	-5.060465000
H	-2.298564000	0.589073000	-4.663623000
H	-0.285451000	1.120631000	-6.005155000
C	-2.426577000	-0.433050000	-2.122117000

H	-2.104864000	-0.592092000	-1.083924000
C	-3.032903000	-1.756123000	-2.617350000
H	-2.296736000	-2.574202000	-2.576805000
H	-3.897456000	-2.043278000	-1.997498000
H	-3.377973000	-1.667373000	-3.660332000
C	-3.466540000	0.694383000	-2.099294000
H	-3.035088000	1.631459000	-1.719292000
H	-3.887249000	0.884263000	-3.099739000
H	-4.304295000	0.418043000	-1.439383000
C	2.662969000	-0.147862000	-2.578219000
H	2.549356000	-0.610584000	-1.587356000
C	3.342822000	1.213755000	-2.365118000
H	3.496819000	1.738739000	-3.322019000
H	2.730273000	1.852891000	-1.710986000
H	4.328752000	1.080979000	-1.891038000
C	3.525705000	-1.089697000	-3.430432000
H	4.504989000	-1.251842000	-2.952624000
H	3.041642000	-2.070468000	-3.560821000
H	3.712142000	-0.672783000	-4.433187000

#### NHC1 (S<sub>1</sub>)

N	-1.102213000	-0.047265000	-0.856665000
C	0.000000000	0.000012000	-0.011096000
B	-0.000078000	0.000144000	1.438654000
N	-0.000208000	0.000357000	4.069320000
C	-0.675830000	-0.031756000	-2.190610000
C	0.675934000	0.031112000	-2.190590000
H	1.390320000	0.069111000	-3.006908000
C	-2.440738000	-0.120322000	-0.369626000
C	-2.930478000	-1.365281000	0.076583000
C	-2.095731000	-2.633968000	-0.014060000
H	-1.092865000	-2.349453000	-0.359497000
C	-1.927845000	-3.308850000	1.354266000
H	-1.254900000	-4.176841000	1.270984000
H	-2.890265000	-3.670593000	1.750982000
H	-1.493772000	-2.613077000	2.087548000
C	-2.681443000	-3.599852000	-1.055886000
H	-2.044523000	-4.493488000	-1.155479000
H	-2.756977000	-3.121630000	-2.045070000
H	-3.690597000	-3.937070000	-0.768754000
C	-4.234552000	-1.406723000	0.588367000
H	-4.643632000	-2.356062000	0.940446000

C	-5.015715000	-0.254601000	0.649304000
H	-6.030330000	-0.306369000	1.051633000
C	-4.509442000	0.966842000	0.202580000
H	-5.132707000	1.860246000	0.263831000
C	-3.210240000	1.062681000	-0.310134000
C	-2.621915000	2.402265000	-0.731728000
H	-1.813938000	2.197665000	-1.449855000
C	-3.635784000	3.311483000	-1.436108000
H	-3.131040000	4.209145000	-1.826178000
H	-4.424366000	3.658161000	-0.749453000
H	-4.123594000	2.798643000	-2.279801000
C	-1.984872000	3.111336000	0.476850000
H	-1.508934000	4.055468000	0.165419000
H	-1.219413000	2.480685000	0.952992000
H	-2.748103000	3.347406000	1.236082000
C	-0.000156000	0.000276000	2.890183000
H	-1.390176000	-0.069927000	-3.006954000
N	1.102260000	0.047064000	-0.856622000
C	2.440780000	0.120258000	-0.369582000
C	3.210395000	-1.062676000	-0.310084000
C	2.930418000	1.365273000	0.076591000
C	4.509615000	-0.966700000	0.202557000
C	4.234500000	1.406837000	0.588350000
C	5.015781000	0.254798000	0.649258000
H	5.132982000	-1.860032000	0.263783000
H	4.643502000	2.356219000	0.940403000
H	6.030409000	0.306666000	1.051541000
C	2.095614000	2.633920000	-0.014130000
H	1.092742000	2.349345000	-0.359490000
C	2.681260000	3.599711000	-1.056084000
H	2.756774000	3.121383000	-2.045217000
H	2.044310000	4.493318000	-1.155752000
H	3.690415000	3.936988000	-0.769022000
C	1.927772000	3.308936000	1.354134000
H	1.493721000	2.613236000	2.087498000
H	2.890200000	3.670721000	1.750788000
H	1.254826000	4.176919000	1.270788000
C	2.622130000	-2.402319000	-0.731596000
H	1.814445000	-2.197832000	-1.450083000
C	1.984586000	-3.111081000	0.476896000
H	2.747531000	-3.347059000	1.236445000
H	1.219011000	-2.480292000	0.952668000

H	1.508689000	-4.055240000	0.165485000
C	3.636190000	-3.311793000	-1.435368000
H	3.131522000	-4.209524000	-1.825374000
H	4.124340000	-2.799224000	-2.279030000
H	4.424497000	-3.658332000	-0.748328000

**[LHB:], L = CAAC, singlet**

N	-0.512517912	-0.181010503	0.165885179
C	-1.292951589	-0.410680917	-0.971392620
B	-0.911214203	-0.448066491	-2.328428273
C	-1.223739777	-0.400940125	1.450996217
C	-0.463249481	-1.357546732	2.379334881
H	-1.016505150	-1.482684859	3.322890402
H	0.532998718	-0.958896523	2.623657853
H	-0.339135354	-2.348757194	1.926011391
C	-1.451372747	0.909106363	2.227624738
H	-1.979563377	0.702013513	3.171257963
H	-2.046226116	1.634899260	1.660268493
H	-0.488142562	1.376262345	2.478745637
C	-2.542759479	-1.035694652	0.955103317
H	-3.398332451	-0.762106119	1.590826727
H	-2.443570337	-2.131432437	0.988236967
C	-2.749730168	-0.601894712	-0.517648296
C	-3.524965842	0.727051471	-0.619896089
H	-4.509289067	0.642835717	-0.129148410
H	-3.684828246	0.996083655	-1.674657431
H	-2.978811518	1.556409626	-0.151859887
C	0.860230838	0.181571148	0.039366939
C	-3.493716306	-1.676524332	-1.319623377
H	-4.514129076	-1.818817617	-0.926992686
H	-2.964288386	-2.639615585	-1.278293385
H	-3.588371521	-1.385976467	-2.379336331
C	1.855070773	-0.824589242	-0.063060771
C	1.508257127	-2.303024188	-0.167225831
H	0.424899077	-2.395551909	-0.020536024
C	1.814726395	-2.830894898	-1.578925663
H	1.510955354	-3.886495346	-1.670404264
H	2.891480306	-2.768307285	-1.806299326
H	1.267658293	-2.256138602	-2.340813248
C	2.220276339	-3.155501838	0.893001721
H	1.871928254	-4.199887427	0.844952929
H	2.036266228	-2.780462227	1.910068312

H	3.310563911	-3.167088967	0.734655457
C	3.199853183	-0.437295131	-0.144731259
H	3.974820781	-1.204356194	-0.210489143
C	3.564142881	0.906613208	-0.159815566
H	4.618457397	1.188764362	-0.217170100
C	2.577161631	1.889271017	-0.134737629
H	2.864475640	2.941506003	-0.194097241
C	1.220214303	1.550717992	-0.053239490
C	0.175017776	2.650534697	-0.159275148
H	-0.801099053	2.185318906	0.013832145
C	0.367710510	3.762705976	0.879887375
H	-0.458886926	4.489327184	0.824015677
H	1.303925043	4.318629838	0.710906861
H	0.399199623	3.361655737	1.903961596
C	0.148799019	3.227800934	-1.584584574
H	-0.651425676	3.979682634	-1.682531975
H	-0.038737413	2.433973072	-2.322716339
H	1.104085927	3.716628698	-1.836958882
H	-0.680528234	-0.454726044	-3.487991836

**[LHB:], L = CAAC, triplet**

N	-0.551223382	-0.114120034	0.133660672
C	-1.364729096	-0.195871185	-0.960185938
B	-0.925000413	-0.111453109	-2.389034605
C	-1.251865680	-0.219044997	1.455113766
C	-0.555639578	-1.206842661	2.395983448
H	-1.105721677	-1.244894627	3.348409499
H	0.476862181	-0.895634208	2.612494134
H	-0.535382069	-2.221199166	1.979495563
C	-1.321564192	1.142710098	2.162848871
H	-1.863397070	1.030347443	3.114029100
H	-1.844691125	1.897545968	1.563035206
H	-0.313840562	1.516073064	2.391244777
C	-2.639936499	-0.727109146	1.012427263
H	-3.442941273	-0.316066811	1.641451728
H	-2.670106852	-1.822183465	1.119482149
C	-2.806869373	-0.358706154	-0.481140847
C	-3.564070241	0.970817114	-0.673309129
H	-4.596164133	0.884730114	-0.294965036
H	-3.604101870	1.231703895	-1.741450305
H	-3.075138742	1.802686406	-0.145788914
C	0.866007871	0.088182423	0.029163631

C	-3.537532304	-1.465340365	-1.252794958
H	-4.559189175	-1.599929259	-0.860078223
H	-3.004060210	-2.424775003	-1.167207322
H	-3.603164740	-1.212201734	-2.321391004
C	1.716620743	-1.039368386	-0.037955274
C	1.180261765	-2.457052371	-0.182665157
H	0.098490393	-2.425570018	-0.000647192
C	1.371277982	-2.949595351	-1.627381170
H	0.937269012	-3.954867142	-1.752949592
H	2.440614490	-3.006667551	-1.887998996
H	0.883887193	-2.270710916	-2.341466158
C	1.803561231	-3.438949466	0.818595383
H	1.316856716	-4.424360172	0.742159540
H	1.701372844	-3.085796970	1.855533755
H	2.876785758	-3.590556250	0.622519829
C	3.100611531	-0.825920339	-0.069344165
H	3.773736697	-1.684323801	-0.115948513
C	3.631255119	0.461951376	-0.064035702
H	4.713903801	0.608628540	-0.083400011
C	2.777309341	1.561691556	-0.070728385
H	3.197913151	2.568196336	-0.118950246
C	1.385296633	1.400999238	-0.041322809
C	0.497215718	2.627900241	-0.196808214
H	-0.541248232	2.310717123	-0.050494773
C	0.807779027	3.727827538	0.827374947
H	0.084231790	4.553383523	0.734205402
H	1.811226665	4.154450247	0.670956143
H	0.764225792	3.351997775	1.860515430
C	0.594307342	3.174762302	-1.631411336
H	-0.091978515	4.026601706	-1.765691402
H	0.331392064	2.400394754	-2.365746943
H	1.615270911	3.524094176	-1.855228986
H	0.174868466	0.036042980	-2.851125651

**[LHB:], L = NHC, singlet**

N	-1.103338866	-0.004465136	0.625909718
C	0.000597748	-0.003947235	-0.241814659
B	0.000741607	-0.003899417	-1.690081588
C	-0.676634236	-0.003570197	1.956171076
C	0.677322515	-0.002645372	1.956319415
H	1.389797434	-0.001993042	2.775442705
C	-2.447090371	-0.002660639	0.159678013

C	-3.083324051	1.233108326	-0.082176844
C	-2.363396459	2.553118409	0.148340875
H	-1.382561639	2.319635750	0.585475533
C	-2.103805803	3.281257419	-1.179233584
H	-1.531012463	4.206820512	-1.006038580
H	-3.047464402	3.556617589	-1.678357825
H	-1.523078498	2.643571603	-1.862760544
C	-3.113740778	3.444950463	1.147528109
H	-2.541311692	4.364690966	1.348719981
H	-3.273833570	2.925492698	2.105351566
H	-4.100725638	3.747246475	0.761368203
C	-4.399633005	1.209738721	-0.560845846
H	-4.918631339	2.151070787	-0.755257359
C	-5.053697477	0.000835369	-0.797531647
H	-6.080304430	0.002216503	-1.172339658
C	-4.402035110	-1.209785405	-0.563130537
H	-4.922870377	-2.149741621	-0.759265200
C	-3.085807972	-1.236649585	-0.084371004
C	-2.368537808	-2.558451479	0.144011823
H	-1.387335776	-2.327530016	0.581680205
C	-3.120928259	-3.450450811	1.141529366
H	-2.550533886	-4.371789249	1.341172167
H	-4.108529346	-3.749894341	0.754720461
H	-3.280014498	-2.932338558	2.100251176
C	-2.110036029	-3.284782814	-1.184750246
H	-1.539234613	-4.211848489	-1.012989387
H	-1.527708418	-2.647066792	-1.866915358
H	-3.054045653	-3.557319564	-1.684782053
H	-1.389399715	-0.003851059	2.775011156
N	1.104420801	-0.003317380	0.626257170
C	2.448099993	0.000993451	0.159784640
C	3.080474728	1.238099250	-0.084350829
C	3.090388086	-1.231602060	-0.081845107
C	4.396162920	1.217847420	-0.564881822
C	4.405894474	-1.201697714	-0.562477378
C	5.053423204	0.010452721	-0.800516752
H	4.912158343	2.160349995	-0.761436366
H	4.929475483	-2.140402955	-0.757139177
H	6.079407951	0.014197072	-1.176998408
C	2.377245874	-2.554976504	0.150782936
H	1.399498782	-2.326231526	0.597414158
C	3.138629810	-3.448187748	1.140211588

H	3.307116316	-2.931145829	2.097909609
H	2.569362881	-4.369243657	1.344171073
H	4.122198645	-3.748524190	0.744039818
C	2.108692643	-3.278975533	-1.177459099
H	1.518268599	-2.641385688	-1.852695820
H	3.049253778	-3.546960390	-1.686343507
H	1.542372819	-4.208318861	-1.002914841
C	2.356531003	2.555972193	0.145854178
H	1.378047344	2.319429577	0.586846054
C	2.089892357	3.279991267	-1.182708633
H	3.031116942	3.556767130	-1.685589270
H	1.508810228	2.638645603	-1.862459299
H	1.514810765	4.204268655	-1.009961329
C	3.106022347	3.453044028	1.140912097
H	2.529473770	4.370079572	1.342557919
H	3.272155560	2.935940837	2.098990173
H	4.089964644	3.760202962	0.750961901
H	-0.000238083	-0.003839360	-2.870780935

**[LHB:], L = NHC, triplet**

N	-1.092078000	-0.000045000	0.611250000
C	0.001651000	-0.000024000	-0.258478000
B	0.009946000	-0.000013000	-1.749338000
C	-0.672297000	-0.000043000	1.931860000
C	0.688645000	-0.000025000	1.925363000
H	1.404857000	-0.000016000	2.741178000
C	-2.452931000	-0.000056000	0.178135000
C	-3.093897000	1.235240000	-0.037391000
C	-2.361880000	2.555527000	0.152107000
H	-1.402055000	2.335515000	0.641081000
C	-2.039035000	3.196887000	-1.206895000
H	-1.456621000	4.122372000	-1.069381000
H	-2.961489000	3.453783000	-1.753023000
H	-1.450950000	2.509354000	-1.832038000
C	-3.129746000	3.520096000	1.065911000
H	-2.537750000	4.431922000	1.244325000
H	-3.351119000	3.059146000	2.041364000
H	-4.086533000	3.832891000	0.617939000
C	-4.424286000	1.209634000	-0.475197000
H	-4.949461000	2.149789000	-0.656306000
C	-5.083534000	-0.000071000	-0.691321000
H	-6.120576000	-0.000076000	-1.035892000



C	-4.424229000	-1.209768000	-0.475331000
H	-4.949359000	-2.149928000	-0.656544000
C	-3.093839000	-1.235358000	-0.037524000
C	-2.361766000	-2.555635000	0.151830000
H	-1.401910000	-2.335627000	0.640742000
C	-3.129540000	-3.520279000	1.065633000
H	-2.537518000	-4.432111000	1.243930000
H	-4.086364000	-3.833049000	0.617724000
H	-3.350830000	-3.059401000	2.041138000
C	-2.039009000	-3.196898000	-1.207237000
H	-1.456549000	-4.122371000	-1.069828000
H	-1.450999000	-2.509304000	-1.832383000
H	-2.961496000	-3.453797000	-1.753309000
H	-1.380579000	-0.000056000	2.754859000
N	1.098131000	-0.000012000	0.602053000
C	2.459137000	0.000042000	0.165516000
C	3.102517000	1.235378000	-0.042485000
C	3.102675000	-1.235240000	-0.042326000
C	4.438117000	1.209750000	-0.463770000
C	4.438272000	-1.209494000	-0.463611000
C	5.100455000	0.000158000	-0.670689000
H	4.965039000	2.149967000	-0.639355000
H	4.965318000	-2.149664000	-0.639073000
H	6.141912000	0.000203000	-1.001696000
C	2.366783000	-2.555256000	0.131913000
H	1.402122000	-2.336669000	0.612050000
C	3.122201000	-3.528670000	1.046443000
H	3.333046000	-3.076417000	2.028345000
H	2.526653000	-4.440969000	1.210226000
H	4.083566000	-3.839606000	0.607083000
C	2.057227000	-3.183243000	-1.236377000
H	1.487104000	-2.480525000	-1.863219000
H	2.985059000	-3.445681000	-1.770730000
H	1.462190000	-4.103093000	-1.115292000
C	2.366476000	2.555328000	0.131616000
H	1.401750000	2.336658000	0.611583000
C	2.057101000	3.183296000	-1.236721000
H	2.984995000	3.445825000	-1.770921000
H	1.487141000	2.480531000	-1.863659000
H	1.461961000	4.103092000	-1.115730000
C	3.121661000	3.528792000	1.046287000
H	2.526037000	4.441065000	1.209944000

H	3.332331000	3.076557000	2.028236000
H	4.083102000	3.839762000	0.607116000
H	-0.935704000	-0.000019000	-2.490491000

**NHC2-dib**

N	2.636915000	-1.080178000	1.252068000
C	1.988663000	-0.001641000	0.730597000
B	0.749615000	-0.000614000	-0.259409000
N	1.383193000	-0.001592000	-2.889790000
C	3.660933000	-0.682436000	2.099658000
C	3.661858000	0.676363000	2.099914000
H	4.290711000	1.395510000	2.613072000
C	2.440507000	-2.449700000	0.848499000
C	1.556333000	-3.256663000	1.586018000
C	0.849483000	-2.727048000	2.821424000
H	0.761376000	-1.637977000	2.719351000
C	-0.572185000	-3.264314000	2.978537000
H	-1.076750000	-2.734238000	3.798325000
H	-0.586925000	-4.342600000	3.207907000
H	-1.153078000	-3.097899000	2.064323000
C	1.686444000	-3.017074000	4.079652000
H	1.194756000	-2.595162000	4.970383000
H	2.695141000	-2.581842000	4.013842000
H	1.801178000	-4.102895000	4.232575000
C	1.411356000	-4.587712000	1.175402000
H	0.718765000	-5.239080000	1.709112000
C	2.138917000	-5.089203000	0.096921000
H	2.010849000	-6.131091000	-0.206922000
C	3.028783000	-4.270978000	-0.596158000
H	3.594449000	-4.676864000	-1.436383000
C	3.196354000	-2.926234000	-0.240542000
C	4.213067000	-2.052900000	-0.963737000
H	4.002914000	-1.007636000	-0.701580000
C	5.632626000	-2.374124000	-0.465108000
H	6.368519000	-1.699271000	-0.931178000
H	5.912447000	-3.409534000	-0.718646000
H	5.714642000	-2.265023000	0.627183000
C	4.127328000	-2.142917000	-2.491689000
H	4.882890000	-1.480272000	-2.943035000
H	3.143669000	-1.816593000	-2.852745000
H	4.326568000	-3.163143000	-2.856601000
C	1.120134000	-0.001200000	-1.747948000

H	4.288767000	-1.402644000	2.612576000
N	2.638358000	1.075830000	1.252512000
C	2.444107000	2.445684000	0.849005000
C	1.561354000	3.254110000	1.586632000
C	3.200500000	2.920928000	-0.240214000
C	1.418337000	4.585323000	1.175875000
C	3.034867000	4.265866000	-0.596015000
C	2.146384000	5.085535000	0.097128000
H	0.726883000	5.237834000	1.709659000
H	3.601001000	4.670783000	-1.436390000
H	2.019810000	6.127564000	-0.206854000
C	4.215996000	2.046042000	-0.963250000
H	4.004413000	1.001116000	-0.700895000
C	5.635970000	2.365421000	-0.464605000
H	5.717768000	2.256476000	0.627717000
H	6.370958000	1.689438000	-0.930466000
H	5.917232000	3.400383000	-0.718375000
C	4.130500000	2.135859000	-2.491227000
H	3.146474000	1.810702000	-2.852332000
H	4.331075000	3.155753000	-2.856330000
H	4.885271000	1.472164000	-2.942359000
C	0.853902000	2.725698000	2.822207000
H	0.763970000	1.636773000	2.720149000
C	-0.566842000	3.265329000	2.979633000
H	-0.579718000	4.343597000	3.209209000
H	-1.148151000	3.100071000	2.065471000
H	-1.072174000	2.735959000	3.799405000
C	1.691581000	3.014351000	4.080273000
H	1.199342000	2.593292000	4.971103000
H	2.699533000	2.577426000	4.014313000
H	1.808155000	4.099984000	4.233138000
N	-2.636449000	1.080153000	-1.252501000
C	-1.988638000	0.001606000	-0.730483000
B	-0.749711000	0.000666000	0.259690000
N	-1.383702000	0.001271000	2.889968000
C	-3.660511000	0.682397000	-2.100034000
C	-3.661874000	-0.676399000	-2.099750000
H	-4.290864000	-1.395555000	-2.612728000
C	-2.439878000	2.449717000	-0.849116000
C	-3.195438000	2.926363000	0.240083000
C	-4.212309000	2.053221000	0.963292000
H	-4.002171000	1.007895000	0.701375000

C	-4.126931000	2.143477000	2.491243000
H	-4.882670000	1.480964000	2.942487000
H	-4.326179000	3.163765000	2.855973000
H	-3.143404000	1.817093000	2.852600000
C	-5.631748000	2.374473000	0.464321000
H	-6.367777000	1.699723000	0.930327000
H	-5.713566000	2.265246000	-0.627967000
H	-5.911535000	3.409935000	0.717683000
C	-3.027549000	4.271063000	0.595701000
H	-3.592947000	4.677023000	1.436068000
C	-2.137747000	5.089173000	-0.097600000
H	-2.009434000	6.131030000	0.206245000
C	-1.410573000	4.587609000	-1.176302000
H	-0.718048000	5.238899000	-1.710193000
C	-1.555801000	3.256573000	-1.586864000
C	-0.849221000	2.726833000	-2.822370000
H	-0.761038000	1.637780000	-2.720150000
C	-1.686446000	3.016667000	-4.080468000
H	-1.194896000	2.594695000	-4.971247000
H	-1.801275000	4.102464000	-4.233486000
H	-2.695102000	2.581380000	-4.014448000
C	0.572376000	3.264176000	-2.979913000
H	1.076845000	2.733868000	-3.799614000
H	1.153470000	3.098164000	-2.065753000
H	0.586951000	4.342384000	-3.209677000
C	-1.120445000	0.001024000	1.748173000
H	-4.288068000	1.402589000	-2.613311000
N	-2.638631000	-1.075855000	-1.252030000
C	-2.444635000	-2.445696000	-0.848362000
C	-3.201280000	-2.920798000	0.240746000
C	-1.561923000	-3.254296000	-1.585846000
C	-3.036051000	-4.265797000	0.596498000
C	-1.419257000	-4.585551000	-1.175095000
C	-2.147640000	-5.085651000	-0.096523000
H	-3.602392000	-4.670600000	1.436789000
H	-0.727852000	-5.238194000	-1.708786000
H	-2.021370000	-6.127723000	0.207437000
C	-0.854205000	-2.726064000	-2.821340000
H	-0.764258000	-1.637129000	-2.719440000
C	-1.691656000	-3.014865000	-4.079524000
H	-2.699607000	-2.577895000	-4.013798000
H	-1.199238000	-2.593930000	-4.970313000

H	-1.808237000	-4.100512000	-4.232275000
C	0.566552000	-3.265764000	-2.978394000
H	1.147723000	-3.100318000	-2.064178000
H	0.579449000	-4.344086000	-3.207720000
H	1.072032000	-2.736588000	-3.798199000
C	-4.216490000	-2.045632000	0.963836000
H	-4.004513000	-1.000756000	0.701605000
C	-4.131002000	-2.135676000	2.491801000
H	-4.332081000	-3.155517000	2.856779000
H	-3.146802000	-1.811048000	2.852911000
H	-4.885423000	-1.471657000	2.943040000
C	-5.636580000	-2.364426000	0.465158000
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H	-5.918211000	-3.399330000	0.718757000

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C	4.887946000	-2.283289000	-3.340467000
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N	-1.762117000	-1.656256000	0.344713000
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