

## **Supporting Information: Theoretical Study of Photoinduced Cross-Linking Reaction of 5-Fluoro-4-Thiouridine with Thymidine**

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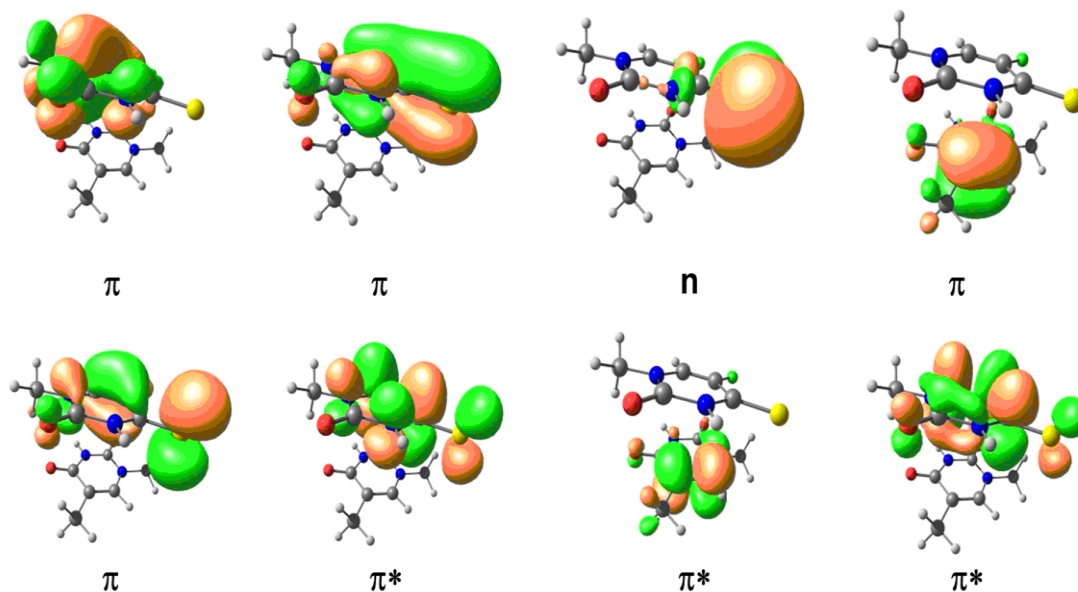
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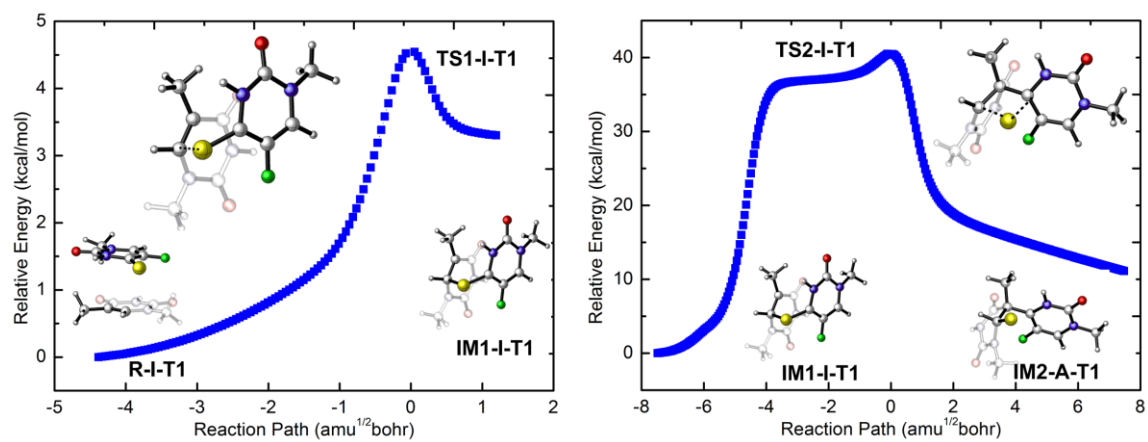
## 1. Active orbitals



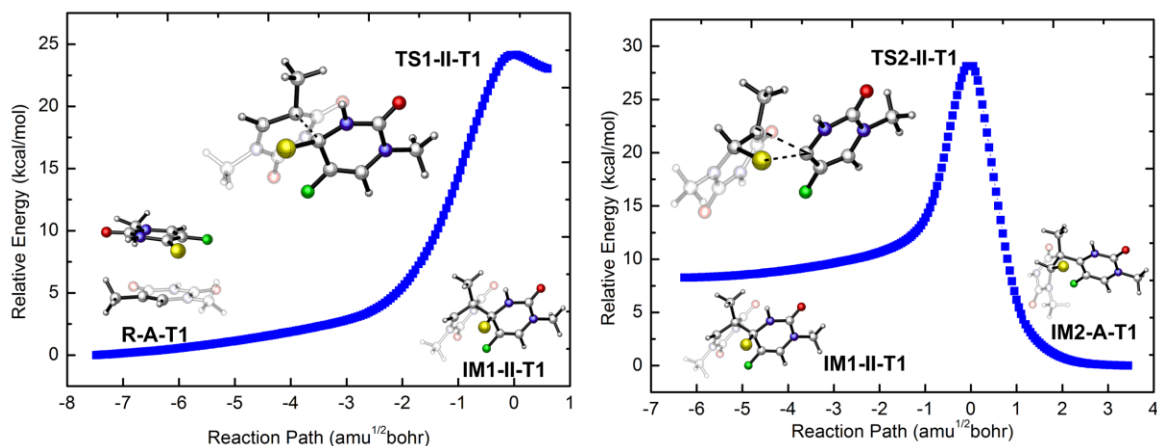
**Fig. S1.** Active space used in CASSCF and CASPT2 computations for photoinduced cross-linking of 5-fluoro-4-thiouridine with thymidine.

## 2. IRC paths

a.

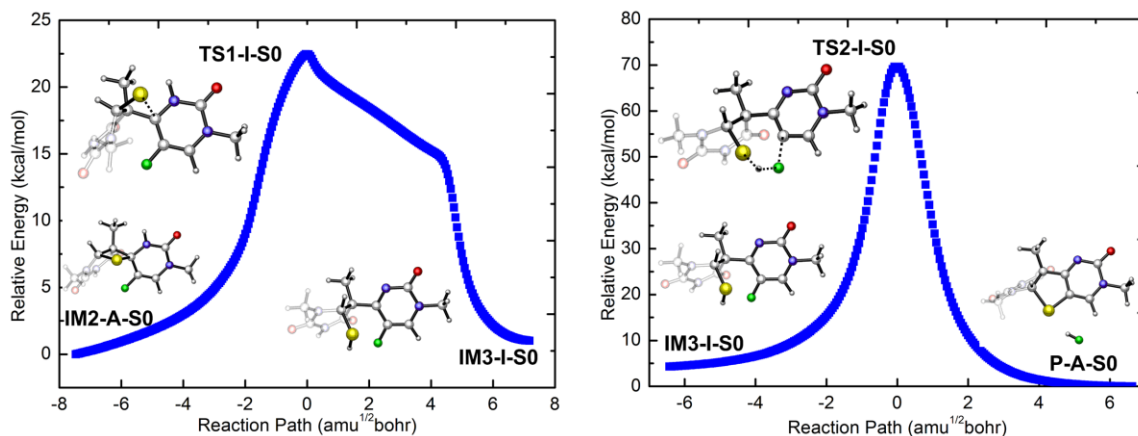


b.

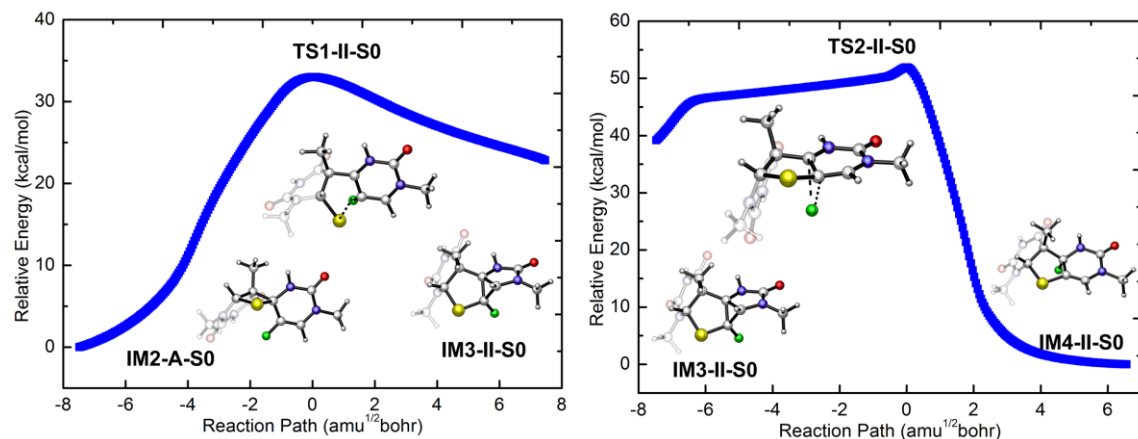


**Fig. S2.** B3LYP-D3/6-31G\* computed IRC paths for transition states in  $T_1$  state: (left of a) connecting R-A-T1 and IM1-I-T1 via TS1-I-T1; (right of a) connecting IM1-I-T1 and IM2-A-T1 via TS2-I-T1; (left of b) connecting R-A-T1 and IM1-II-T1 via TS1-II-T1; (right of b) connecting IM1-II-T1 and IM2-A-T1 via TS2-II-T1.

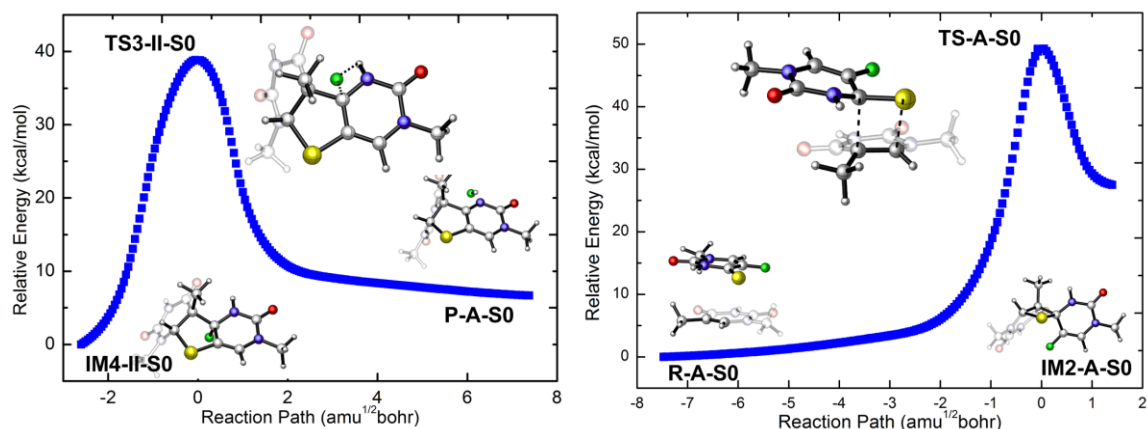
a.



b.

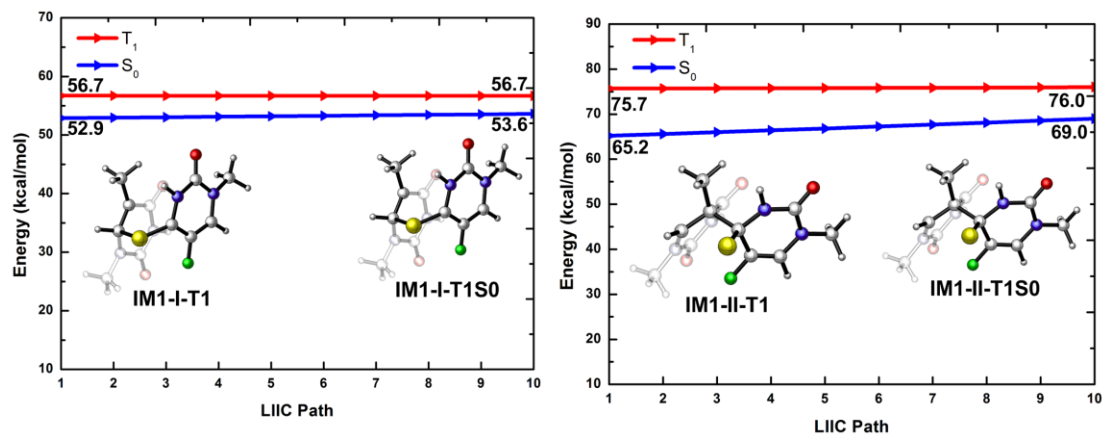


C.

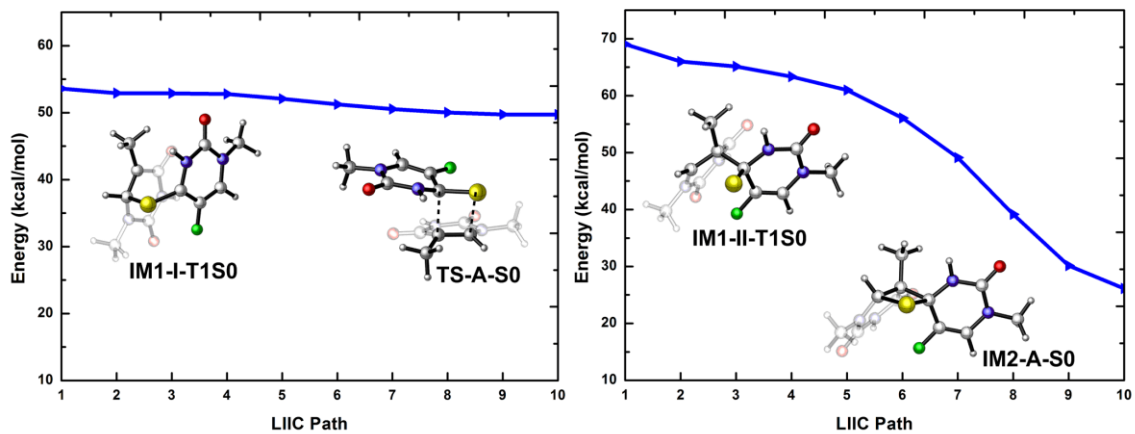


**Fig. S3.** B3LYP-D3/6-31G\* computed IRC paths for transition states in  $S_0$  state: (left of a) connecting IM2-A-S0 and IM3-I-S0 via TS1-I-S0; (right of a) connecting IM3-I-S0 and P-A-S0 via TS2-I-S0; (left of b) connecting IM2-A-S0 and IM3-II-S0 via TS1-II-S0; (right of b) connecting IM3-II-S0 and IM4-II-S0 via TS2-II-S0; (left of c) connecting IM4-II-S0 and P-A-S0 via TS3-II-S0; (right of c) connecting R-A-S0 and IM2-A-S0 via TS-A-S0.

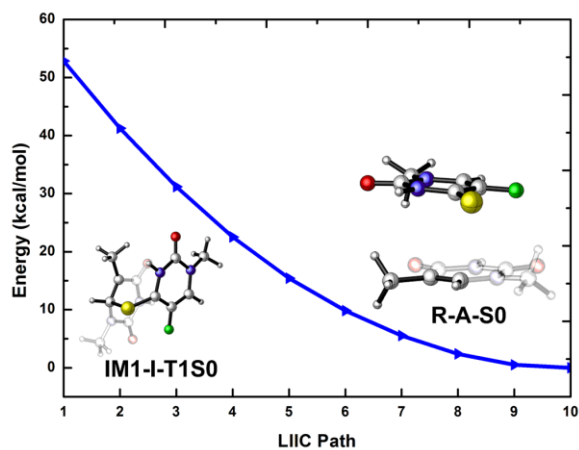
### 3. LIIC paths



**Fig. S4.** B3LYP-D3/6-311++G\*\* computed LIIC paths: (left) connecting IM1-I-T1 and IM1-I-T1S0; (right) connecting IM1-II-T1 and IM1-II-T1S0.

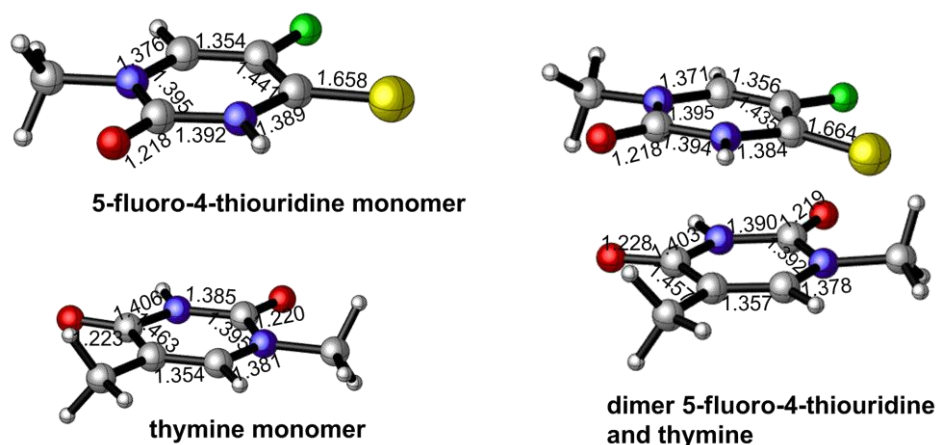


**Fig. S5.** B3LYP-D3/6-311++G\*\* computed LIIC paths: (left) connecting IM1-I-T1S0 and TS-A-S0; (right) connecting IM1-II-T1S0 and IM2-A-S0.



**Fig. S6.** B3LYP-D3/6-311++G\*\* computed LIIC path that connected IM1-I-T1S0 and R-A-S0.

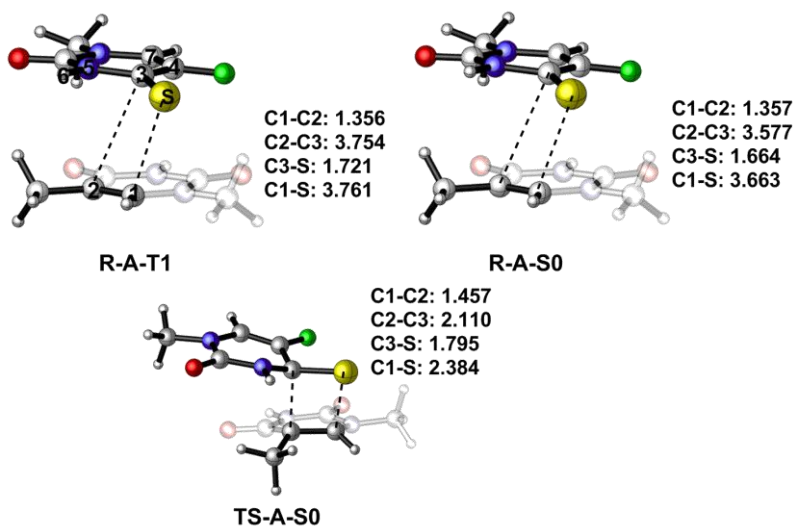
#### 4. Additional structures



**Fig. S7.** B3LYP-D3/6-31G\* optimized  $S_0$  minima of two monomers (i.e. thymine and 5-fluoro-4-thiouridine) and dimer 5-fluoro-4-thiouridine and thymine. Selected distances are given in Å.

**Table S1.** Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) of the Dimer 5-Fluoro-4-Thiouridine and Thymine Relative to the Separated Two Monomers (i.e. Thymine and 5-Fluoro-4-Thiouridine). First Value: Gas phase (B3LYP-D3/6-31G\*); Second Value: Aqueous Solution (B3LYP-D3/6-311++G\*\*/PCM).

|   | Thymine + 5-Fluoro-4-Thiouridine | Dimer      |
|---|----------------------------------|------------|
| E | 0.0/0.0                          | -16.9/-9.0 |
| H | 0.0/0.0                          | -15.3/-7.3 |
| G | 0.0/0.0                          | -2.4/5.0   |



**Fig. S8.** B3LYP-D3/6-31G\* optimized  $S_0$  transition states and  $S_0$  and  $T_1$  minima dimer 5-fluoro-4-thiouridine and thymine. Selected distances are given in Å.

## 5. SOC matrix elements

**Table S2.** CASPT2(10,8)/cc-pVDZ/PCM Calculated SOC Matrix Elements ( $\hat{H}'$ : SOC operator; unit:  $\text{cm}^{-1}$ ) of Dimer 5-Fluoro-4-Thiouridine and Thymine at Selected Points.

| S1-MIN                                 | X and Y | Z      |
|--|---------|--------|
| $\langle S_1   \hat{H}'   T_1 \rangle$ | 75.129  | 45.759 |
| $\langle S_1   \hat{H}'   T_2 \rangle$ | 74.448  | 46.046 |

**Table S3.** CASPT2(10,8)/cc-pVDZ/PCM (First Value) and TD-B3LYP-D3/cc-pVDZ/PCM (Second Value) Calculated SOC Matrix Elements ( $\hat{H}'$ : SOC operator; unit:  $\text{cm}^{-1}$ ) of Dimer 5-Fluoro-4-Thiouridine and Thymine at Selected Points.

| IM1-I-T1S0                             | X and Y      | Z                   |
|--|--------------|---------------------|
| $\langle T_1   \hat{H}'   S_0 \rangle$ | 1.210/2.307  | $\langle 1.0/0.521$ |
| IM1-II-T1S0                            | X,Y          | Z                   |
| $\langle T_1   \hat{H}'   S_0 \rangle$ | 29.329/6.375 | 11.973/8.157        |

The effective singlet–triplet SOC values reported in the main text are computed as:

SOC=

$$\frac{1}{3} \sqrt{|\langle S_{ms=0} | \hat{H}' | T_{ms=-1} \rangle_{1,1}|^2 + |\langle S_{ms=0} | \hat{H}' | T_{ms=-1} \rangle_{1,-1}|^2 + |\langle S_0 | \hat{H}' | T_{ms=0} \rangle_{1,0}|^2}$$

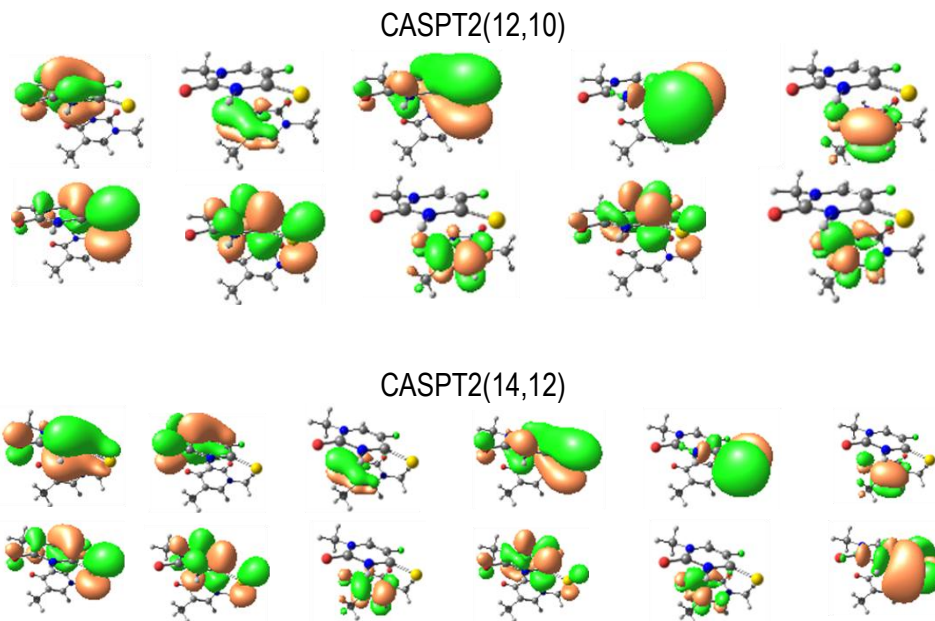
## 6. Tables

**Table S4.** CASPT2(12,10)/6-31G\*/PCM Computed Vertical and Adiabatic Excitation Energies (kcal/mol and [eV]) to the Lowest Four Electronic States (i.e.  $S_2$ ,  $S_1$ ,  $T_2$ , and  $T_1$ ) of Dimer 5-Fluoro-4-Thiouridine and Thymine in Aqueous Solution (PCM model).

|                      | $S_2$       | $S_1$       | $T_2$       | $T_1$       |
|----------------------|-------------|-------------|-------------|-------------|
| vertical excitation  | 93.9 [4.07] | 64.6 [2.80] | 62.5 [2.71] | 61.4 [2.66] |
| adiabatic excitation | 73.2 [3.17] | 57.3 [2.49] | 54.2 [2.35] | 54.1 [2.35] |

**Table S5.** CASPT2(14,12)/6-31G\*/PCM Computed Vertical and Adiabatic Excitation Energies (kcal/mol and [eV]) to the Lowest Four Electronic States (i.e.  $S_2$ ,  $S_1$ ,  $T_2$ , and  $T_1$ ) of Dimer 5-Fluoro-4-Thiouridine and Thymine in Aqueous Solution (PCM model).

|                      | $S_2$       | $S_1$       | $T_2$       | $T_1$       |
|----------------------|-------------|-------------|-------------|-------------|
| vertical excitation  | 93.8 [4.07] | 65.2 [2.83] | 62.6 [2.71] | 61.9 [2.69] |
| adiabatic excitation | 75.1 [3.26] | 56.7 [2.46] | 55.1 [2.39] | 54.2 [2.35] |



**Fig. S9.** Active space used in CASPT2 computations for photoinduced cross-linking of 5-fluoro-4-thiouridines with thymidine.

**Table S6.** CASPT2(10,8)/6-31G\*/PCM Computed Energies (kcal/mol and [eV]) to the Lowest Five Electronic States (i.e.  $S_2$ ,  $S_1$ ,  $T_2$ ,  $T_1$ , and  $S_0$ ) at All the Characterized Critical Points ( $S_0$ -MIN,  $S_1$ -MIN,  $T_1$ -MIN,  $S_2$ -MIN,  $S_2S_1$ -MIN, IM1-I-T1S0) of Dimer 5-Fluoro-4-Thiouridine and Thymine in Aqueous Solution (PCM model).

| geometry      | state       |             |              |             |              |
|---------------|-------------|-------------|--------------|-------------|--------------|
|               | $S_0$       | $S_1$       | $S_2$        | $T_1$       | $T_2$        |
| $S_0$ -MIN    | 0.0 [0.00]  | 64.6 [2.80] | 94.2 [4.09]  | 61.4 [2.66] | 62.3 [2.70]  |
| $S_1$ -MIN    | 7.0 [0.30]  | 57.4 [2.49] | 78.1 [3.39]  | 54.2 [2.35] | 55.9 [2.42]  |
| $T_1$ -MIN    | 8.1 [0.35]  | 57.2 [2.48] | 78.8 [3.42]  | 53.7 [2.33] | 55.3 [2.40]  |
| $T_2$ -MIN    | 6.3 [0.27]  | 55.9 [2.42] | 79.8 [3.46]  | 54.0 [2.34] | 54.1 [2.35]  |
| $S_2$ -MIN    | 16.4 [0.71] | 61.0 [2.65] | 73.4 [3.18]  | 57.0 [2.47] | 59.8 [2.59]  |
| $S_2S_1$ -MIN | 31.5 [1.36] | 77.3 [3.35] | 80.1 [3.47]  | 70.4 [3.05] | 74.7 [3.24]  |
| IM1-I-T1S0    | 40.1 [1.74] | 66.0 [2.86] | 105.0 [4.55] | 45.2 [1.96] | 106.5 [4.62] |

**Table S7.** CASPT2(10,8)/cc-pVDZ/PCM Calculated Weights and Singly Occupied Orbitals Involved in Electronic Transition of  $T_1$  and  $T_2$  States of Dimer 5-Fluoro-4-Thiouridine and Thymine at  $S_1$  Minimum.

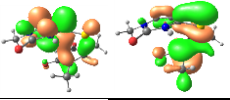
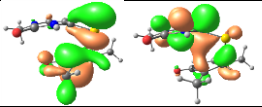
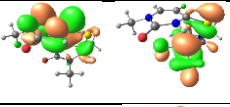
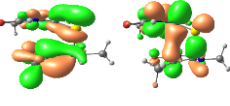
|       | transition              | weight | singly occupied orbitals |     |         |
|-------|-------------------------|--------|--------------------------|-----|---------|
|       |                         |        | $\pi$                    | $n$ | $\pi^*$ |
| $T_1$ | $\pi \rightarrow \pi^*$ | 0.36   |                          |     |         |
|       | $n \rightarrow \pi^*$   | 0.39   |                          |     |         |
| $T_2$ | $\pi \rightarrow \pi^*$ | 0.30   |                          |     |         |
|       | $n \rightarrow \pi^*$   | 0.43   |                          |     |         |



**Table S8.** CASPT2(10,8)/6-31G\*/PCM and UMP2/6-311++G\*\*/PCM Computed Energies (kcal/mol) of the B3LYP-D3 Optimized Structures on the Reactive Path from R-A-T1 to IM2-A-S0.

|             | R-A-S0 | TS-A-S0 | IM2-A-S0 | R-A-T1 | TS1-I-T1 | IM1-I-T1 | IM1-I-T1S0 |
|-------------|--------|---------|----------|--------|----------|----------|------------|
| G(B3LYP-D3) | 0.0    | 48.2    | 28.4     | 50.0   | 55.5     | 54.9     | 56.7/53.6  |
| E(CASPT2)   | 0.0    | 46.2    | 13.0     | 54.6   | 52.4     | 45.2     | 45.2/40.1  |
| E(UMP2)     | 0.0    | 44.1    | 13.8     | 72.3   | 79.3     | 70.4     | 70.4/54.0  |

**Table S9.** CASPT2(10,8)/6-31G\*/PCM and B3LYP-D3/PCM Calculated Weights and Singly Occupied Orbitals Involved in Electronic Transition of T<sub>1</sub> State that Crosses with the S<sub>0</sub> of Dimer 5-Fluoro-4-Thiouridine and Thymine at IM1-I-T1S0.

|                               | weight | singly occupied orbitals  |
|-------------------------------|--------|---|
| T <sub>1</sub> (CASPT2/PCM)   | 0.83   |                 |
| S <sub>0</sub> (CASPT2/PCM)   | 0.17   |                 |
| T <sub>1</sub> (B3LYP-D3/PCM) | -      |                |
| S <sub>0</sub> (B3LYP-D3/PCM) | -      | <br>HOMO LUMO |

**Table S10.** CASPT2(10,8)/6-31G\*/PCM Computed Energies (kcal/mol) of Conical Intersection S<sub>1</sub>/S<sub>0</sub> and Singlet-Triplet Crossing T<sub>1</sub>/S<sub>0</sub> in Franck-Condon Region that will Drive the System Back to the Original Ground State Minimum of Dimer 5-Fluoro-4-Thiouridine and Thymine.

|   | S <sub>1</sub> /S <sub>0</sub> | T <sub>1</sub> /S <sub>0</sub> |
|---|--------------------------------|--------------------------------|
| E | 86.1/80.0                      | 75.3/67.7                      |

**Table S11.** CASPT2(10,8)/6-31G\*/PCM Computed Vertical and Adiabatic Excitation Energies (kcal/mol and [eV]) to the Lowest Four Electronic States (i.e. S<sub>2</sub>, S<sub>1</sub>, T<sub>2</sub>, and T<sub>1</sub>) of Isolated Thymine in Aqueous Solution (PCM model).

| Thymine              | S <sub>2</sub>                          | S <sub>1</sub>                          | T <sub>2</sub>                          | T <sub>1</sub>                          |
|----------------------|---|---|---|---|
| Vertical excitation  | 116.2 [5.04]                            | 115.3 [5.00]                            | 110.0 [4.77]                            | 88.4 [3.83]                             |
|                      | [4.89] <sup>a</sup> [4.92] <sup>b</sup> | [4.77] <sup>a</sup> [4.77] <sup>b</sup> | [4.75] <sup>a</sup> [4.77] <sup>b</sup> | [3.59] <sup>a</sup> [3.75] <sup>b</sup> |
| Adiabatic excitation | 111.9 [4.85]                            | 100.4 [4.35]                            | 92.6 [4.01]                             | 71.5 [3.10]                             |

a. See ref. J. Phys. Chem. B 2007, 111, 11880-11883, CASPT2//CASSCF(14,10)/ANO-S.

b. See ref. J. Phys. Chem. B 2013, 117, 1999-2004, CASPT2//CASSCF(6,6)/ANO-S.

**Table S12.** CASPT2(10,8)/6-31G\*/PCM Computed Vertical and Adiabatic Excitation Energies (kcal/mol and [eV]) to the Lowest Four Electronic States (i.e. S<sub>2</sub>, S<sub>1</sub>, T<sub>2</sub>, and T<sub>1</sub>) of Dimer 5-Fluoro-4-Thiouridine and Thymine in Aqueous Solution (PCM model).

| Dimer                | S <sub>2</sub> | S <sub>1</sub> | T <sub>2</sub> | T <sub>1</sub> |
|----------------------|----------------|----------------|----------------|----------------|
| Vertical excitation  | 94.2 [4.08]    | 64.6 [2.80]    | 62.3 [2.70]    | 61.4 [2.66]    |
| Adiabatic excitation | 73.4 [3.18]    | 57.4 [2.49]    | 54.1 [2.35]    | 53.7 [2.33]    |

**Table S13.** CASPT2(10,8)/6-31G\*/PCM Computed Vertical and Adiabatic Excitation Energies (kcal/mol and [eV]) to the Lowest Four Electronic States (i.e. S<sub>2</sub>, S<sub>1</sub>, T<sub>2</sub>, and T<sub>1</sub>) of Isolated 5-Fluoro-4-Thiouridine in Aqueous Solution (PCM model).

| 5-Fluoro-4-Thiouridine | S <sub>2</sub> | S <sub>1</sub> | T <sub>2</sub> | T <sub>1</sub> |
|------------------------|----------------|----------------|----------------|----------------|
| Vertical excitation    | 92.3 [4.00]    | 61.8 [2.68]    | 59.6 [2.58]    | 59.6 [2.58]    |
| Adiabatic excitation   | 76.8 [3.33]    | 56.0 [2.43]    | 56.3 [2.44]    | 54.0 [2.34]    |

## 7. Cartesian coordinates

In xyz format (unit: Ångstrom)

### CASSCF/6-31G\*

Dimer 5-Fluoro-4-Thiouridine and Thymine

S0-MIN

```

C 2.350278190 1.652327850 0.339580680
C 0.165489580 2.367479390 -0.592281960
C 0.321500990 1.343809540 -1.636956010
C 1.430316830 0.582743640 -1.601779300
N 2.437939490 0.721685000 -0.653569990
H 1.161740190 3.138465430 1.003227470
H 1.606205870 -0.187373390 -2.326490350
C 3.545048200 -0.227645390 -0.607468950
H 4.429913450 0.277368740 -0.257829610
H 3.719905830 -0.606401860 -1.604580990
H 3.318195590 -1.051780720 0.056518170
O 3.171191400 1.796192760 1.198084750
N 1.219599570 2.440959470 0.291456510
O -0.785141860 3.087177590 -0.478069840
C -0.759681960 1.214261920 -2.674757650
H -1.718068600 1.001312860 -2.215701200
H -0.869747560 2.138108300 -3.230921640
H -0.528961360 0.418482150 -3.373316420

```

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.746384490 | -1.028086840 | 0.238695910  |
| C | -0.604480150 | -2.292938490 | 0.316527100  |
| C | -0.194357250 | -1.340683270 | 1.333128900  |
| C | -1.005145670 | -0.354532620 | 1.738049230  |
| N | -2.281847020 | -0.196541600 | 1.213987780  |
| H | -2.252317130 | -2.649503830 | -0.829125460 |
| H | -0.699569000 | 0.349480630  | 2.484692210  |
| C | -3.079366710 | 0.959625840  | 1.614628930  |
| H | -4.093111610 | 0.802919930  | 1.290124720  |
| H | -2.690227340 | 1.863543430  | 1.164082790  |
| H | -3.057939670 | 1.048687540  | 2.693008690  |
| O | -3.814759080 | -0.921682150 | -0.289280710 |
| N | -1.883449660 | -2.045887380 | -0.125431890 |
| S | 0.315731440  | -3.515344470 | -0.257850630 |
| F | 1.020073490  | -1.455079010 | 1.844067770  |

S2-MIN (1ππ\*)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.415148590  | 1.503170880  | 0.325017990  |
| C | 0.159521980  | 2.075483680  | -0.532322510 |
| C | 0.401693330  | 1.165729620  | -1.660807310 |
| C | 1.574025630  | 0.504592990  | -1.687322990 |
| N | 2.574451830  | 0.661728420  | -0.736036660 |
| H | 1.098505900  | 2.808207770  | 1.114080220  |
| H | 1.810212940  | -0.187703520 | -2.470308340 |
| C | 3.754276280  | -0.195839760 | -0.758565200 |
| H | 4.597859410  | 0.353132590  | -0.374732380 |
| H | 3.951753060  | -0.488202370 | -1.780134440 |
| H | 3.597334350  | -1.081132140 | -0.156011370 |
| O | 3.231257690  | 1.662737980  | 1.184877500  |
| N | 1.215812420  | 2.185823030  | 0.342856910  |
| O | -0.861058150 | 2.676869100  | -0.345378830 |
| C | -0.664844730 | 1.031405740  | -2.713214380 |
| H | -1.611643580 | 0.735065220  | -2.277721660 |
| H | -0.828541390 | 1.977837910  | -3.216312670 |
| H | -0.381978560 | 0.293284940  | -3.454325520 |
| C | -2.809654090 | -0.853492940 | 0.254271290  |
| C | -0.612678220 | -1.932603280 | 0.344649980  |
| C | -0.252830440 | -1.132260830 | 1.358864570  |
| C | -1.188163670 | -0.174445980 | 1.907784700  |
| N | -2.417494600 | -0.085363550 | 1.323891430  |
| H | -2.179641860 | -2.395328720 | -0.881793870 |
| H | -1.041298290 | 0.295690250  | 2.857084340  |
| C | -3.337046510 | 0.971522110  | 1.749388410  |
| H | -4.349575060 | 0.621427660  | 1.646561100  |
| H | -3.186145650 | 1.848841800  | 1.135338100  |
| H | -3.130056450 | 1.208193020  | 2.782766130  |
| O | -3.867192080 | -0.734659670 | -0.293341570 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -1.887436310 | -1.795090650 | -0.140378820 |
| S | 0.388810810  | -3.104223790 | -0.620637100 |
| F | 0.985189420  | -1.089246520 | 1.836361970  |

S1-MIN ( $1n\pi^*$ )

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.269286730  | 1.733079060  | 0.324906870  |
| C | 0.146426840  | 2.535928440  | -0.671138580 |
| C | 0.235096740  | 1.437376050  | -1.646214690 |
| C | 1.289737200  | 0.607795450  | -1.556276050 |
| N | 2.300870670  | 0.740125860  | -0.609117330 |
| H | 1.177446600  | 3.328683940  | 0.892098450  |
| H | 1.414876420  | -0.217295680 | -2.228905880 |
| C | 3.367275880  | -0.247888740 | -0.501580410 |
| H | 4.313509650  | 0.251178570  | -0.364494680 |
| H | 3.396532010  | -0.825556150 | -1.414032570 |
| H | 3.194925300  | -0.909870310 | 0.336935600  |
| O | 3.097214770  | 1.865947340  | 1.179586290  |
| N | 1.197752660  | 2.591588540  | 0.219284890  |
| O | -0.747560830 | 3.329778970  | -0.616706590 |
| C | -0.857408640 | 1.305732950  | -2.671738090 |
| H | -1.817832010 | 1.137911860  | -2.198871160 |
| H | -0.940290410 | 2.211989990  | -3.260308520 |
| H | -0.656990970 | 0.477604480  | -3.341628310 |
| C | -2.574071700 | -1.020449030 | 0.126499420  |
| C | -0.586019490 | -2.439182990 | 0.455433110  |
| C | -0.159322260 | -1.576165730 | 1.437332750  |
| C | -0.896598160 | -0.465377260 | 1.788585370  |
| N | -2.115668940 | -0.224227170 | 1.138510080  |
| H | -2.215400400 | -2.734191800 | -0.818404390 |
| H | -0.616995920 | 0.191053130  | 2.583684230  |
| C | -2.878795270 | 0.957828260  | 1.517181560  |
| H | -3.854972270 | 0.896421250  | 1.069334730  |
| H | -2.385536620 | 1.859598760  | 1.175844390  |
| H | -2.980619490 | 0.987849570  | 2.595233570  |
| O | -3.609617780 | -0.837210980 | -0.450831490 |
| N | -1.764730600 | -2.080220810 | -0.218627920 |
| S | 0.399379950  | -3.731865710 | -0.245490800 |
| F | 1.006674330  | -1.806819120 | 2.038365160  |

T2-MIN ( $3n\pi^*$ )

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.261442740 | 1.713563830  | 0.323032390  |
| C | 0.139575250 | 2.525473260  | -0.667341080 |
| C | 0.227106250 | 1.433579930  | -1.650140680 |
| C | 1.280170680 | 0.601331630  | -1.565176790 |
| N | 2.289741930 | 0.724393410  | -0.615209250 |
| H | 1.172295160 | 3.307519320  | 0.900192920  |
| H | 1.404598480 | -0.218829570 | -2.243986130 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.357864720  | -0.262440910 | -0.514349920 |
| H | 4.308323190  | 0.236557290  | -0.407853140 |
| H | 3.365308250  | -0.856899710 | -1.416332470 |
| H | 3.204143090  | -0.908105490 | 0.340294850  |
| O | 3.091366340  | 1.840598110  | 1.176501050  |
| N | 1.191107020  | 2.574199510  | 0.223200680  |
| O | -0.753620680 | 3.319813370  | -0.607545370 |
| C | -0.864401650 | 1.311689770  | -2.678124820 |
| H | -1.824738530 | 1.134415200  | -2.208540530 |
| H | -0.949412870 | 2.225221160  | -3.254952430 |
| H | -0.660296520 | 0.493247610  | -3.358853470 |
| C | -2.552033850 | -1.007081860 | 0.120697650  |
| C | -0.560513610 | -2.419824400 | 0.462884500  |
| C | -0.151781360 | -1.559548360 | 1.459202050  |
| C | -0.903788980 | -0.461377470 | 1.811175960  |
| N | -2.124374230 | -0.231366170 | 1.161979880  |
| H | -2.106194230 | -2.645471140 | -0.928003540 |
| H | -0.639055280 | 0.187135300  | 2.617953510  |
| C | -2.892647740 | 0.952720110  | 1.525031750  |
| H | -3.884704680 | 0.859014090  | 1.119262310  |
| H | -2.430412810 | 1.850466610  | 1.133095260  |
| H | -2.951861080 | 1.018402100  | 2.604278510  |
| O | -3.558665080 | -0.799097690 | -0.498278650 |
| N | -1.745245790 | -2.073799960 | -0.198287180 |
| S | 0.404657630  | -3.746159670 | -0.178921640 |
| F | 1.004622220  | -1.788188220 | 2.077562810  |

T1-MIN (3ππ\*)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.261868730  | 1.751475790  | 0.336294830  |
| C | 0.138650490  | 2.534672740  | -0.675927970 |
| C | 0.250365670  | 1.444070100  | -1.657876340 |
| C | 1.317070730  | 0.630445870  | -1.565126070 |
| N | 2.318242000  | 0.768813670  | -0.608338530 |
| H | 1.144192010  | 3.329369960  | 0.902161650  |
| H | 1.463124310  | -0.184331930 | -2.246528080 |
| C | 3.384124360  | -0.219976030 | -0.497658020 |
| H | 4.301068440  | 0.272222210  | -0.218200870 |
| H | 3.514808830  | -0.698522300 | -1.457960510 |
| H | 3.143635480  | -0.967371130 | 0.247955680  |
| O | 3.074262360  | 1.887664700  | 1.204878500  |
| N | 1.181369510  | 2.598418150  | 0.223325800  |
| O | -0.766689530 | 3.315750260  | -0.624687310 |
| C | -0.831265440 | 1.305528210  | -2.693977230 |
| H | -1.793167200 | 1.120219210  | -2.230302080 |
| H | -0.922656620 | 2.215560890  | -3.275277830 |
| H | -0.613402960 | 0.486499790  | -3.369682010 |
| C | -2.606316310 | -1.037116230 | 0.157503280  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.602932950 | -2.455067350 | 0.427036940  |
| C | -0.146320870 | -1.602990520 | 1.385337600  |
| C | -0.878245150 | -0.456859020 | 1.755942940  |
| N | -2.121570020 | -0.241096320 | 1.166415440  |
| H | -2.210870160 | -2.711138990 | -0.866369370 |
| H | -0.592504550 | 0.164591310  | 2.576213020  |
| C | -2.867669560 | 0.958089980  | 1.530181980  |
| H | -3.893768620 | 0.832404320  | 1.231968400  |
| H | -2.457534580 | 1.833099390  | 1.041514850  |
| H | -2.818516750 | 1.087972740  | 2.603684920  |
| O | -3.635843470 | -0.817241180 | -0.417430970 |
| N | -1.833940350 | -2.122314350 | -0.158511670 |
| S | 0.235562810  | -3.887570490 | -0.151706370 |
| F | 1.013443380  | -1.804122450 | 1.989594410  |

S<sub>2</sub> (<sup>1</sup>ππ\*)/ S<sub>1</sub> (<sup>1</sup>ππ\*)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.369883900  | 1.494807000  | 0.334441300  |
| C | 0.131556000  | 2.119077200  | -0.535641200 |
| C | 0.361117300  | 1.193604900  | -1.653698100 |
| C | 1.514723100  | 0.497344700  | -1.666613500 |
| N | 2.510897000  | 0.631847100  | -0.710201900 |
| H | 1.088426000  | 2.850607900  | 1.103610700  |
| H | 1.733074800  | -0.209157900 | -2.441778200 |
| C | 3.684171700  | -0.237043400 | -0.711905500 |
| H | 4.566651100  | 0.359013600  | -0.535942400 |
| H | 3.752681900  | -0.711649400 | -1.678007900 |
| H | 3.584748900  | -0.999527200 | 0.045470700  |
| O | 3.186131200  | 1.650586000  | 1.194973200  |
| N | 1.188304500  | 2.208673100  | 0.343534800  |
| O | -0.874410500 | 2.745353700  | -0.351705700 |
| C | -0.704281900 | 1.083215700  | -2.711919700 |
| H | -1.663301200 | 0.811234300  | -2.285714400 |
| H | -0.844612500 | 2.030349000  | -3.220722700 |
| H | -0.438885000 | 0.332740800  | -3.445512700 |
| C | -2.708525800 | -0.830508400 | 0.215883900  |
| C | -0.565674200 | -1.993968500 | 0.347556200  |
| C | -0.240401900 | -1.193396900 | 1.350889400  |
| C | -1.174635000 | -0.177520800 | 1.939289500  |
| N | -2.334818300 | -0.073048100 | 1.304187800  |
| H | -2.009553600 | -2.412887400 | -0.882733100 |
| H | -1.079420600 | 0.288623500  | 2.904016300  |
| C | -3.259845000 | 0.976726500  | 1.720064600  |
| H | -4.269884300 | 0.614699000  | 1.600204900  |
| H | -3.091217400 | 1.817289800  | 1.059587700  |
| H | -3.047535300 | 1.240972400  | 2.742894600  |
| O | -3.770598000 | -0.666308300 | -0.346653900 |
| N | -1.795024700 | -1.787839400 | -0.131334700 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| S | 0.369083600 | -3.224899600 | -0.683085000 |
| F | 0.979748200 | -1.097859800 | 1.851014100  |

S<sub>1</sub> (1nπ\*)/ T<sub>2</sub> (3nπ\*)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.279974400  | 1.751928300  | 0.327397000  |
| C | 0.155041100  | 2.543727800  | -0.672620500 |
| C | 0.236018800  | 1.428206000  | -1.627830000 |
| C | 1.286286100  | 0.594317800  | -1.526924500 |
| N | 2.301723900  | 0.740807600  | -0.586093500 |
| H | 1.195400800  | 3.360582400  | 0.872527500  |
| H | 1.401866000  | -0.247996600 | -2.178900600 |
| C | 3.375808600  | -0.237916500 | -0.473416700 |
| H | 4.327406500  | 0.267333300  | -0.412812100 |
| H | 3.358931800  | -0.870262100 | -1.348681000 |
| H | 3.245765600  | -0.847692700 | 0.410581100  |
| O | 3.115725700  | 1.899112400  | 1.172557400  |
| N | 1.208938300  | 2.610026300  | 0.214571900  |
| O | -0.735889300 | 3.341865800  | -0.628281200 |
| C | -0.860335900 | 1.282842000  | -2.647462300 |
| H | -1.822816600 | 1.148612000  | -2.168327100 |
| H | -0.927656500 | 2.170425700  | -3.265991400 |
| H | -0.676158700 | 0.429086700  | -3.289092400 |
| C | -2.587390300 | -1.023375100 | 0.115641200  |
| C | -0.614633600 | -2.463059700 | 0.437299200  |
| C | -0.176778300 | -1.581880200 | 1.428966900  |
| C | -0.898789500 | -0.490788200 | 1.778189800  |
| N | -2.108084000 | -0.218945900 | 1.105604400  |
| H | -2.335142600 | -2.818890900 | -0.668703300 |
| H | -0.603479300 | 0.186625300  | 2.550701700  |
| C | -2.862548400 | 0.963203600  | 1.500489100  |
| H | -3.812609400 | 0.949654200  | 0.995493700  |
| H | -2.327698400 | 1.865283100  | 1.229856300  |
| H | -3.027605800 | 0.948378600  | 2.571603900  |
| O | -3.640721900 | -0.858553800 | -0.431191400 |
| N | -1.785558400 | -2.096144800 | -0.255586800 |
| S | 0.455876300  | -3.550835300 | -0.454171100 |
| F | 1.007706900  | -1.844526400 | 1.989053900  |

S<sub>1</sub> (1nπ\*)/ T<sub>1</sub> (3ππ\*)

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.262087400 | 1.751510600  | 0.335851400  |
| C | 0.140281000 | 2.535840800  | -0.677633800 |
| C | 0.251247400 | 1.443567300  | -1.657304200 |
| C | 1.315309900 | 0.627238100  | -1.564341400 |
| N | 2.317479900 | 0.769133900  | -0.608745300 |
| H | 1.144661300 | 3.328847200  | 0.901768800  |
| H | 1.459181000 | -0.191559300 | -2.240919300 |
| C | 3.382183800 | -0.218065100 | -0.499410700 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 4.299238600  | 0.273056800  | -0.217541300 |
| H | 3.510364400  | -0.698836900 | -1.458580400 |
| H | 3.140316400  | -0.966053200 | 0.245479700  |
| O | 3.076043600  | 1.886983300  | 1.204054800  |
| N | 1.182494000  | 2.598513900  | 0.222546900  |
| O | -0.762232600 | 3.320417200  | -0.629282500 |
| C | -0.830392300 | 1.305521500  | -2.693133000 |
| H | -1.791681600 | 1.122115600  | -2.227228500 |
| H | -0.921425500 | 2.214642200  | -3.276290100 |
| H | -0.612286700 | 0.485035800  | -3.367458100 |
| C | -2.607086600 | -1.034908000 | 0.161826300  |
| C | -0.601891800 | -2.416111000 | 0.456040200  |
| C | -0.139884900 | -1.560358500 | 1.425047200  |
| C | -0.863413600 | -0.478461300 | 1.752187200  |
| N | -2.133987500 | -0.243613300 | 1.160594300  |
| H | -2.255735500 | -2.685603200 | -0.884887100 |
| H | -0.576651200 | 0.144560300  | 2.568596200  |
| C | -2.874864000 | 0.955217300  | 1.520862800  |
| H | -3.904091000 | 0.838359600  | 1.229135100  |
| H | -2.467616200 | 1.838698900  | 1.043176900  |
| H | -2.827898500 | 1.082903800  | 2.595745200  |
| O | -3.631527200 | -0.842516100 | -0.430116900 |
| N | -1.839024300 | -2.131088400 | -0.171985100 |
| S | 0.248358800  | -3.860697400 | -0.135763100 |
| F | 1.061017400  | -1.863141400 | 1.982156700  |

|   | $T_2$ ( $^3n\pi^*$ ) | $T_1$ ( $^3\pi\pi^*$ ) |              |
|---|----------------------|------------------------|--------------|
| C | 2.261694400          | 1.749601500            | 0.329147800  |
| C | 0.137080700          | 2.531977500            | -0.680705700 |
| C | 0.238380100          | 1.430149500            | -1.650859300 |
| C | 1.300904100          | 0.611589800            | -1.554667700 |
| N | 2.309192600          | 0.757765800            | -0.606071500 |
| H | 1.153094800          | 3.337289800            | 0.885468500  |
| H | 1.438261700          | -0.213244000           | -2.225543800 |
| C | 3.371975000          | -0.233289900           | -0.491544900 |
| H | 4.291926500          | 0.258586400            | -0.221463100 |
| H | 3.495059900          | -0.722512200           | -1.447377600 |
| H | 3.132936100          | -0.971813800           | 0.263348600  |
| O | 3.079768100          | 1.891118700            | 1.191801400  |
| N | 1.184151400          | 2.599689200            | 0.213550900  |
| O | -0.763555500         | 3.318628900            | -0.633999100 |
| C | -0.848827800         | 1.285663100            | -2.680453300 |
| H | -1.809515200         | 1.110358000            | -2.210627600 |
| H | -0.937739500         | 2.189714400            | -3.271454500 |
| H | -0.637501400         | 0.458044500            | -3.347798700 |
| C | -2.585386900         | -1.012999000           | 0.140845600  |
| C | -0.584670000         | -2.425387800           | 0.415512500  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.146628000 | -1.578253300 | 1.406850400  |
| C | -0.879136400 | -0.469135500 | 1.774598700  |
| N | -2.123430400 | -0.239073200 | 1.168824100  |
| H | -2.171825500 | -2.647113700 | -0.931217800 |
| H | -0.595647400 | 0.164857800  | 2.586639000  |
| C | -2.871798700 | 0.955101800  | 1.540462600  |
| H | -3.892712800 | 0.837549700  | 1.220649400  |
| H | -2.452282200 | 1.839834300  | 1.077128100  |
| H | -2.844630900 | 1.064720000  | 2.617249600  |
| O | -3.605481200 | -0.795234000 | -0.451465200 |
| N | -1.800621800 | -2.091366200 | -0.194651500 |
| S | 0.286934100  | -3.838803300 | -0.170464900 |
| F | 1.018606300  | -1.822863800 | 2.002738000  |

$S_1$  ( $1n\pi^*$ ) /  $S_0$

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.337045400  | 1.828857000  | 0.294836100  |
| C | 0.209109700  | 2.604590100  | -0.707924000 |
| C | 0.280109400  | 1.469250900  | -1.636523700 |
| C | 1.328820800  | 0.633793200  | -1.526983400 |
| N | 2.355436000  | 0.806223900  | -0.603630800 |
| H | 1.247230900  | 3.438948800  | 0.829123900  |
| H | 1.427734500  | -0.232737900 | -2.145676200 |
| C | 3.449891100  | -0.150456500 | -0.504695800 |
| H | 4.392350000  | 0.374434800  | -0.474412800 |
| H | 3.422091300  | -0.794744400 | -1.369224000 |
| H | 3.352477000  | -0.749300300 | 0.390142300  |
| O | 3.179387300  | 1.992922400  | 1.131725100  |
| N | 1.264230800  | 2.684883900  | 0.175631700  |
| O | -0.680603900 | 3.408389500  | -0.675396400 |
| C | -0.828198800 | 1.297976500  | -2.639888700 |
| H | -1.783623600 | 1.151889400  | -2.148695800 |
| H | -0.918479900 | 2.179310500  | -3.264477000 |
| H | -0.638103600 | 0.442762700  | -3.278203800 |
| C | -2.650166000 | -1.078882300 | 0.180294200  |
| C | -0.763402300 | -2.523699600 | 0.518564600  |
| C | -0.270945400 | -1.756777800 | 1.430034200  |
| C | -1.062616800 | -0.626328000 | 1.979988800  |
| N | -2.059178000 | -0.218063400 | 1.074468600  |
| H | -2.644446800 | -3.044258900 | -0.207215700 |
| H | -1.339273600 | -0.602545100 | 3.015532600  |
| C | -2.734408200 | 1.048905000  | 1.357262100  |
| H | -3.701919100 | 1.050850700  | 0.886948900  |
| H | -2.151973000 | 1.881721500  | 0.991203100  |
| H | -2.859273000 | 1.146888500  | 2.430734000  |
| O | -3.686528400 | -0.853791900 | -0.371160800 |
| N | -1.996738200 | -2.308393700 | -0.063053300 |
| S | 0.586983600  | -3.379982300 | -0.489694800 |

F 1.085554800 -1.791486300 1.484816200

T<sub>1</sub> (<sup>3</sup>ππ\*)/ S<sub>0</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.517747900  | 1.657382800  | 0.305803200  |
| C | 0.305281900  | 2.471979500  | -0.453550800 |
| C | 0.346990900  | 1.464117100  | -1.523423500 |
| C | 1.422836100  | 0.659597300  | -1.583213000 |
| N | 2.502050000  | 0.749042900  | -0.710868900 |
| H | 1.426451100  | 3.154537300  | 1.098373600  |
| H | 1.508946000  | -0.108768700 | -2.324814800 |
| C | 3.599325900  | -0.206449400 | -0.765153100 |
| H | 4.543839700  | 0.314904800  | -0.737974100 |
| H | 3.525109100  | -0.764925300 | -1.686884500 |
| H | 3.552699900  | -0.887852500 | 0.073861400  |
| O | 3.410627900  | 1.748205200  | 1.097812500  |
| N | 1.418641400  | 2.486028000  | 0.357253900  |
| O | -0.603296900 | 3.230252800  | -0.265959300 |
| C | -0.811285900 | 1.388512500  | -2.479566200 |
| H | -1.736487000 | 1.184746200  | -1.953897800 |
| H | -0.938671900 | 2.329101500  | -3.003155300 |
| H | -0.654525400 | 0.604862600  | -3.211286700 |
| C | -2.748860400 | -1.275250000 | 0.254744300  |
| C | -0.580872700 | -2.335334100 | 0.682279200  |
| C | -0.182195600 | -1.330796200 | 1.423687200  |
| C | -1.140573700 | -0.279895300 | 1.800081300  |
| N | -2.284157400 | -0.219969200 | 0.988359000  |
| H | -2.369183600 | -3.244817500 | 0.183703600  |
| H | -1.254637900 | 0.048612700  | 2.818457500  |
| C | -3.144485000 | 0.948923500  | 1.150532100  |
| H | -3.935497500 | 0.906443900  | 0.422329500  |
| H | -2.558819100 | 1.844305000  | 1.002829400  |
| H | -3.579466100 | 0.957257400  | 2.144740500  |
| O | -3.822564300 | -1.319845000 | -0.264384900 |
| N | -1.881130100 | -2.372205700 | 0.172063500  |
| S | 0.184359300  | -3.373711600 | -0.607948700 |
| F | 1.110377300  | -1.097841800 | 1.659618900  |

LIIC path connecting S2-MIN and S<sub>2</sub> (<sup>1</sup>ππ\*)/ S<sub>1</sub> (<sup>1</sup>ππ\*)

Coord\_1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.480000000  | 0.000000000  | 0.000000000  |
| C | 2.439920000  | 0.000000000  | 1.469070000  |
| C | 1.230250000  | -0.026870000 | 2.059110000  |
| N | 0.027740000  | -0.016230000 | 1.363160000  |
| H | 1.225900000  | 0.056460000  | -1.597890000 |
| H | 1.126350000  | -0.046340000 | 3.125390000  |
| C | -1.235460000 | -0.190690000 | 2.071550000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2.008720000 | 0.352690000  | 1.554710000  |
| H | -1.129380000 | 0.202200000  | 3.072780000  |
| H | -1.505320000 | -1.237540000 | 2.123700000  |
| O | -1.002700000 | -0.011640000 | -0.652160000 |
| N | 1.242200000  | 0.037110000  | -0.600260000 |
| O | 3.482400000  | -0.043150000 | -0.656910000 |
| C | 3.742780000  | 0.033830000  | 2.220410000  |
| H | 4.384980000  | -0.789350000 | 1.930840000  |
| H | 4.284000000  | 0.949170000  | 2.008560000  |
| H | 3.571370000  | -0.024000000 | 3.288750000  |
| C | 4.232700000  | -3.788400000 | 0.767970000  |
| C | 1.954220000  | -3.791500000 | 1.666800000  |
| C | 1.461010000  | -3.578560000 | 0.437950000  |
| C | 2.342990000  | -3.509130000 | -0.706980000 |
| N | 3.683510000  | -3.616250000 | -0.479690000 |
| H | 3.696610000  | -4.110260000 | 2.684690000  |
| H | 1.989740000  | -3.594970000 | -1.712770000 |
| C | 4.616670000  | -3.400960000 | -1.587170000 |
| H | 5.492350000  | -4.007760000 | -1.434390000 |
| H | 4.894160000  | -2.356450000 | -1.626330000 |
| H | 4.125780000  | -3.683840000 | -2.506800000 |
| O | 5.411290000  | -3.824860000 | 0.972860000  |
| N | 3.313050000  | -3.931730000 | 1.781160000  |
| S | 1.106670000  | -3.777930000 | 3.275810000  |
| F | 0.179860000  | -3.312340000 | 0.213640000  |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.480150000  | 0.000000000  | 0.000000000  |
| C | 2.439200000  | 0.000000000  | 1.469030000  |
| C | 1.229350000  | -0.027620000 | 2.059000000  |
| N | 0.027100000  | -0.017650000 | 1.363020000  |
| H | 1.226070000  | 0.057940000  | -1.598150000 |
| H | 1.125550000  | -0.047560000 | 3.125250000  |
| C | -1.237590000 | -0.190470000 | 2.069430000  |
| H | -2.004590000 | 0.373200000  | 1.564620000  |
| H | -1.124530000 | 0.180480000  | 3.077970000  |
| H | -1.518540000 | -1.234850000 | 2.101810000  |
| O | -1.002280000 | -0.010700000 | -0.652840000 |
| N | 1.242210000  | 0.037120000  | -0.600340000 |
| O | 3.482340000  | -0.043670000 | -0.657180000 |
| C | 3.742230000  | 0.034360000  | 2.220350000  |
| H | 4.384990000  | -0.788780000 | 1.931630000  |
| H | 4.283680000  | 0.949510000  | 2.008280000  |
| H | 3.570870000  | -0.023590000 | 3.288570000  |
| C | 4.210560000  | -3.785380000 | 0.781200000  |
| C | 1.932840000  | -3.793720000 | 1.679630000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 1.445030000 | -3.582460000 | 0.450390000  |
| C | 2.328120000 | -3.514280000 | -0.701250000 |
| N | 3.663790000 | -3.616790000 | -0.468130000 |
| H | 3.663080000 | -4.106340000 | 2.698730000  |
| H | 1.979830000 | -3.604620000 | -1.709110000 |
| C | 4.598990000 | -3.405870000 | -1.574060000 |
| H | 5.473240000 | -4.014370000 | -1.417310000 |
| H | 4.878070000 | -2.361520000 | -1.608040000 |
| H | 4.108640000 | -3.686010000 | -2.494490000 |
| O | 5.391160000 | -3.819940000 | 0.985380000  |
| N | 3.288420000 | -3.929920000 | 1.790690000  |
| S | 1.091420000 | -3.780150000 | 3.296760000  |
| F | 0.166840000 | -3.311290000 | 0.218800000  |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.480290000  | 0.000000000  | 0.000000000  |
| C | 2.438480000  | 0.000000000  | 1.468980000  |
| C | 1.228440000  | -0.028370000 | 2.058880000  |
| N | 0.026460000  | -0.019070000 | 1.362870000  |
| H | 1.226230000  | 0.059430000  | -1.598420000 |
| H | 1.124760000  | -0.048780000 | 3.125120000  |
| C | -1.239720000 | -0.190250000 | 2.067300000  |
| H | -2.000190000 | 0.393380000  | 1.574940000  |
| H | -1.119990000 | 0.158510000  | 3.082710000  |
| H | -1.531720000 | -1.231670000 | 2.079970000  |
| O | -1.001860000 | -0.009750000 | -0.653520000 |
| N | 1.242220000  | 0.037120000  | -0.600410000 |
| O | 3.482280000  | -0.044200000 | -0.657440000 |
| C | 3.741680000  | 0.034890000  | 2.220280000  |
| H | 4.384990000  | -0.788220000 | 1.932420000  |
| H | 4.283350000  | 0.949850000  | 2.008010000  |
| H | 3.570360000  | -0.023180000 | 3.288390000  |
| C | 4.188540000  | -3.782230000 | 0.794620000  |
| C | 1.911560000  | -3.795750000 | 1.692600000  |
| C | 1.429170000  | -3.586200000 | 0.462990000  |
| C | 2.313370000  | -3.519310000 | -0.695370000 |
| N | 3.644170000  | -3.617200000 | -0.456440000 |
| H | 3.629520000  | -4.102010000 | 2.712890000  |
| H | 1.970110000  | -3.614140000 | -1.705260000 |
| C | 4.581450000  | -3.410620000 | -1.560780000 |
| H | 5.454240000  | -4.020820000 | -1.400010000 |
| H | 4.862090000  | -2.366450000 | -1.589530000 |
| H | 4.091700000  | -3.688000000 | -2.482020000 |
| O | 5.371150000  | -3.814870000 | 0.998060000  |
| N | 3.263870000  | -3.927840000 | 1.800390000  |
| S | 1.076300000  | -3.782070000 | 3.317800000  |

F 0.154020000 -3.310120000 0.224080000

Coord\_4

C 0.000000000 0.000000000 0.000000000  
C 2.480440000 0.000000000 0.000000000  
C 2.437760000 0.000000000 1.468940000  
C 1.227540000 -0.029120000 2.058770000  
N 0.025820000 -0.020490000 1.362730000  
H 1.226390000 0.060910000 -1.598680000  
H 1.123970000 -0.050000000 3.124990000  
C -1.241830000 -0.190020000 2.065180000  
H -1.995520000 0.413220000 1.585640000  
H -1.115750000 0.136310000 3.086980000  
H -1.544850000 -1.227990000 2.058170000  
O -1.001430000 -0.008810000 -0.654200000  
N 1.242230000 0.037130000 -0.600490000  
O 3.482210000 -0.044720000 -0.657710000  
C 3.741120000 0.035410000 2.220210000  
H 4.385000000 -0.787650000 1.933200000  
H 4.283030000 0.950200000 2.007740000  
H 3.569860000 -0.022770000 3.288200000  
C 4.166640000 -3.778950000 0.808210000  
C 1.890390000 -3.797600000 1.705710000  
C 1.413450000 -3.589780000 0.475730000  
C 2.298750000 -3.524230000 -0.689320000  
N 3.624640000 -3.617480000 -0.444620000  
H 3.595940000 -4.097270000 2.727170000  
H 1.960560000 -3.623510000 -1.701230000  
C 4.564030000 -3.415230000 -1.547320000  
H 5.435350000 -4.027100000 -1.382510000  
H 4.846220000 -2.371240000 -1.570800000  
H 4.074950000 -3.689830000 -2.469400000  
O 5.351250000 -3.809650000 1.010900000  
N 3.239400000 -3.925490000 1.810270000  
S 1.061310000 -3.783670000 3.338950000  
F 0.141400000 -3.308820000 0.229470000

Coord\_5

C 0.000000000 0.000000000 0.000000000  
C 2.480580000 0.000000000 0.000000000  
C 2.437040000 0.000000000 1.468890000  
C 1.226640000 -0.029870000 2.058650000  
N 0.025180000 -0.021910000 1.362580000  
H 1.226550000 0.062390000 -1.598930000  
H 1.123180000 -0.051220000 3.124850000  
C -1.243950000 -0.189780000 2.063050000  
H -1.990580000 0.432710000 1.596730000

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.111820000 | 0.113900000  | 3.090800000  |
| H | -1.557920000 | -1.223820000 | 2.036420000  |
| O | -1.001010000 | -0.007870000 | -0.654880000 |
| N | 1.242240000  | 0.037130000  | -0.600560000 |
| O | 3.482150000  | -0.045240000 | -0.657980000 |
| C | 3.740570000  | 0.035940000  | 2.220150000  |
| H | 4.385010000  | -0.787070000 | 1.933990000  |
| H | 4.282710000  | 0.950540000  | 2.007460000  |
| H | 3.569350000  | -0.022360000 | 3.288020000  |
| C | 4.144840000  | -3.775530000 | 0.821980000  |
| C | 1.869330000  | -3.799280000 | 1.718960000  |
| C | 1.397860000  | -3.593210000 | 0.488620000  |
| C | 2.284280000  | -3.529040000 | -0.683120000 |
| N | 3.605200000  | -3.617630000 | -0.432680000 |
| H | 3.562340000  | -4.092120000 | 2.741570000  |
| H | 1.951190000  | -3.632750000 | -1.697000000 |
| C | 4.546740000  | -3.419670000 | -1.533680000 |
| H | 5.416570000  | -4.033220000 | -1.364800000 |
| H | 4.830460000  | -2.375910000 | -1.551860000 |
| H | 4.058390000  | -3.691490000 | -2.456640000 |
| O | 5.331460000  | -3.804270000 | 1.023900000  |
| N | 3.215020000  | -3.922870000 | 1.820310000  |
| S | 1.046460000  | -3.784970000 | 3.360190000  |
| F | 0.128980000  | -3.307390000 | 0.234970000  |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.480730000  | 0.000000000  | 0.000000000  |
| C | 2.436310000  | 0.000000000  | 1.468850000  |
| C | 1.225740000  | -0.030620000 | 2.058540000  |
| N | 0.024540000  | -0.023330000 | 1.362430000  |
| H | 1.226720000  | 0.063870000  | -1.599190000 |
| H | 1.122390000  | -0.052440000 | 3.124720000  |
| C | -1.246050000 | -0.189530000 | 2.060920000  |
| H | -1.985390000 | 0.451830000  | 1.608200000  |
| H | -1.108200000 | 0.091280000  | 3.094150000  |
| H | -1.570920000 | -1.219160000 | 2.014740000  |
| O | -1.000580000 | -0.006920000 | -0.655550000 |
| N | 1.242250000  | 0.037130000  | -0.600640000 |
| O | 3.482080000  | -0.045770000 | -0.658240000 |
| C | 3.740020000  | 0.036470000  | 2.220080000  |
| H | 4.385010000  | -0.786500000 | 1.934780000  |
| H | 4.282390000  | 0.950890000  | 2.007190000  |
| H | 3.568850000  | -0.021940000 | 3.287830000  |
| C | 4.123170000  | -3.771980000 | 0.835920000  |
| C | 1.848390000  | -3.800770000 | 1.732340000  |
| C | 1.382400000  | -3.596470000 | 0.501660000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.269930000 | -3.533730000 | -0.676760000 |
| N | 3.585870000 | -3.617640000 | -0.420630000 |
| H | 3.528730000 | -4.086560000 | 2.756080000  |
| H | 1.942000000 | -3.641850000 | -1.692590000 |
| C | 4.529580000 | -3.423970000 | -1.519860000 |
| H | 5.397900000 | -4.039170000 | -1.346890000 |
| H | 4.814800000 | -2.380440000 | -1.532690000 |
| H | 4.042030000 | -3.692980000 | -2.443720000 |
| O | 5.311790000 | -3.798750000 | 1.037050000  |
| N | 3.190720000 | -3.919990000 | 1.830510000  |
| S | 1.031740000 | -3.785950000 | 3.381520000  |
| F | 0.116760000 | -3.305840000 | 0.240600000  |

Coord\_7

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.480870000  | 0.000000000  | 0.000000000  |
| C | 2.435590000  | 0.000000000  | 1.468800000  |
| C | 1.224840000  | -0.031370000 | 2.058420000  |
| N | 0.023910000  | -0.024750000 | 1.362280000  |
| H | 1.226880000  | 0.065350000  | -1.599450000 |
| H | 1.121600000  | -0.053650000 | 3.124580000  |
| C | -1.248150000 | -0.189280000 | 2.058800000  |
| H | -1.979960000 | 0.470570000  | 1.620050000  |
| H | -1.104890000 | 0.068470000  | 3.097030000  |
| H | -1.583840000 | -1.214010000 | 1.993130000  |
| O | -1.000160000 | -0.005970000 | -0.656230000 |
| N | 1.242260000  | 0.037140000  | -0.600720000 |
| O | 3.482020000  | -0.046290000 | -0.658510000 |
| C | 3.739460000  | 0.037000000  | 2.220010000  |
| H | 4.385020000  | -0.785930000 | 1.935570000  |
| H | 4.282060000  | 0.951230000  | 2.006910000  |
| H | 3.568340000  | -0.021530000 | 3.287650000  |
| C | 4.101610000  | -3.768290000 | 0.850030000  |
| C | 1.827560000  | -3.802070000 | 1.745850000  |
| C | 1.367080000  | -3.599580000 | 0.514840000  |
| C | 2.255730000  | -3.538300000 | -0.670250000 |
| N | 3.566630000  | -3.617530000 | -0.408460000 |
| H | 3.495110000  | -4.080580000 | 2.770690000  |
| H | 1.932990000  | -3.650810000 | -1.687990000 |
| C | 4.512540000  | -3.428100000 | -1.505880000 |
| H | 5.379340000  | -4.044940000 | -1.328780000 |
| H | 4.799250000  | -2.384840000 | -1.513320000 |
| H | 4.025860000  | -3.694300000 | -2.430670000 |
| O | 5.292240000  | -3.793070000 | 1.050350000  |
| N | 3.166520000  | -3.916830000 | 1.840890000  |
| S | 1.017160000  | -3.786630000 | 3.402940000  |
| F | 0.104740000  | -3.304160000 | 0.246330000  |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.481010000  | 0.000000000  | 0.000000000  |
| C | 2.434870000  | 0.000000000  | 1.468750000  |
| C | 1.223940000  | -0.032120000 | 2.058310000  |
| N | 0.023270000  | -0.026170000 | 1.362120000  |
| H | 1.227040000  | 0.066840000  | -1.599700000 |
| H | 1.120810000  | -0.054870000 | 3.124440000  |
| C | -1.250240000 | -0.189010000 | 2.056670000  |
| H | -1.974270000 | 0.488930000  | 1.632250000  |
| H | -1.101890000 | 0.045480000  | 3.099440000  |
| H | -1.596690000 | -1.208360000 | 1.971590000  |
| O | -0.999730000 | -0.005020000 | -0.656900000 |
| N | 1.242270000  | 0.037140000  | -0.600800000 |
| O | 3.481960000  | -0.046820000 | -0.658770000 |
| C | 3.738910000  | 0.037530000  | 2.219940000  |
| H | 4.385020000  | -0.785350000 | 1.936350000  |
| H | 4.281740000  | 0.951570000  | 2.006640000  |
| H | 3.567830000  | -0.021110000 | 3.287460000  |
| C | 4.080170000  | -3.764470000 | 0.864310000  |
| C | 1.806840000  | -3.803200000 | 1.759490000  |
| C | 1.351890000  | -3.602530000 | 0.528170000  |
| C | 2.241660000  | -3.542760000 | -0.663580000 |
| N | 3.547480000  | -3.617280000 | -0.396170000 |
| H | 3.461490000  | -4.074200000 | 2.785410000  |
| H | 1.924160000  | -3.659630000 | -1.683200000 |
| C | 4.495640000  | -3.432080000 | -1.491720000 |
| H | 5.360890000  | -4.050550000 | -1.310480000 |
| H | 4.783800000  | -2.389100000 | -1.493730000 |
| H | 4.009890000  | -3.695450000 | -2.417470000 |
| O | 5.272810000  | -3.787230000 | 1.063800000  |
| N | 3.142420000  | -3.913410000 | 1.851430000  |
| S | 1.002720000  | -3.786990000 | 3.424460000  |
| F | 0.092930000  | -3.302370000 | 0.252180000  |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.481160000  | 0.000000000  | 0.000000000  |
| C | 2.434150000  | 0.000000000  | 1.468710000  |
| C | 1.223040000  | -0.032870000 | 2.058190000  |
| N | 0.022630000  | -0.027590000 | 1.361970000  |
| H | 1.227200000  | 0.068320000  | -1.599950000 |
| H | 1.120030000  | -0.056080000 | 3.124300000  |
| C | -1.252320000 | -0.188740000 | 2.054550000  |
| H | -1.968350000 | 0.506890000  | 1.644820000  |
| H | -1.099200000 | 0.022330000  | 3.101370000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.609450000 | -1.202240000 | 1.950150000  |
| O | -0.999300000 | -0.004060000 | -0.657570000 |
| N | 1.242280000  | 0.037150000  | -0.600880000 |
| O | 3.481890000  | -0.047340000 | -0.659040000 |
| C | 3.738360000  | 0.038060000  | 2.219870000  |
| H | 4.385030000  | -0.784770000 | 1.937140000  |
| H | 4.281420000  | 0.951920000  | 2.006360000  |
| H | 3.567330000  | -0.020700000 | 3.287280000  |
| C | 4.058860000  | -3.760500000 | 0.878750000  |
| C | 1.786240000  | -3.804150000 | 1.773260000  |
| C | 1.336840000  | -3.605320000 | 0.541630000  |
| C | 2.227730000  | -3.547110000 | -0.656770000 |
| N | 3.528440000  | -3.616910000 | -0.383770000 |
| H | 3.427880000  | -4.067390000 | 2.800220000  |
| H | 1.915510000  | -3.668310000 | -1.678230000 |
| C | 4.478870000  | -3.435900000 | -1.477390000 |
| H | 5.342540000  | -4.055980000 | -1.291990000 |
| H | 4.768450000  | -2.393230000 | -1.473940000 |
| H | 3.994110000  | -3.696430000 | -2.404130000 |
| O | 5.253490000  | -3.781240000 | 1.077400000  |
| N | 3.118420000  | -3.909720000 | 1.862130000  |
| S | 0.988410000  | -3.787040000 | 3.446060000  |
| F | 0.081320000  | -3.300460000 | 0.258140000  |

Coord\_10

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.481300000  | 0.000000000  | 0.000000000  |
| C | 2.433430000  | 0.000000000  | 1.468660000  |
| C | 1.222150000  | -0.033620000 | 2.058070000  |
| N | 0.021990000  | -0.029010000 | 1.361810000  |
| H | 1.227370000  | 0.069810000  | -1.600200000 |
| H | 1.119240000  | -0.057290000 | 3.124170000  |
| C | -1.254400000 | -0.188460000 | 2.052430000  |
| H | -1.962200000 | 0.524450000  | 1.657730000  |
| H | -1.096830000 | -0.000960000 | 3.102810000  |
| H | -1.622120000 | -1.195630000 | 1.928800000  |
| O | -0.998880000 | -0.003110000 | -0.658240000 |
| N | 1.242290000  | 0.037150000  | -0.600960000 |
| O | 3.481830000  | -0.047870000 | -0.659300000 |
| C | 3.737800000  | 0.038590000  | 2.219800000  |
| H | 4.385030000  | -0.784190000 | 1.937930000  |
| H | 4.281100000  | 0.952260000  | 2.006080000  |
| H | 3.566820000  | -0.020280000 | 3.287090000  |
| C | 4.037660000  | -3.756400000 | 0.893360000  |
| C | 1.765760000  | -3.804910000 | 1.787160000  |
| C | 1.321930000  | -3.607960000 | 0.555240000  |
| C | 2.213940000  | -3.551350000 | -0.649800000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 3.509500000 | -3.616400000 | -0.371260000 |
| H | 3.394270000 | -4.060180000 | 2.815130000  |
| H | 1.907040000 | -3.676860000 | -1.673080000 |
| C | 4.462230000 | -3.439570000 | -1.462900000 |
| H | 5.324310000 | -4.061240000 | -1.273310000 |
| H | 4.753190000 | -2.397220000 | -1.453940000 |
| H | 3.978530000 | -3.697240000 | -2.390650000 |
| O | 5.234300000 | -3.775090000 | 1.091130000  |
| N | 3.094510000 | -3.905760000 | 1.873000000  |
| S | 0.974250000 | -3.786780000 | 3.467750000  |
| F | 0.069920000 | -3.298430000 | 0.264220000  |

LIIC path connecting S1-MIN and T2-MIN

Coord\_1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478550000  | 0.000000000  | 0.000000000  |
| C | 2.438610000  | 0.000000000  | 1.471010000  |
| C | 1.230460000  | -0.003890000 | 2.061690000  |
| N | 0.026660000  | 0.007660000  | 1.363300000  |
| H | 1.224070000  | 0.030710000  | -1.600160000 |
| H | 1.126320000  | -0.010790000 | 3.128450000  |
| C | -1.249960000 | -0.094870000 | 2.059490000  |
| H | -1.953830000 | 0.602700000  | 1.633850000  |
| H | -1.095450000 | 0.144050000  | 3.101690000  |
| H | -1.653740000 | -1.095440000 | 1.976690000  |
| O | -1.009540000 | -0.025100000 | -0.643260000 |
| N | 1.238290000  | 0.022040000  | -0.602100000 |
| O | 3.479510000  | -0.024080000 | -0.655640000 |
| C | 3.743820000  | -0.004450000 | 2.218680000  |
| H | 4.322020000  | -0.891470000 | 1.988370000  |
| H | 4.344890000  | 0.854330000  | 1.943350000  |
| H | 3.573120000  | 0.023920000  | 3.288620000  |
| C | 3.336120000  | -4.000450000 | 1.986490000  |
| C | 1.041620000  | -4.020750000 | 2.885510000  |
| C | 0.561110000  | -3.899090000 | 1.602810000  |
| C | 1.411230000  | -3.838930000 | 0.519080000  |
| N | 2.794720000  | -3.920670000 | 0.733970000  |
| H | 2.853530000  | -4.244330000 | 3.901170000  |
| H | 1.064860000  | -3.799450000 | -0.490740000 |
| C | 3.679040000  | -3.848640000 | -0.421790000 |
| H | 4.675220000  | -4.109840000 | -0.110870000 |
| H | 3.685840000  | -2.849220000 | -0.839060000 |
| H | 3.342750000  | -4.551800000 | -1.174080000 |
| O | 4.514420000  | -4.067100000 | 2.201900000  |
| N | 2.438340000  | -3.997110000 | 3.031110000  |
| S | 0.060590000  | -3.844010000 | 4.348270000  |
| F | -0.753800000 | -3.808040000 | 1.411250000  |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478530000  | 0.000000000  | 0.000000000  |
| C | 2.438600000  | 0.000000000  | 1.471020000  |
| C | 1.230440000  | -0.004050000 | 2.061720000  |
| N | 0.026660000  | 0.007170000  | 1.363310000  |
| H | 1.224060000  | 0.030920000  | -1.600170000 |
| H | 1.126330000  | -0.010890000 | 3.128490000  |
| C | -1.250120000 | -0.095020000 | 2.059250000  |
| H | -1.952790000 | 0.605260000  | 1.636010000  |
| H | -1.095040000 | 0.140180000  | 3.102200000  |
| H | -1.655870000 | -1.094510000 | 1.973160000  |
| O | -1.009590000 | -0.024780000 | -0.643180000 |
| N | 1.238290000  | 0.022100000  | -0.602110000 |
| O | 3.479500000  | -0.024070000 | -0.655630000 |
| C | 3.743820000  | -0.004180000 | 2.218700000  |
| H | 4.321830000  | -0.891520000 | 1.989120000  |
| H | 4.345050000  | 0.854260000  | 1.942690000  |
| H | 3.573110000  | 0.025140000  | 3.288620000  |
| C | 3.333210000  | -3.997890000 | 1.983320000  |
| C | 1.037590000  | -4.018790000 | 2.879810000  |
| C | 0.558640000  | -3.898470000 | 1.596020000  |
| C | 1.410180000  | -3.839470000 | 0.513610000  |
| N | 2.793280000  | -3.922390000 | 0.729880000  |
| H | 2.848540000  | -4.225900000 | 3.900150000  |
| H | 1.064880000  | -3.801500000 | -0.496640000 |
| C | 3.679510000  | -3.848840000 | -0.424380000 |
| H | 4.674050000  | -4.116320000 | -0.113520000 |
| H | 3.691730000  | -2.847560000 | -0.837100000 |
| H | 3.340630000  | -4.546900000 | -1.180180000 |
| O | 4.511530000  | -4.058670000 | 2.200480000  |
| N | 2.432790000  | -3.997400000 | 3.025310000  |
| S | 0.054030000  | -3.850380000 | 4.340680000  |
| F | -0.755970000 | -3.808750000 | 1.402390000  |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478510000  | 0.000000000  | 0.000000000  |
| C | 2.438580000  | 0.000000000  | 1.471030000  |
| C | 1.230420000  | -0.004210000 | 2.061750000  |
| N | 0.026660000  | 0.006680000  | 1.363320000  |
| H | 1.224050000  | 0.031140000  | -1.600180000 |
| H | 1.126330000  | -0.010990000 | 3.128520000  |
| C | -1.250280000 | -0.095180000 | 2.059010000  |
| H | -1.951740000 | 0.607800000  | 1.638170000  |
| H | -1.094650000 | 0.136300000  | 3.102710000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.658000000 | -1.093570000 | 1.969630000  |
| O | -1.009640000 | -0.024460000 | -0.643090000 |
| N | 1.238280000  | 0.022150000  | -0.602120000 |
| O | 3.479490000  | -0.024060000 | -0.655610000 |
| C | 3.743820000  | -0.003910000 | 2.218710000  |
| H | 4.321640000  | -0.891570000 | 1.989880000  |
| H | 4.345220000  | 0.854190000  | 1.942030000  |
| H | 3.573090000  | 0.026360000  | 3.288610000  |
| C | 3.330330000  | -3.995320000 | 1.980150000  |
| C | 1.033580000  | -4.016830000 | 2.874100000  |
| C | 0.556200000  | -3.897860000 | 1.589220000  |
| C | 1.409160000  | -3.840020000 | 0.508150000  |
| N | 2.791870000  | -3.924110000 | 0.725800000  |
| H | 2.843630000  | -4.207440000 | 3.899000000  |
| H | 1.064930000  | -3.803560000 | -0.502540000 |
| C | 3.679980000  | -3.849030000 | -0.426970000 |
| H | 4.672870000  | -4.122790000 | -0.116220000 |
| H | 3.697590000  | -2.845950000 | -0.835110000 |
| H | 3.338530000  | -4.541970000 | -1.186260000 |
| O | 4.508630000  | -4.050230000 | 2.199060000  |
| N | 2.427500000  | -3.997730000 | 3.019700000  |
| S | 0.047470000  | -3.856720000 | 4.333020000  |
| F | -0.758110000 | -3.809470000 | 1.393530000  |

Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478490000  | 0.000000000  | 0.000000000  |
| C | 2.438570000  | 0.000000000  | 1.471050000  |
| C | 1.230400000  | -0.004370000 | 2.061780000  |
| N | 0.026660000  | 0.006180000  | 1.363330000  |
| H | 1.224050000  | 0.031360000  | -1.600190000 |
| H | 1.126330000  | -0.011080000 | 3.128560000  |
| C | -1.250440000 | -0.095330000 | 2.058770000  |
| H | -1.950680000 | 0.610340000  | 1.640350000  |
| H | -1.094260000 | 0.132410000  | 3.103200000  |
| H | -1.660130000 | -1.092610000 | 1.966110000  |
| O | -1.009690000 | -0.024140000 | -0.643000000 |
| N | 1.238270000  | 0.022200000  | -0.602130000 |
| O | 3.479480000  | -0.024050000 | -0.655600000 |
| C | 3.743820000  | -0.003640000 | 2.218730000  |
| H | 4.321450000  | -0.891620000 | 1.990640000  |
| H | 4.345380000  | 0.854110000  | 1.941370000  |
| H | 3.573080000  | 0.027580000  | 3.288610000  |
| C | 3.327460000  | -3.992750000 | 1.976980000  |
| C | 1.029590000  | -4.014870000 | 2.868380000  |
| C | 0.553780000  | -3.897250000 | 1.582410000  |
| C | 1.408160000  | -3.840570000 | 0.502680000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 2.790480000  | -3.925830000 | 0.721740000  |
| H | 2.838790000  | -4.188960000 | 3.897730000  |
| H | 1.065010000  | -3.805620000 | -0.508450000 |
| C | 3.680440000  | -3.849220000 | -0.429560000 |
| H | 4.671660000  | -4.129230000 | -0.118990000 |
| H | 3.703440000  | -2.844380000 | -0.833100000 |
| H | 3.336440000  | -4.537000000 | -1.192310000 |
| O | 4.505720000  | -4.041780000 | 2.197640000  |
| N | 2.422490000  | -3.998080000 | 3.014290000  |
| S | 0.040920000  | -3.863040000 | 4.325280000  |
| F | -0.760220000 | -3.810190000 | 1.384660000  |

Coord\_5

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478470000  | 0.000000000  | 0.000000000  |
| C | 2.438550000  | 0.000000000  | 1.471060000  |
| C | 1.230390000  | -0.004530000 | 2.061810000  |
| N | 0.026660000  | 0.005690000  | 1.363340000  |
| H | 1.224040000  | 0.031580000  | -1.600200000 |
| H | 1.126330000  | -0.011180000 | 3.128590000  |
| C | -1.250610000 | -0.095480000 | 2.058530000  |
| H | -1.949620000 | 0.612870000  | 1.642540000  |
| H | -1.093880000 | 0.128530000  | 3.103680000  |
| H | -1.662260000 | -1.091640000 | 1.962580000  |
| O | -1.009730000 | -0.023830000 | -0.642920000 |
| N | 1.238260000  | 0.022250000  | -0.602130000 |
| O | 3.479470000  | -0.024050000 | -0.655580000 |
| C | 3.743820000  | -0.003380000 | 2.218740000  |
| H | 4.321260000  | -0.891670000 | 1.991390000  |
| H | 4.345550000  | 0.854040000  | 1.940710000  |
| H | 3.573060000  | 0.028800000  | 3.288600000  |
| C | 3.324610000  | -3.990180000 | 1.973810000  |
| C | 1.025620000  | -4.012910000 | 2.862650000  |
| C | 0.551390000  | -3.896640000 | 1.575600000  |
| C | 1.407190000  | -3.841110000 | 0.497220000  |
| N | 2.789100000  | -3.927540000 | 0.717680000  |
| H | 2.834020000  | -4.170450000 | 3.896330000  |
| H | 1.065130000  | -3.807680000 | -0.514350000 |
| C | 3.680900000  | -3.849410000 | -0.432140000 |
| H | 4.670430000  | -4.135660000 | -0.121820000 |
| H | 3.709260000  | -2.842850000 | -0.831060000 |
| H | 3.334350000  | -4.532000000 | -1.198330000 |
| O | 4.502800000  | -4.033330000 | 2.196220000  |
| N | 2.417740000  | -3.998460000 | 3.009070000  |
| S | 0.034370000  | -3.869340000 | 4.317460000  |
| F | -0.762300000 | -3.810920000 | 1.375770000  |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478450000  | 0.000000000  | 0.000000000  |
| C | 2.438530000  | 0.000000000  | 1.471070000  |
| C | 1.230370000  | -0.004690000 | 2.061840000  |
| N | 0.026660000  | 0.005190000  | 1.363350000  |
| H | 1.224040000  | 0.031800000  | -1.600210000 |
| H | 1.126330000  | -0.011280000 | 3.128620000  |
| C | -1.250770000 | -0.095630000 | 2.058290000  |
| H | -1.948560000 | 0.615380000  | 1.644730000  |
| H | -1.093500000 | 0.124640000  | 3.104150000  |
| H | -1.664380000 | -1.090650000 | 1.959070000  |
| O | -1.009780000 | -0.023510000 | -0.642830000 |
| N | 1.238250000  | 0.022300000  | -0.602140000 |
| O | 3.479460000  | -0.024040000 | -0.655570000 |
| C | 3.743820000  | -0.003110000 | 2.218760000  |
| H | 4.321060000  | -0.891710000 | 1.992150000  |
| H | 4.345720000  | 0.853970000  | 1.940050000  |
| H | 3.573040000  | 0.030020000  | 3.288600000  |
| C | 3.321780000  | -3.987600000 | 1.970640000  |
| C | 1.021670000  | -4.010950000 | 2.856900000  |
| C | 0.549020000  | -3.896030000 | 1.568770000  |
| C | 1.406250000  | -3.841660000 | 0.491740000  |
| N | 2.787750000  | -3.929260000 | 0.713650000  |
| H | 2.829320000  | -4.151910000 | 3.894810000  |
| H | 1.065270000  | -3.809740000 | -0.520250000 |
| C | 3.681350000  | -3.849590000 | -0.434720000 |
| H | 4.669170000  | -4.142080000 | -0.124700000 |
| H | 3.715070000  | -2.841360000 | -0.829000000 |
| H | 3.332280000  | -4.526970000 | -1.204330000 |
| O | 4.499860000  | -4.024870000 | 2.194790000  |
| N | 2.413250000  | -3.998850000 | 3.004050000  |
| S | 0.027820000  | -3.875610000 | 4.309560000  |
| F | -0.764350000 | -3.811660000 | 1.366880000  |

Coord\_7

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478440000  | 0.000000000  | 0.000000000  |
| C | 2.438520000  | 0.000000000  | 1.471080000  |
| C | 1.230350000  | -0.004850000 | 2.061870000  |
| N | 0.026650000  | 0.004700000  | 1.363360000  |
| H | 1.224030000  | 0.032020000  | -1.600220000 |
| H | 1.126330000  | -0.011380000 | 3.128660000  |
| C | -1.250930000 | -0.095780000 | 2.058060000  |
| H | -1.947480000 | 0.617890000  | 1.646930000  |
| H | -1.093140000 | 0.120740000  | 3.104600000  |
| H | -1.666500000 | -1.089650000 | 1.955550000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -1.009830000 | -0.023190000 | -0.642740000 |
| N | 1.238240000  | 0.022350000  | -0.602150000 |
| O | 3.479450000  | -0.024030000 | -0.655560000 |
| C | 3.743820000  | -0.002840000 | 2.218770000  |
| H | 4.320870000  | -0.891760000 | 1.992910000  |
| H | 4.345880000  | 0.853900000  | 1.939400000  |
| H | 3.573030000  | 0.031240000  | 3.288590000  |
| C | 3.318970000  | -3.985020000 | 1.967460000  |
| C | 1.017740000  | -4.008990000 | 2.851150000  |
| C | 0.546680000  | -3.895430000 | 1.561940000  |
| C | 1.405330000  | -3.842210000 | 0.486270000  |
| N | 2.786410000  | -3.930970000 | 0.709620000  |
| H | 2.824690000  | -4.133360000 | 3.893170000  |
| H | 1.065440000  | -3.811800000 | -0.526150000 |
| C | 3.681800000  | -3.849780000 | -0.437310000 |
| H | 4.667890000  | -4.148470000 | -0.127650000 |
| H | 3.720850000  | -2.839920000 | -0.826920000 |
| H | 3.330210000  | -4.521900000 | -1.210300000 |
| O | 4.496900000  | -4.016400000 | 2.193370000  |
| N | 2.409030000  | -3.999250000 | 2.999230000  |
| S | 0.021280000  | -3.881860000 | 4.301590000  |
| F | -0.766370000 | -3.812400000 | 1.357970000  |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478420000  | 0.000000000  | 0.000000000  |
| C | 2.438500000  | 0.000000000  | 1.471100000  |
| C | 1.230330000  | -0.005010000 | 2.061900000  |
| N | 0.026650000  | 0.004210000  | 1.363370000  |
| H | 1.224030000  | 0.032240000  | -1.600230000 |
| H | 1.126330000  | -0.011480000 | 3.128690000  |
| C | -1.251090000 | -0.095940000 | 2.057820000  |
| H | -1.946410000 | 0.620390000  | 1.649140000  |
| H | -1.092780000 | 0.116840000  | 3.105050000  |
| H | -1.668620000 | -1.088630000 | 1.952040000  |
| O | -1.009880000 | -0.022870000 | -0.642650000 |
| N | 1.238230000  | 0.022400000  | -0.602160000 |
| O | 3.479440000  | -0.024020000 | -0.655540000 |
| C | 3.743820000  | -0.002570000 | 2.218790000  |
| H | 4.320680000  | -0.891810000 | 1.993670000  |
| H | 4.346050000  | 0.853820000  | 1.938740000  |
| H | 3.573010000  | 0.032460000  | 3.288580000  |
| C | 3.316180000  | -3.982440000 | 1.964280000  |
| C | 1.013820000  | -4.007040000 | 2.845390000  |
| C | 0.544360000  | -3.894830000 | 1.555100000  |
| C | 1.404440000  | -3.842750000 | 0.480800000  |
| N | 2.785100000  | -3.932680000 | 0.705610000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2.820150000  | -4.114780000 | 3.891410000  |
| H | 1.065650000  | -3.813860000 | -0.532060000 |
| C | 3.682240000  | -3.849960000 | -0.439890000 |
| H | 4.666590000  | -4.154850000 | -0.130650000 |
| H | 3.726620000  | -2.838510000 | -0.824810000 |
| H | 3.328150000  | -4.516790000 | -1.216250000 |
| O | 4.493930000  | -4.007930000 | 2.191940000  |
| N | 2.405070000  | -3.999650000 | 2.994620000  |
| S | 0.014750000  | -3.888090000 | 4.293540000  |
| F | -0.768360000 | -3.813150000 | 1.349060000  |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478400000  | 0.000000000  | 0.000000000  |
| C | 2.438490000  | 0.000000000  | 1.471110000  |
| C | 1.230310000  | -0.005170000 | 2.061930000  |
| N | 0.026650000  | 0.003710000  | 1.363380000  |
| H | 1.224020000  | 0.032450000  | -1.600240000 |
| H | 1.126340000  | -0.011580000 | 3.128730000  |
| C | -1.251250000 | -0.096090000 | 2.057580000  |
| H | -1.945320000 | 0.622870000  | 1.651360000  |
| H | -1.092430000 | 0.112940000  | 3.105480000  |
| H | -1.670730000 | -1.087600000 | 1.948530000  |
| O | -1.009930000 | -0.022560000 | -0.642560000 |
| N | 1.238220000  | 0.022450000  | -0.602170000 |
| O | 3.479430000  | -0.024020000 | -0.655530000 |
| C | 3.743820000  | -0.002300000 | 2.218800000  |
| H | 4.320490000  | -0.891850000 | 1.994420000  |
| H | 4.346210000  | 0.853750000  | 1.938080000  |
| H | 3.573000000  | 0.033670000  | 3.288570000  |
| C | 3.313400000  | -3.979860000 | 1.961090000  |
| C | 1.009930000  | -4.005090000 | 2.839620000  |
| C | 0.542070000  | -3.894240000 | 1.548250000  |
| C | 1.403580000  | -3.843300000 | 0.475320000  |
| N | 2.783800000  | -3.934390000 | 0.701610000  |
| H | 2.815670000  | -4.096170000 | 3.889530000  |
| H | 1.065880000  | -3.815930000 | -0.537960000 |
| C | 3.682680000  | -3.850140000 | -0.442470000 |
| H | 4.665260000  | -4.161220000 | -0.133710000 |
| H | 3.732360000  | -2.837140000 | -0.822690000 |
| H | 3.326090000  | -4.511650000 | -1.222170000 |
| O | 4.490950000  | -3.999450000 | 2.190520000  |
| N | 2.401370000  | -4.000040000 | 2.990200000  |
| S | 0.008210000  | -3.894290000 | 4.285420000  |
| F | -0.770320000 | -3.813910000 | 1.340140000  |

Coord\_10



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.00000000  | 0.00000000  | 0.00000000  |
| C | 2.47838000  | 0.00000000  | 0.00000000  |
| C | 2.43847000  | 0.00000000  | 1.47112000  |
| C | 1.23029000  | -0.00533000 | 2.06195000  |
| N | 0.02665000  | 0.00322000  | 1.36339000  |
| H | 1.22402000  | 0.03267000  | -1.60024000 |
| H | 1.12634000  | -0.01168000 | 3.12876000  |
| C | -1.25142000 | -0.09624000 | 2.05734000  |
| H | -1.94424000 | 0.62535000  | 1.65358000  |
| H | -1.09209000 | 0.10904000  | 3.10590000  |
| H | -1.67285000 | -1.08655000 | 1.94503000  |
| O | -1.00997000 | -0.02224000 | -0.64248000 |
| N | 1.23821000  | 0.02250000  | -0.60218000 |
| O | 3.47942000  | -0.02401000 | -0.65551000 |
| C | 3.74382000  | -0.00204000 | 2.21882000  |
| H | 4.32030000  | -0.89189000 | 1.99518000  |
| H | 4.34638000  | 0.85367000  | 1.93742000  |
| H | 3.57298000  | 0.03489000  | 3.28856000  |
| C | 3.31065000  | -3.97727000 | 1.95790000  |
| C | 1.00605000  | -4.00314000 | 2.83384000  |
| C | 0.53981000  | -3.89365000 | 1.54139000  |
| C | 1.40274000  | -3.84385000 | 0.46984000  |
| N | 2.78252000  | -3.93609000 | 0.69763000  |
| H | 2.81128000  | -4.07755000 | 3.88752000  |
| H | 1.06615000  | -3.81799000 | -0.54386000 |
| C | 3.68311000  | -3.85032000 | -0.44505000 |
| H | 4.66391000  | -4.16756000 | -0.13684000 |
| H | 3.73808000  | -2.83582000 | -0.82054000 |
| H | 3.32405000  | -4.50648000 | -1.22806000 |
| O | 4.48796000  | -3.99097000 | 2.18909000  |
| N | 2.39793000  | -4.00041000 | 2.98598000  |
| S | 0.00169000  | -3.90046000 | 4.27722000  |
| F | -0.77225000 | -3.81467000 | 1.33120000  |

LIIC path connecting S1-MIN and T1-MIN

Coord\_1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.00000000  | 0.00000000  | 0.00000000  |
| C | 2.47855000  | 0.00000000  | 0.00000000  |
| C | 2.43861000  | 0.00000000  | 1.47101000  |
| C | 1.23046000  | -0.00389000 | 2.06169000  |
| N | 0.02666000  | 0.00766000  | 1.36330000  |
| H | 1.22407000  | 0.03071000  | -1.60016000 |
| H | 1.12632000  | -0.01079000 | 3.12845000  |
| C | -1.24996000 | -0.09487000 | 2.05949000  |
| H | -1.95383000 | 0.60270000  | 1.63385000  |
| H | -1.09545000 | 0.14405000  | 3.10169000  |
| H | -1.65374000 | -1.09544000 | 1.97669000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -1.009540000 | -0.025100000 | -0.643260000 |
| N | 1.238290000  | 0.022040000  | -0.602100000 |
| O | 3.479510000  | -0.024080000 | -0.655640000 |
| C | 3.743820000  | -0.004450000 | 2.218680000  |
| H | 4.322020000  | -0.891470000 | 1.988370000  |
| H | 4.344890000  | 0.854330000  | 1.943350000  |
| H | 3.573120000  | 0.023920000  | 3.288620000  |
| C | 3.336120000  | -4.000450000 | 1.986490000  |
| C | 1.041620000  | -4.020750000 | 2.885510000  |
| C | 0.561110000  | -3.899090000 | 1.602810000  |
| C | 1.411230000  | -3.838930000 | 0.519080000  |
| N | 2.794720000  | -3.920670000 | 0.733970000  |
| H | 2.853530000  | -4.244330000 | 3.901170000  |
| H | 1.064860000  | -3.799450000 | -0.490740000 |
| C | 3.679040000  | -3.848640000 | -0.421790000 |
| H | 4.675220000  | -4.109840000 | -0.110870000 |
| H | 3.685840000  | -2.849220000 | -0.839060000 |
| H | 3.342750000  | -4.551800000 | -1.174080000 |
| O | 4.514420000  | -4.067100000 | 2.201900000  |
| N | 2.438340000  | -3.997110000 | 3.031110000  |
| S | 0.060590000  | -3.844010000 | 4.348270000  |
| F | -0.753800000 | -3.808040000 | 1.411250000  |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478610000  | 0.000000000  | 0.000000000  |
| C | 2.438750000  | 0.000000000  | 1.471030000  |
| C | 1.230560000  | -0.003370000 | 2.061640000  |
| N | 0.026700000  | 0.008350000  | 1.363370000  |
| H | 1.224130000  | 0.030770000  | -1.600080000 |
| H | 1.126410000  | -0.009450000 | 3.128430000  |
| C | -1.249250000 | -0.095710000 | 2.060660000  |
| H | -1.957920000 | 0.591240000  | 1.626060000  |
| H | -1.097050000 | 0.157540000  | 3.099860000  |
| H | -1.645480000 | -1.100300000 | 1.990170000  |
| O | -1.009300000 | -0.025790000 | -0.643560000 |
| N | 1.238380000  | 0.022320000  | -0.602020000 |
| O | 3.479600000  | -0.024240000 | -0.655600000 |
| C | 3.744000000  | -0.004620000 | 2.218630000  |
| H | 4.321960000  | -0.891850000 | 1.988380000  |
| H | 4.345300000  | 0.853910000  | 1.943060000  |
| H | 3.573440000  | 0.024050000  | 3.288590000  |
| C | 3.338730000  | -4.008370000 | 1.977640000  |
| C | 1.046390000  | -4.025170000 | 2.883640000  |
| C | 0.562190000  | -3.898780000 | 1.604450000  |
| C | 1.411020000  | -3.835560000 | 0.515530000  |
| N | 2.793540000  | -3.924840000 | 0.726210000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2.859850000  | -4.245320000 | 3.895540000  |
| H | 1.060440000  | -3.798090000 | -0.492870000 |
| C | 3.676230000  | -3.847770000 | -0.430670000 |
| H | 4.669480000  | -4.127370000 | -0.126400000 |
| H | 3.695840000  | -2.842640000 | -0.833540000 |
| H | 3.327860000  | -4.535160000 | -1.191850000 |
| O | 4.517970000  | -4.072800000 | 2.188430000  |
| N | 2.442650000  | -4.012650000 | 3.022470000  |
| S | 0.072080000  | -3.876880000 | 4.352400000  |
| F | -0.751470000 | -3.806140000 | 1.411810000  |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478680000  | 0.000000000  | 0.000000000  |
| C | 2.438890000  | 0.000000000  | 1.471060000  |
| C | 1.230660000  | -0.002850000 | 2.061580000  |
| N | 0.026730000  | 0.009030000  | 1.363430000  |
| H | 1.224200000  | 0.030830000  | -1.600010000 |
| H | 1.126490000  | -0.008110000 | 3.128410000  |
| C | -1.248540000 | -0.096540000 | 2.061820000  |
| H | -1.961920000 | 0.579640000  | 1.618410000  |
| H | -1.098790000 | 0.170980000  | 3.097870000  |
| H | -1.637180000 | -1.104960000 | 2.003680000  |
| O | -1.009060000 | -0.026480000 | -0.643850000 |
| N | 1.238470000  | 0.022600000  | -0.601940000 |
| O | 3.479690000  | -0.024400000 | -0.655550000 |
| C | 3.744180000  | -0.004790000 | 2.218570000  |
| H | 4.321890000  | -0.892230000 | 1.988380000  |
| H | 4.345710000  | 0.853490000  | 1.942770000  |
| H | 3.573760000  | 0.024180000  | 3.288560000  |
| C | 3.341400000  | -4.016280000 | 1.968790000  |
| C | 1.051240000  | -4.029620000 | 2.881780000  |
| C | 0.563360000  | -3.898540000 | 1.606130000  |
| C | 1.410880000  | -3.832240000 | 0.512040000  |
| N | 2.792410000  | -3.929030000 | 0.718460000  |
| H | 2.866210000  | -4.246270000 | 3.889860000  |
| H | 1.056120000  | -3.796820000 | -0.494950000 |
| C | 3.673450000  | -3.846920000 | -0.439520000 |
| H | 4.663530000  | -4.144760000 | -0.142230000 |
| H | 3.705950000  | -2.836490000 | -0.827990000 |
| H | 3.313150000  | -4.518280000 | -1.209280000 |
| O | 4.521560000  | -4.078430000 | 2.174960000  |
| N | 2.447220000  | -4.028160000 | 3.013930000  |
| S | 0.083290000  | -3.909840000 | 4.355700000  |
| F | -0.749040000 | -3.804310000 | 1.412430000  |

Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478740000  | 0.000000000  | 0.000000000  |
| C | 2.439020000  | 0.000000000  | 1.471090000  |
| C | 1.230760000  | -0.002330000 | 2.061530000  |
| N | 0.026770000  | 0.009720000  | 1.363500000  |
| H | 1.224260000  | 0.030890000  | -1.599940000 |
| H | 1.126570000  | -0.006770000 | 3.128390000  |
| C | -1.247820000 | -0.097370000 | 2.062990000  |
| H | -1.965840000 | 0.567890000  | 1.610870000  |
| H | -1.100650000 | 0.184350000  | 3.095690000  |
| H | -1.628840000 | -1.109400000 | 2.017240000  |
| O | -1.008820000 | -0.027180000 | -0.644150000 |
| N | 1.238550000  | 0.022870000  | -0.601860000 |
| O | 3.479790000  | -0.024560000 | -0.655500000 |
| C | 3.744370000  | -0.004960000 | 2.218520000  |
| H | 4.321820000  | -0.892600000 | 1.988390000  |
| H | 4.346120000  | 0.853080000  | 1.942480000  |
| H | 3.574090000  | 0.024310000  | 3.288530000  |
| C | 3.344100000  | -4.024170000 | 1.959930000  |
| C | 1.056170000  | -4.034090000 | 2.879940000  |
| C | 0.564640000  | -3.898380000 | 1.607850000  |
| C | 1.410820000  | -3.828980000 | 0.508580000  |
| N | 2.791330000  | -3.933230000 | 0.710720000  |
| H | 2.872620000  | -4.247160000 | 3.884130000  |
| H | 1.051900000  | -3.795640000 | -0.496970000 |
| C | 3.670710000  | -3.846080000 | -0.448340000 |
| H | 4.657360000  | -4.162000000 | -0.158340000 |
| H | 3.716180000  | -2.830750000 | -0.822400000 |
| H | 3.298630000  | -4.501160000 | -1.226360000 |
| O | 4.525160000  | -4.083990000 | 2.161490000  |
| N | 2.452030000  | -4.043630000 | 3.005510000  |
| S | 0.094200000  | -3.942860000 | 4.358180000  |
| F | -0.746500000 | -3.802570000 | 1.413090000  |

Coord\_5

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478810000  | 0.000000000  | 0.000000000  |
| C | 2.439160000  | 0.000000000  | 1.471110000  |
| C | 1.230860000  | -0.001800000 | 2.061470000  |
| N | 0.026800000  | 0.010410000  | 1.363570000  |
| H | 1.224330000  | 0.030950000  | -1.599860000 |
| H | 1.126660000  | -0.005430000 | 3.128370000  |
| C | -1.247100000 | -0.098200000 | 2.064150000  |
| H | -1.969660000 | 0.556000000  | 1.603470000  |
| H | -1.102640000 | 0.197650000  | 3.093350000  |
| H | -1.620460000 | -1.113640000 | 2.030830000  |
| O | -1.008580000 | -0.027870000 | -0.644440000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 1.238640000  | 0.023150000  | -0.601780000 |
| O | 3.479880000  | -0.024720000 | -0.655450000 |
| C | 3.744550000  | -0.005140000 | 2.218470000  |
| H | 4.321750000  | -0.892980000 | 1.988400000  |
| H | 4.346530000  | 0.852660000  | 1.942200000  |
| H | 3.574410000  | 0.024440000  | 3.288490000  |
| C | 3.346860000  | -4.032030000 | 1.951060000  |
| C | 1.061190000  | -4.038590000 | 2.878120000  |
| C | 0.566010000  | -3.898290000 | 1.609600000  |
| C | 1.410830000  | -3.825770000 | 0.505180000  |
| N | 2.790280000  | -3.937450000 | 0.703000000  |
| H | 2.879060000  | -4.248000000 | 3.878360000  |
| H | 1.047780000  | -3.794540000 | -0.498930000 |
| C | 3.668010000  | -3.845270000 | -0.457130000 |
| H | 4.650980000  | -4.179090000 | -0.174720000 |
| H | 3.726520000  | -2.825430000 | -0.816780000 |
| H | 3.284310000  | -4.483800000 | -1.243090000 |
| O | 4.528790000  | -4.089490000 | 2.148030000  |
| N | 2.457090000  | -4.059060000 | 2.997190000  |
| S | 0.104810000  | -3.975900000 | 4.359830000  |
| F | -0.743860000 | -3.800890000 | 1.413790000  |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478870000  | 0.000000000  | 0.000000000  |
| C | 2.439290000  | 0.000000000  | 1.471140000  |
| C | 1.230960000  | -0.001280000 | 2.061410000  |
| N | 0.026840000  | 0.011090000  | 1.363630000  |
| H | 1.224400000  | 0.031010000  | -1.599790000 |
| H | 1.126740000  | -0.004090000 | 3.128350000  |
| C | -1.246380000 | -0.099020000 | 2.065320000  |
| H | -1.973390000 | 0.543970000  | 1.596190000  |
| H | -1.104750000 | 0.210880000  | 3.090820000  |
| H | -1.612040000 | -1.117670000 | 2.044440000  |
| O | -1.008340000 | -0.028560000 | -0.644730000 |
| N | 1.238730000  | 0.023430000  | -0.601700000 |
| O | 3.479970000  | -0.024880000 | -0.655400000 |
| C | 3.744730000  | -0.005310000 | 2.218410000  |
| H | 4.321680000  | -0.893360000 | 1.988410000  |
| H | 4.346930000  | 0.852240000  | 1.941910000  |
| H | 3.574730000  | 0.024570000  | 3.288460000  |
| C | 3.349660000  | -4.039880000 | 1.942170000  |
| C | 1.066300000  | -4.043110000 | 2.876300000  |
| C | 0.567490000  | -3.898270000 | 1.611400000  |
| C | 1.410920000  | -3.822600000 | 0.501810000  |
| N | 2.789290000  | -3.941690000 | 0.695290000  |
| H | 2.885540000  | -4.248780000 | 3.872550000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1.043760000  | -3.793530000 | -0.500830000 |
| C | 3.665340000  | -3.844480000 | -0.465890000 |
| H | 4.644380000  | -4.196020000 | -0.191380000 |
| H | 3.736970000  | -2.820530000 | -0.811150000 |
| H | 3.270170000  | -4.466210000 | -1.259470000 |
| O | 4.532440000  | -4.094930000 | 2.134570000  |
| N | 2.462390000  | -4.074440000 | 2.988980000  |
| S | 0.115120000  | -4.008950000 | 4.360670000  |
| F | -0.741120000 | -3.799300000 | 1.414540000  |

Coord\_7

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478930000  | 0.000000000  | 0.000000000  |
| C | 2.439430000  | 0.000000000  | 1.471170000  |
| C | 1.231060000  | -0.000760000 | 2.061360000  |
| N | 0.026870000  | 0.011780000  | 1.363700000  |
| H | 1.224460000  | 0.031070000  | -1.599720000 |
| H | 1.126830000  | -0.002750000 | 3.128330000  |
| C | -1.245650000 | -0.099840000 | 2.066490000  |
| H | -1.977030000 | 0.531790000  | 1.589040000  |
| H | -1.106990000 | 0.224050000  | 3.088130000  |
| H | -1.603590000 | -1.121480000 | 2.058090000  |
| O | -1.008100000 | -0.029260000 | -0.645020000 |
| N | 1.238810000  | 0.023710000  | -0.601620000 |
| O | 3.480060000  | -0.025040000 | -0.655350000 |
| C | 3.744910000  | -0.005480000 | 2.218360000  |
| H | 4.321620000  | -0.893730000 | 1.988420000  |
| H | 4.347340000  | 0.851830000  | 1.941620000  |
| H | 3.575050000  | 0.024700000  | 3.288430000  |
| C | 3.352510000  | -4.047720000 | 1.933280000  |
| C | 1.071480000  | -4.047660000 | 2.874500000  |
| C | 0.569070000  | -3.898320000 | 1.613220000  |
| C | 1.411080000  | -3.819500000 | 0.498480000  |
| N | 2.788330000  | -3.945940000 | 0.687580000  |
| H | 2.892070000  | -4.249510000 | 3.866690000  |
| H | 1.039850000  | -3.792600000 | -0.502690000 |
| C | 3.662710000  | -3.843700000 | -0.474610000 |
| H | 4.637580000  | -4.212780000 | -0.208310000 |
| H | 3.747510000  | -2.816040000 | -0.805510000 |
| H | 3.256240000  | -4.448410000 | -1.275490000 |
| O | 4.536110000  | -4.100310000 | 2.121120000  |
| N | 2.467940000  | -4.089770000 | 2.980870000  |
| S | 0.125110000  | -4.041970000 | 4.360710000  |
| F | -0.738270000 | -3.797780000 | 1.415340000  |

Coord\_8

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
|---|-------------|-------------|-------------|

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.479000000  | 0.000000000  | 0.000000000  |
| C | 2.439570000  | 0.000000000  | 1.471190000  |
| C | 1.231160000  | -0.000240000 | 2.061300000  |
| N | 0.026900000  | 0.012460000  | 1.363760000  |
| H | 1.224530000  | 0.031130000  | -1.599640000 |
| H | 1.126920000  | -0.001410000 | 3.128300000  |
| C | -1.244930000 | -0.100660000 | 2.067660000  |
| H | -1.980570000 | 0.519480000  | 1.582020000  |
| H | -1.109360000 | 0.237130000  | 3.085270000  |
| H | -1.595100000 | -1.125080000 | 2.071770000  |
| O | -1.007860000 | -0.029950000 | -0.645310000 |
| N | 1.238900000  | 0.023980000  | -0.601540000 |
| O | 3.480150000  | -0.025200000 | -0.655300000 |
| C | 3.745090000  | -0.005650000 | 2.218310000  |
| H | 4.321550000  | -0.894110000 | 1.988420000  |
| H | 4.347750000  | 0.851410000  | 1.941330000  |
| H | 3.575370000  | 0.024830000  | 3.288400000  |
| C | 3.355410000  | -4.055530000 | 1.924380000  |
| C | 1.076760000  | -4.052240000 | 2.872710000  |
| C | 0.570750000  | -3.898450000 | 1.615090000  |
| C | 1.411320000  | -3.816440000 | 0.495200000  |
| N | 2.787420000  | -3.950210000 | 0.679900000  |
| H | 2.898630000  | -4.250180000 | 3.860790000  |
| H | 1.036030000  | -3.791760000 | -0.504480000 |
| C | 3.660120000  | -3.842950000 | -0.483310000 |
| H | 4.630560000  | -4.229370000 | -0.225500000 |
| H | 3.758160000  | -2.811970000 | -0.799870000 |
| H | 3.242510000  | -4.430390000 | -1.291140000 |
| O | 4.539810000  | -4.105620000 | 2.107670000  |
| N | 2.473730000  | -4.105040000 | 2.972870000  |
| S | 0.134790000  | -4.074940000 | 4.359940000  |
| F | -0.735320000 | -3.796340000 | 1.416170000  |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.479060000  | 0.000000000  | 0.000000000  |
| C | 2.439700000  | 0.000000000  | 1.471220000  |
| C | 1.231260000  | 0.000290000  | 2.061250000  |
| N | 0.026940000  | 0.013150000  | 1.363830000  |
| H | 1.224600000  | 0.031190000  | -1.599570000 |
| H | 1.127000000  | -0.000070000 | 3.128280000  |
| C | -1.244190000 | -0.101480000 | 2.068830000  |
| H | -1.984020000 | 0.507040000  | 1.575140000  |
| H | -1.111850000 | 0.250140000  | 3.082240000  |
| H | -1.586590000 | -1.128470000 | 2.085470000  |
| O | -1.007620000 | -0.030650000 | -0.645600000 |
| N | 1.238990000  | 0.024260000  | -0.601460000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | 3.480240000  | -0.025360000 | -0.655250000 |
| C | 3.745280000  | -0.005820000 | 2.218250000  |
| H | 4.321480000  | -0.894480000 | 1.988430000  |
| H | 4.348160000  | 0.850990000  | 1.941040000  |
| H | 3.575700000  | 0.024960000  | 3.288360000  |
| C | 3.358350000  | -4.063320000 | 1.915470000  |
| C | 1.082120000  | -4.056840000 | 2.870930000  |
| C | 0.572530000  | -3.898640000 | 1.616980000  |
| C | 1.411630000  | -3.813440000 | 0.491950000  |
| N | 2.786550000  | -3.954500000 | 0.672220000  |
| H | 2.905230000  | -4.250800000 | 3.854840000  |
| H | 1.032320000  | -3.791000000 | -0.506230000 |
| C | 3.657560000  | -3.842210000 | -0.491970000 |
| H | 4.623320000  | -4.245770000 | -0.242950000 |
| H | 3.768900000  | -2.808320000 | -0.794230000 |
| H | 3.228980000  | -4.412170000 | -1.306440000 |
| O | 4.543530000  | -4.110880000 | 2.094230000  |
| N | 2.479770000  | -4.120250000 | 2.964970000  |
| S | 0.144150000  | -4.107820000 | 4.358370000  |
| F | -0.732270000 | -3.794970000 | 1.417050000  |

Coord\_10

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.479130000  | 0.000000000  | 0.000000000  |
| C | 2.439840000  | 0.000000000  | 1.471250000  |
| C | 1.231360000  | 0.000810000  | 2.061190000  |
| N | 0.026970000  | 0.013830000  | 1.363890000  |
| H | 1.224660000  | 0.031250000  | -1.599490000 |
| H | 1.127090000  | 0.001270000  | 3.128260000  |
| C | -1.243460000 | -0.102290000 | 2.070000000  |
| H | -1.987370000 | 0.494470000  | 1.568390000  |
| H | -1.114470000 | 0.263060000  | 3.079030000  |
| H | -1.578040000 | -1.131650000 | 2.099190000  |
| O | -1.007380000 | -0.031350000 | -0.645880000 |
| N | 1.239070000  | 0.024540000  | -0.601380000 |
| O | 3.480330000  | -0.025520000 | -0.655200000 |
| C | 3.745460000  | -0.006000000 | 2.218200000  |
| H | 4.321410000  | -0.894860000 | 1.988440000  |
| H | 4.348570000  | 0.850570000  | 1.940750000  |
| H | 3.576020000  | 0.025090000  | 3.288330000  |
| C | 3.361350000  | -4.071100000 | 1.906560000  |
| C | 1.087560000  | -4.061460000 | 2.869160000  |
| C | 0.574410000  | -3.898910000 | 1.618910000  |
| C | 1.412020000  | -3.810480000 | 0.488750000  |
| N | 2.785730000  | -3.958800000 | 0.664550000  |
| H | 2.911860000  | -4.251370000 | 3.848850000  |
| H | 1.028720000  | -3.790340000 | -0.507920000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.655040000  | -3.841500000 | -0.500600000 |
| H | 4.615880000  | -4.261990000 | -0.260660000 |
| H | 3.779740000  | -2.805090000 | -0.788610000 |
| H | 3.215660000  | -4.393760000 | -1.321370000 |
| O | 4.547280000  | -4.116070000 | 2.080790000  |
| N | 2.486050000  | -4.135390000 | 2.957180000  |
| S | 0.153190000  | -4.140590000 | 4.356030000  |
| F | -0.729120000 | -3.793680000 | 1.417960000  |

LIIC path connecting T2-MIN and T1-MIN

Coord\_1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478380000  | 0.000000000  | 0.000000000  |
| C | 2.438470000  | 0.000000000  | 1.471120000  |
| C | 1.230290000  | -0.005330000 | 2.061950000  |
| N | 0.026650000  | 0.003220000  | 1.363390000  |
| H | 1.224010000  | 0.032670000  | -1.600240000 |
| H | 1.126340000  | -0.011680000 | 3.128760000  |
| C | -1.251410000 | -0.096240000 | 2.057340000  |
| H | -1.944240000 | 0.625350000  | 1.653580000  |
| H | -1.092090000 | 0.109040000  | 3.105900000  |
| H | -1.672840000 | -1.086550000 | 1.945030000  |
| O | -1.009970000 | -0.022240000 | -0.642480000 |
| N | 1.238200000  | 0.022500000  | -0.602180000 |
| O | 3.479420000  | -0.024010000 | -0.655510000 |
| C | 3.743820000  | -0.002040000 | 2.218810000  |
| H | 4.320290000  | -0.891900000 | 1.995180000  |
| H | 4.346380000  | 0.853670000  | 1.937420000  |
| H | 3.572980000  | 0.034890000  | 3.288560000  |
| C | 3.310640000  | -3.977270000 | 1.957900000  |
| C | 1.006050000  | -4.003140000 | 2.833840000  |
| C | 0.539800000  | -3.893650000 | 1.541390000  |
| C | 1.402740000  | -3.843850000 | 0.469830000  |
| N | 2.782520000  | -3.936100000 | 0.697630000  |
| H | 2.811270000  | -4.077560000 | 3.887520000  |
| H | 1.066150000  | -3.817990000 | -0.543860000 |
| C | 3.683110000  | -3.850320000 | -0.445050000 |
| H | 4.663910000  | -4.167570000 | -0.136840000 |
| H | 3.738080000  | -2.835820000 | -0.820540000 |
| H | 3.324050000  | -4.506490000 | -1.228070000 |
| O | 4.487950000  | -3.990970000 | 2.189090000  |
| N | 2.397930000  | -4.000410000 | 2.985980000  |
| S | 0.001680000  | -3.900470000 | 4.277210000  |
| F | -0.772250000 | -3.814680000 | 1.331200000  |

Coord\_2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
|---|-------------|-------------|-------------|

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.478460000  | 0.000000000  | 0.000000000  |
| C | 2.438620000  | 0.000000000  | 1.471130000  |
| C | 1.230410000  | -0.004650000 | 2.061870000  |
| N | 0.026680000  | 0.004400000  | 1.363450000  |
| H | 1.224090000  | 0.032510000  | -1.600160000 |
| H | 1.126420000  | -0.010240000 | 3.128710000  |
| C | -1.250550000 | -0.096930000 | 2.058740000  |
| H | -1.949590000 | 0.611730000  | 1.643320000  |
| H | -1.093780000 | 0.126550000  | 3.104030000  |
| H | -1.662570000 | -1.092900000 | 1.961920000  |
| O | -1.009690000 | -0.023250000 | -0.642860000 |
| N | 1.238300000  | 0.022730000  | -0.602090000 |
| O | 3.479520000  | -0.024180000 | -0.655480000 |
| C | 3.744000000  | -0.002480000 | 2.218750000  |
| H | 4.320420000  | -0.892230000 | 1.994430000  |
| H | 4.346620000  | 0.853330000  | 1.937790000  |
| H | 3.573320000  | 0.033810000  | 3.288530000  |
| C | 3.316090000  | -3.987760000 | 1.952300000  |
| C | 1.014700000  | -4.009600000 | 2.837830000  |
| C | 0.543060000  | -3.894020000 | 1.549910000  |
| C | 1.403310000  | -3.840010000 | 0.471730000  |
| N | 2.782790000  | -3.938560000 | 0.693720000  |
| H | 2.822120000  | -4.097010000 | 3.883520000  |
| H | 1.061380000  | -3.814680000 | -0.540150000 |
| C | 3.680070000  | -3.849170000 | -0.451410000 |
| H | 4.659150000  | -4.178230000 | -0.150200000 |
| H | 3.742540000  | -2.831500000 | -0.816930000 |
| H | 3.311980000  | -4.494160000 | -1.239450000 |
| O | 4.494510000  | -4.005080000 | 2.177330000  |
| N | 2.407430000  | -4.015490000 | 2.982960000  |
| S | 0.018940000  | -3.926880000 | 4.287950000  |
| F | -0.768080000 | -3.812170000 | 1.340730000  |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478540000  | 0.000000000  | 0.000000000  |
| C | 2.438770000  | 0.000000000  | 1.471150000  |
| C | 1.230530000  | -0.003970000 | 2.061780000  |
| N | 0.026720000  | 0.005580000  | 1.363510000  |
| H | 1.224160000  | 0.032350000  | -1.600080000 |
| H | 1.126500000  | -0.008810000 | 3.128650000  |
| C | -1.249690000 | -0.097620000 | 2.060140000  |
| H | -1.954810000 | 0.597870000  | 1.633250000  |
| H | -1.095670000 | 0.143970000  | 3.101870000  |
| H | -1.652220000 | -1.098930000 | 1.978880000  |
| O | -1.009400000 | -0.024250000 | -0.643250000 |
| N | 1.238400000  | 0.022950000  | -0.602000000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | 3.479620000  | -0.024350000 | -0.655440000 |
| C | 3.744190000  | -0.002920000 | 2.218680000  |
| H | 4.320540000  | -0.892560000 | 1.993680000  |
| H | 4.346870000  | 0.852990000  | 1.938160000  |
| H | 3.573660000  | 0.032720000  | 3.288510000  |
| C | 3.321590000  | -3.998230000 | 1.946670000  |
| C | 1.023450000  | -4.016070000 | 2.841800000  |
| C | 0.546470000  | -3.894450000 | 1.558450000  |
| C | 1.404000000  | -3.836210000 | 0.473670000  |
| N | 2.783070000  | -3.941040000 | 0.689880000  |
| H | 2.833040000  | -4.116440000 | 3.879440000  |
| H | 1.056760000  | -3.811430000 | -0.536360000 |
| C | 3.677010000  | -3.848060000 | -0.457730000 |
| H | 4.654250000  | -4.188860000 | -0.163670000 |
| H | 3.747030000  | -2.827400000 | -0.813320000 |
| H | 3.299920000  | -4.481770000 | -1.250580000 |
| O | 4.501070000  | -4.019130000 | 2.165500000  |
| N | 2.417010000  | -4.030550000 | 2.979900000  |
| S | 0.036100000  | -3.953400000 | 4.298190000  |
| F | -0.763750000 | -3.809700000 | 1.350290000  |

Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478630000  | 0.000000000  | 0.000000000  |
| C | 2.438920000  | 0.000000000  | 1.471160000  |
| C | 1.230650000  | -0.003290000 | 2.061700000  |
| N | 0.026760000  | 0.006760000  | 1.363570000  |
| H | 1.224230000  | 0.032200000  | -1.599990000 |
| H | 1.126580000  | -0.007370000 | 3.128600000  |
| C | -1.248810000 | -0.098300000 | 2.061540000  |
| H | -1.959900000 | 0.583780000  | 1.623380000  |
| H | -1.097760000 | 0.161300000  | 3.099430000  |
| H | -1.641800000 | -1.104620000 | 1.995900000  |
| O | -1.009110000 | -0.025260000 | -0.643630000 |
| N | 1.238490000  | 0.023180000  | -0.601910000 |
| O | 3.479720000  | -0.024510000 | -0.655410000 |
| C | 3.744370000  | -0.003360000 | 2.218610000  |
| H | 4.320670000  | -0.892890000 | 1.992930000  |
| H | 4.347110000  | 0.852640000  | 1.938530000  |
| H | 3.574000000  | 0.031630000  | 3.288480000  |
| C | 3.327130000  | -4.008690000 | 1.941020000  |
| C | 1.032310000  | -4.022540000 | 2.845760000  |
| C | 0.550020000  | -3.894920000 | 1.567020000  |
| C | 1.404800000  | -3.832440000 | 0.475670000  |
| N | 2.783380000  | -3.943530000 | 0.686090000  |
| H | 2.844060000  | -4.135820000 | 3.875290000  |
| H | 1.052300000  | -3.808230000 | -0.532500000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.673930000  | -3.846990000 | -0.463990000 |
| H | 4.649210000  | -4.199440000 | -0.177250000 |
| H | 3.751580000  | -2.823530000 | -0.809730000 |
| H | 3.287860000  | -4.469330000 | -1.261460000 |
| O | 4.507650000  | -4.033130000 | 2.153600000  |
| N | 2.426660000  | -4.045590000 | 2.976780000  |
| S | 0.053170000  | -3.979990000 | 4.307930000  |
| F | -0.759260000 | -3.807280000 | 1.359880000  |

Coord\_5

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478710000  | 0.000000000  | 0.000000000  |
| C | 2.439080000  | 0.000000000  | 1.471180000  |
| C | 1.230760000  | -0.002610000 | 2.061610000  |
| N | 0.026790000  | 0.007940000  | 1.363630000  |
| H | 1.224300000  | 0.032040000  | -1.599910000 |
| H | 1.126660000  | -0.005930000 | 3.128540000  |
| C | -1.247940000 | -0.098980000 | 2.062950000  |
| H | -1.964840000 | 0.569450000  | 1.613700000  |
| H | -1.100050000 | 0.178540000  | 3.096720000  |
| H | -1.631310000 | -1.109970000 | 2.012990000  |
| O | -1.008830000 | -0.026280000 | -0.644010000 |
| N | 1.238590000  | 0.023410000  | -0.601820000 |
| O | 3.479820000  | -0.024680000 | -0.655370000 |
| C | 3.744550000  | -0.003800000 | 2.218540000  |
| H | 4.320790000  | -0.893220000 | 1.992180000  |
| H | 4.347350000  | 0.852300000  | 1.938900000  |
| H | 3.574330000  | 0.030540000  | 3.288460000  |
| C | 3.332720000  | -4.019130000 | 1.935340000  |
| C | 1.041260000  | -4.029020000 | 2.849710000  |
| C | 0.553720000  | -3.895460000 | 1.575610000  |
| C | 1.405710000  | -3.828690000 | 0.477730000  |
| N | 2.783710000  | -3.946030000 | 0.682360000  |
| H | 2.855150000  | -4.155170000 | 3.871060000  |
| H | 1.047980000  | -3.805100000 | -0.528570000 |
| C | 3.670830000  | -3.845970000 | -0.470210000 |
| H | 4.644020000  | -4.209980000 | -0.190920000 |
| H | 3.756160000  | -2.819890000 | -0.806150000 |
| H | 3.275800000  | -4.456840000 | -1.272080000 |
| O | 4.514230000  | -4.047090000 | 2.141630000  |
| N | 2.436380000  | -4.060600000 | 2.973630000  |
| S | 0.070130000  | -4.006660000 | 4.317170000  |
| F | -0.754620000 | -3.804900000 | 1.369500000  |

Coord\_6

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| C | 2.478790000 | 0.000000000 | 0.000000000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.439230000  | 0.000000000  | 1.471190000  |
| C | 1.230880000  | -0.001920000 | 2.061530000  |
| N | 0.026830000  | 0.009110000  | 1.363680000  |
| H | 1.224370000  | 0.031880000  | -1.599830000 |
| H | 1.126750000  | -0.004490000 | 3.128480000  |
| C | -1.247050000 | -0.099650000 | 2.064350000  |
| H | -1.969640000 | 0.554890000  | 1.604220000  |
| H | -1.102540000 | 0.195670000  | 3.093730000  |
| H | -1.620760000 | -1.114990000 | 2.030140000  |
| O | -1.008540000 | -0.027290000 | -0.644390000 |
| N | 1.238690000  | 0.023630000  | -0.601730000 |
| O | 3.479920000  | -0.024850000 | -0.655340000 |
| C | 3.744730000  | -0.004240000 | 2.218470000  |
| H | 4.320910000  | -0.893550000 | 1.991430000  |
| H | 4.347590000  | 0.851950000  | 1.939270000  |
| H | 3.574670000  | 0.029450000  | 3.288430000  |
| C | 3.338360000  | -4.029560000 | 1.929640000  |
| C | 1.050320000  | -4.035500000 | 2.853630000  |
| C | 0.557560000  | -3.896040000 | 1.584230000  |
| C | 1.406740000  | -3.824990000 | 0.479840000  |
| N | 2.784060000  | -3.948560000 | 0.678680000  |
| H | 2.866330000  | -4.174490000 | 3.866770000  |
| H | 1.043820000  | -3.802030000 | -0.524570000 |
| C | 3.667710000  | -3.844990000 | -0.476390000 |
| H | 4.638680000  | -4.220480000 | -0.204690000 |
| H | 3.760790000  | -2.816480000 | -0.802590000 |
| H | 3.263750000  | -4.444300000 | -1.282450000 |
| O | 4.520820000  | -4.060990000 | 2.129600000  |
| N | 2.446170000  | -4.075600000 | 2.970430000  |
| S | 0.086980000  | -4.033380000 | 4.325920000  |
| F | -0.749830000 | -3.802570000 | 1.379140000  |

Coord\_7

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478880000  | 0.000000000  | 0.000000000  |
| C | 2.439380000  | 0.000000000  | 1.471200000  |
| C | 1.231000000  | -0.001240000 | 2.061440000  |
| N | 0.026860000  | 0.010290000  | 1.363740000  |
| H | 1.224450000  | 0.031720000  | -1.599740000 |
| H | 1.126830000  | -0.003050000 | 3.128430000  |
| C | -1.246160000 | -0.100320000 | 2.065760000  |
| H | -1.974300000 | 0.540110000  | 1.594950000  |
| H | -1.105230000 | 0.212700000  | 3.090460000  |
| H | -1.610160000 | -1.119660000 | 2.047330000  |
| O | -1.008250000 | -0.028300000 | -0.644760000 |
| N | 1.238780000  | 0.023860000  | -0.601640000 |
| O | 3.480030000  | -0.025020000 | -0.655310000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.744910000  | -0.004680000 | 2.218400000  |
| H | 4.321040000  | -0.893880000 | 1.990680000  |
| H | 4.347840000  | 0.851610000  | 1.939640000  |
| H | 3.575010000  | 0.028360000  | 3.288400000  |
| C | 3.344030000  | -4.039970000 | 1.923900000  |
| C | 1.059480000  | -4.041990000 | 2.857540000  |
| C | 0.561560000  | -3.896680000 | 1.592870000  |
| C | 1.407890000  | -3.821310000 | 0.481990000  |
| N | 2.784440000  | -3.951090000 | 0.675060000  |
| H | 2.877590000  | -4.193760000 | 3.862400000  |
| H | 1.039810000  | -3.799010000 | -0.520510000 |
| C | 3.664570000  | -3.844050000 | -0.482510000 |
| H | 4.633200000  | -4.230930000 | -0.218550000 |
| H | 3.765460000  | -2.813290000 | -0.799060000 |
| H | 3.251710000  | -4.431720000 | -1.292570000 |
| O | 4.527420000  | -4.074830000 | 2.117490000  |
| N | 2.456040000  | -4.090580000 | 2.967180000  |
| S | 0.103720000  | -4.060150000 | 4.334180000  |
| F | -0.744880000 | -3.800280000 | 1.388810000  |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.478960000  | 0.000000000  | 0.000000000  |
| C | 2.439530000  | 0.000000000  | 1.471220000  |
| C | 1.231120000  | -0.000560000 | 2.061360000  |
| N | 0.026900000  | 0.011470000  | 1.363790000  |
| H | 1.224520000  | 0.031560000  | -1.599660000 |
| H | 1.126920000  | -0.001610000 | 3.128370000  |
| C | -1.245270000 | -0.100980000 | 2.067170000  |
| H | -1.978810000 | 0.525110000  | 1.585880000  |
| H | -1.108110000 | 0.229610000  | 3.086920000  |
| H | -1.599500000 | -1.124000000 | 2.064580000  |
| O | -1.007960000 | -0.029320000 | -0.645140000 |
| N | 1.238880000  | 0.024080000  | -0.601550000 |
| O | 3.480130000  | -0.025180000 | -0.655270000 |
| C | 3.745090000  | -0.005120000 | 2.218330000  |
| H | 4.321160000  | -0.894210000 | 1.989930000  |
| H | 4.348080000  | 0.851260000  | 1.940010000  |
| H | 3.575340000  | 0.027270000  | 3.288380000  |
| C | 3.349760000  | -4.050360000 | 1.918150000  |
| C | 1.068740000  | -4.048470000 | 2.861430000  |
| C | 0.565700000  | -3.897370000 | 1.601530000  |
| C | 1.409150000  | -3.817670000 | 0.484200000  |
| N | 2.784850000  | -3.953640000 | 0.671500000  |
| H | 2.888930000  | -4.213000000 | 3.857950000  |
| H | 1.035960000  | -3.796060000 | -0.516380000 |
| C | 3.661410000  | -3.843150000 | -0.488590000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 4.627580000  | -4.241330000 | -0.232500000 |
| H | 3.770180000  | -2.810330000 | -0.795540000 |
| H | 3.239680000  | -4.419100000 | -1.302430000 |
| O | 4.534030000  | -4.088630000 | 2.105320000  |
| N | 2.465970000  | -4.105530000 | 2.963890000  |
| S | 0.120340000  | -4.086940000 | 4.341950000  |
| F | -0.739780000 | -3.798040000 | 1.398510000  |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.000000000  | 0.000000000  | 0.000000000  |
| C | 2.479040000  | 0.000000000  | 0.000000000  |
| C | 2.439680000  | 0.000000000  | 1.471230000  |
| C | 1.231240000  | 0.000130000  | 2.061270000  |
| N | 0.026940000  | 0.012650000  | 1.363840000  |
| H | 1.224590000  | 0.031400000  | -1.599570000 |
| H | 1.127000000  | -0.000170000 | 3.128310000  |
| C | -1.244360000 | -0.101640000 | 2.068580000  |
| H | -1.983170000 | 0.509890000  | 1.577030000  |
| H | -1.111190000 | 0.246400000  | 3.083110000  |
| H | -1.588790000 | -1.127990000 | 2.081860000  |
| O | -1.007670000 | -0.030330000 | -0.645510000 |
| N | 1.238970000  | 0.024310000  | -0.601470000 |
| O | 3.480230000  | -0.025350000 | -0.655240000 |
| C | 3.745280000  | -0.005560000 | 2.218270000  |
| H | 4.321280000  | -0.894530000 | 1.989180000  |
| H | 4.348320000  | 0.850910000  | 1.940380000  |
| H | 3.575680000  | 0.026180000  | 3.288350000  |
| C | 3.355530000  | -4.060740000 | 1.912360000  |
| C | 1.078100000  | -4.054960000 | 2.865300000  |
| C | 0.569980000  | -3.898110000 | 1.610210000  |
| C | 1.410530000  | -3.814060000 | 0.486450000  |
| N | 2.785270000  | -3.956210000 | 0.668000000  |
| H | 2.900360000  | -4.232200000 | 3.853440000  |
| H | 1.032270000  | -3.793160000 | -0.512180000 |
| C | 3.658230000  | -3.842300000 | -0.494630000 |
| H | 4.621800000  | -4.251680000 | -0.246540000 |
| H | 3.774930000  | -2.807600000 | -0.792060000 |
| H | 3.227660000  | -4.406450000 | -1.312030000 |
| O | 4.540650000  | -4.102370000 | 2.093090000  |
| N | 2.475970000  | -4.120470000 | 2.960560000  |
| S | 0.136830000  | -4.113760000 | 4.349230000  |
| F | -0.734520000 | -3.795840000 | 1.408220000  |

Coord\_10

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| C | 2.479120000 | 0.000000000 | 0.000000000 |
| C | 2.439840000 | 0.000000000 | 1.471250000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.231360000  | 0.000810000  | 2.061190000  |
| N | 0.026970000  | 0.013830000  | 1.363900000  |
| H | 1.224660000  | 0.031250000  | -1.599490000 |
| H | 1.127090000  | 0.001270000  | 3.128260000  |
| C | -1.243460000 | -0.102290000 | 2.070000000  |
| H | -1.987370000 | 0.494470000  | 1.568380000  |
| H | -1.114470000 | 0.263060000  | 3.079030000  |
| H | -1.578040000 | -1.131650000 | 2.099190000  |
| O | -1.007390000 | -0.031350000 | -0.645880000 |
| N | 1.239070000  | 0.024540000  | -0.601380000 |
| O | 3.480330000  | -0.025520000 | -0.655200000 |
| C | 3.745460000  | -0.006000000 | 2.218200000  |
| H | 4.321410000  | -0.894860000 | 1.988430000  |
| H | 4.348570000  | 0.850570000  | 1.940750000  |
| H | 3.576020000  | 0.025090000  | 3.288320000  |
| C | 3.361340000  | -4.071100000 | 1.906550000  |
| C | 1.087570000  | -4.061460000 | 2.869150000  |
| C | 0.574420000  | -3.898910000 | 1.618910000  |
| C | 1.412030000  | -3.810480000 | 0.488740000  |
| N | 2.785730000  | -3.958800000 | 0.664550000  |
| H | 2.911860000  | -4.251360000 | 3.848850000  |
| H | 1.028720000  | -3.790330000 | -0.507930000 |
| C | 3.655040000  | -3.841500000 | -0.500610000 |
| H | 4.615880000  | -4.261980000 | -0.260660000 |
| H | 3.779730000  | -2.805090000 | -0.788610000 |
| H | 3.215660000  | -4.393760000 | -1.321380000 |
| O | 4.547280000  | -4.116060000 | 2.080790000  |
| N | 2.486050000  | -4.135380000 | 2.957180000  |
| S | 0.153190000  | -4.140580000 | 4.356020000  |
| F | -0.729110000 | -3.793680000 | 1.417960000  |

#### Thymine monomer

|                |              |              |              |
|----------------|--------------|--------------|--------------|
| S <sub>0</sub> |              |              |              |
| C              | 2.032539330  | 1.449207830  | 0.499628390  |
| C              | -0.097973010 | 2.176432190  | -0.547364640 |
| C              | 0.105445840  | 1.147577330  | -1.579121650 |
| C              | 1.213121050  | 0.390129820  | -1.499274860 |
| N              | 2.179425200  | 0.530000770  | -0.509236620 |
| H              | 0.801290760  | 2.910917230  | 1.137503180  |
| H              | 1.420744920  | -0.376295930 | -2.219705900 |
| C              | 3.323784400  | -0.364671550 | -0.442479420 |
| H              | 4.221087000  | 0.200215670  | -0.241754370 |
| H              | 3.428054380  | -0.867033520 | -1.393566880 |
| H              | 3.199255940  | -1.104946840 | 0.338651640  |
| O              | 2.822133570  | 1.568457870  | 1.397746490  |
| N              | 0.907535950  | 2.236747190  | 0.410387460  |



|   |              |             |              |
|---|--------------|-------------|--------------|
| O | -1.042746890 | 2.918393920 | -0.502825880 |
| C | -0.931677060 | 1.003515370 | -2.658497130 |
| H | -1.901789090 | 0.771414730 | -2.233867000 |
| H | -1.037774240 | 1.926217930 | -3.217719220 |
| H | -0.662233040 | 0.213243980 | -3.349692610 |

S<sub>1</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.071201490  | 1.506639280  | 0.469015360  |
| C | -0.058128940 | 2.085168900  | -0.553421200 |
| C | 0.068276630  | 1.139488920  | -1.539650420 |
| C | 1.221482060  | 0.354645210  | -1.498777990 |
| N | 2.206054730  | 0.564733540  | -0.517611570 |
| H | 0.766043870  | 2.836771920  | 1.186336990  |
| H | 1.386954600  | -0.474176350 | -2.153657340 |
| C | 3.331949410  | -0.348501320 | -0.468971470 |
| H | 4.081612660  | 0.046549290  | 0.194626520  |
| H | 3.754983450  | -0.452935370 | -1.460982710 |
| H | 3.026215400  | -1.327616870 | -0.113287520 |
| O | 2.837030730  | 1.629312680  | 1.387933100  |
| N | 0.982469480  | 2.352653040  | 0.342560400  |
| O | -1.003148540 | 3.079672060  | -0.564951700 |
| C | -0.972982790 | 0.969206060  | -2.619703420 |
| H | -1.969288260 | 0.882276070  | -2.200640040 |
| H | -0.972355040 | 1.812239680  | -3.303156010 |
| H | -0.778145940 | 0.073397250  | -3.196849980 |

S<sub>2</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.017769100  | 1.418105880  | 0.492954770  |
| C | 0.053951020  | 2.237824800  | -0.699730450 |
| C | 0.031514020  | 1.164937780  | -1.549262490 |
| C | 1.223556660  | 0.275122360  | -1.500019500 |
| N | 2.135926440  | 0.463022950  | -0.473901360 |
| H | 0.954792890  | 3.104117970  | 0.896393210  |
| H | 1.659913630  | -0.089674390 | -2.416665650 |
| C | 3.258524950  | -0.455899740 | -0.338550430 |
| H | 4.158572830  | 0.092195800  | -0.106164610 |
| H | 3.383375190  | -0.983454340 | -1.272520380 |
| H | 3.073015740  | -1.171763700 | 0.452061790  |
| O | 2.744278410  | 1.513788390  | 1.448535540  |
| N | 1.002335500  | 2.331462720  | 0.267135670  |
| O | -0.814422740 | 3.271018520  | -0.608758250 |
| C | -1.017445570 | 0.936561830  | -2.594892550 |
| H | -1.421998880 | -0.071195610 | -2.530029580 |
| H | -1.837359260 | 1.633170410  | -2.473449010 |
| H | -0.626074910 | 1.060182350  | -3.604325740 |

T<sub>1</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.011038570  | 1.450511850  | 0.446895310  |
| C | -0.256028490 | 1.986980630  | -0.399803180 |
| C | -0.032065930 | 1.051936400  | -1.486156720 |
| C | 1.083696690  | 0.082385480  | -1.303818220 |
| N | 2.197432180  | 0.600251770  | -0.626420560 |
| H | 0.640055360  | 2.635386600  | 1.317476380  |
| H | 0.854112270  | -0.961975990 | -1.131287860 |
| C | 3.435250140  | -0.158594260 | -0.677767390 |
| H | 4.248202500  | 0.456384880  | -0.329124220 |
| H | 3.620159830  | -0.448486210 | -1.702797940 |
| H | 3.382158280  | -1.051494170 | -0.060285260 |
| O | 2.879987220  | 1.731705530  | 1.224476350  |
| N | 0.730819340  | 1.959859080  | 0.589636990  |
| O | -1.182997380 | 2.758597760  | -0.334111300 |
| C | -0.770354180 | 1.146498730  | -2.782033780 |
| H | -1.538816670 | 1.904930730  | -2.733789740 |
| H | -0.086090040 | 1.388117320  | -3.592079110 |
| H | -1.236332710 | 0.196524890  | -3.030200730 |

T<sub>2</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.081981700  | 1.519827300  | 0.458610700  |
| C | -0.051575100 | 2.101888700  | -0.562131500 |
| C | 0.073968000  | 1.139482300  | -1.543821600 |
| C | 1.204213400  | 0.338717600  | -1.477256200 |
| N | 2.192961000  | 0.547637300  | -0.501347900 |
| H | 0.796577000  | 2.889666000  | 1.148290300  |
| H | 1.376641800  | -0.482516100 | -2.140563900 |
| C | 3.316718900  | -0.368661500 | -0.456811500 |
| H | 4.034505700  | -0.013017500 | 0.262378800  |
| H | 3.786648700  | -0.420477300 | -1.432881700 |
| H | 2.992319800  | -1.364669600 | -0.170709700 |
| O | 2.863230700  | 1.666682200  | 1.360873300  |
| N | 0.992755100  | 2.362366600  | 0.325855300  |
| O | -0.971188800 | 3.110035700  | -0.593552200 |
| C | -0.976028900 | 0.960873500  | -2.613378700 |
| H | -1.931059100 | 0.668736300  | -2.189307800 |
| H | -1.127318400 | 1.880282300  | -3.169952600 |
| H | -0.675124500 | 0.192667200  | -3.315484000 |

5-Fluoro-4-Thiouridine monomer

S<sub>0</sub>

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | -2.434653470 | -0.723952690 | 0.050777480 |
| C | -0.291589830 | -1.982862460 | 0.084742660 |
| C | 0.088280760  | -1.128017560 | 1.194283760 |
| C | -0.736992220 | -0.180611680 | 1.656900560 |
| N | -1.994578280 | 0.028055530  | 1.101226100 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.889902740 | -2.229303780 | -1.154093170 |
| H | -0.461070840 | 0.452320180  | 2.475356450  |
| C | -2.838220150 | 1.086398290  | 1.638295690  |
| H | -3.788643630 | 1.052780570  | 1.135681650  |
| H | -2.379398130 | 2.054202310  | 1.474375750  |
| H | -2.987390430 | 0.936454040  | 2.700448710  |
| O | -3.499796460 | -0.588042960 | -0.476923420 |
| N | -1.549571090 | -1.690147720 | -0.386544650 |
| S | 0.656885930  | -3.183657750 | -0.564786470 |
| F | 1.274987580  | -1.301984330 | 1.745898900  |

S<sub>1</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.438429850 | -0.726458710 | 0.048421360  |
| C | -0.293340220 | -1.935439830 | 0.134012070  |
| C | 0.096709960  | -1.139088280 | 1.183759290  |
| C | -0.730711770 | -0.155824970 | 1.680306760  |
| N | -1.996368660 | 0.027776930  | 1.101428730  |
| H | -1.915383710 | -2.221935310 | -1.162312210 |
| H | -0.459669280 | 0.478430570  | 2.495785450  |
| C | -2.843328870 | 1.081322540  | 1.631827530  |
| H | -3.789317140 | 1.056548320  | 1.120365230  |
| H | -2.379580470 | 2.050256890  | 1.482044000  |
| H | -3.004246350 | 0.928163920  | 2.692914710  |
| O | -3.509885130 | -0.581531520 | -0.472312880 |
| N | -1.568351380 | -1.690525740 | -0.396808900 |
| S | 0.703567990  | -3.247102020 | -0.593437970 |
| F | 1.296681870  | -1.322962800 | 1.729646820  |

S<sub>2</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.426949920 | -0.718055340 | 0.058260680  |
| C | -0.296302870 | -1.912552960 | 0.155718550  |
| C | 0.108047430  | -1.141951100 | 1.191155090  |
| C | -0.746286160 | -0.133693540 | 1.695252880  |
| N | -1.985468570 | 0.037228470  | 1.111817190  |
| H | -1.835739320 | -2.242535930 | -1.133639930 |
| H | -0.481860650 | 0.501970960  | 2.511704220  |
| C | -2.854377250 | 1.088193760  | 1.632584860  |
| H | -3.798475480 | 1.041560720  | 1.120267970  |
| H | -2.399189890 | 2.057042130  | 1.468350420  |
| H | -3.007346730 | 0.937789660  | 2.693598750  |
| O | -3.490139760 | -0.585331550 | -0.472196300 |
| N | -1.529369180 | -1.681811710 | -0.367056490 |
| S | 0.621320490  | -3.354444650 | -0.754550570 |
| F | 1.290484840  | -1.291778920 | 1.764372690  |

T<sub>1</sub>

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | -2.437251480 | -0.727762780 | 0.046337650 |
|---|--------------|--------------|-------------|

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.288838380 | -1.941639230 | 0.129271850  |
| C | 0.104697410  | -1.161107120 | 1.170208590  |
| C | -0.740124760 | -0.152708850 | 1.685398990  |
| N | -1.993076800 | 0.028502210  | 1.105970930  |
| H | -1.895625950 | -2.231015720 | -1.157290010 |
| H | -0.463524820 | 0.471799510  | 2.505644840  |
| C | -2.843562350 | 1.084115990  | 1.630766080  |
| H | -3.793173620 | 1.046626480  | 1.127380280  |
| H | -2.385717030 | 2.052937090  | 1.465022260  |
| H | -2.992552800 | 0.940924960  | 2.694599750  |
| O | -3.509498560 | -0.572957590 | -0.468363750 |
| N | -1.567069830 | -1.686782410 | -0.391983790 |
| S | 0.687875040  | -3.241593130 | -0.610771600 |
| F | 1.285790940  | -1.307709430 | 1.743447940  |

T<sub>2</sub>

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.440263400 | -0.729850700 | 0.051957300  |
| C | -0.293450500 | -1.936265900 | 0.132193600  |
| C | 0.099178900  | -1.134090200 | 1.179321500  |
| C | -0.726608400 | -0.150568300 | 1.672314800  |
| N | -1.992398100 | 0.033584100  | 1.094974100  |
| H | -1.919921400 | -2.234325400 | -1.150546000 |
| H | -0.453684200 | 0.486919600  | 2.484791400  |
| C | -2.843036700 | 1.080763200  | 1.632504000  |
| H | -3.769915700 | 1.088783400  | 1.086671700  |
| H | -2.358218900 | 2.045511400  | 1.531659600  |
| H | -3.045455200 | 0.896092400  | 2.681657800  |
| O | -3.515924700 | -0.593957000 | -0.462063400 |
| N | -1.568280600 | -1.693411800 | -0.393480500 |
| S | 0.695668000  | -3.242038700 | -0.589002400 |
| F | 1.300657900  | -1.315516300 | 1.722686400  |

### **B3LYP-D3/6-31G\***

#### **X=F**

Dimer 5-Fluoro-4-Thiouridine with Thymidine

R-A-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.054119000  | 1.461909000  | 0.503288000  |
| C | -0.120636000 | 2.160498000  | -0.549566000 |
| C | 0.105432000  | 1.157908000  | -1.582261000 |
| C | 1.233355000  | 0.406919000  | -1.509894000 |
| N | 2.190228000  | 0.534817000  | -0.526684000 |
| H | 0.798146000  | 2.941155000  | 1.127158000  |
| H | 1.435520000  | -0.374002000 | -2.234230000 |
| C | 3.334500000  | -0.380217000 | -0.444091000 |
| H | 4.232357000  | 0.191540000  | -0.206182000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3.450892000  | -0.881431000 | -1.405619000 |
| H | 3.158390000  | -1.125862000 | 0.333613000  |
| O | 2.859981000  | 1.583622000  | 1.410045000  |
| N | 0.904364000  | 2.237242000  | 0.405735000  |
| O | -1.107295000 | 2.885875000  | -0.459044000 |
| C | -0.931193000 | 1.005866000  | -2.659414000 |
| H | -1.920910000 | 0.818292000  | -2.229105000 |
| H | -1.016580000 | 1.924547000  | -3.251369000 |
| H | -0.680443000 | 0.180843000  | -3.333571000 |
| C | -2.425809000 | -0.695313000 | 0.026266000  |
| C | -0.275077000 | -1.984007000 | 0.083666000  |
| C | 0.055265000  | -1.204224000 | 1.242488000  |
| C | -0.782430000 | -0.256156000 | 1.729259000  |
| N | -2.004956000 | -0.003086000 | 1.161574000  |
| H | -1.837145000 | -2.176570000 | -1.232384000 |
| H | -0.500240000 | 0.344686000  | 2.585056000  |
| C | -2.847146000 | 1.107640000  | 1.627108000  |
| H | -3.891937000 | 0.827223000  | 1.496817000  |
| H | -2.628630000 | 2.003318000  | 1.039104000  |
| H | -2.637842000 | 1.284422000  | 2.683958000  |
| O | -3.474307000 | -0.470146000 | -0.551129000 |
| N | -1.534351000 | -1.677630000 | -0.402328000 |
| S | 0.706507000  | -3.112936000 | -0.645297000 |
| F | 1.246445000  | -1.385591000 | 1.831482000  |

TS-A-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.507710000  | -1.277961000 | 0.125753000  |
| C | 0.320188000  | -1.013252000 | 1.315130000  |
| C | 0.491789000  | 0.425557000  | 1.257340000  |
| C | 1.760323000  | 0.951522000  | 0.771897000  |
| N | 2.719778000  | 0.109393000  | 0.287629000  |
| H | 1.201808000  | -2.752183000 | 0.621396000  |
| H | 2.151329000  | 1.867140000  | 1.198384000  |
| C | 3.899734000  | 0.694327000  | -0.348102000 |
| H | 4.634394000  | -0.089864000 | -0.517811000 |
| H | 4.314546000  | 1.466770000  | 0.305166000  |
| H | 3.600834000  | 1.146333000  | -1.301390000 |
| O | 3.311510000  | -1.999327000 | -0.432049000 |
| N | 1.347570000  | -1.753332000 | 0.703166000  |
| O | -0.667401000 | -1.597737000 | 1.753412000  |
| C | -0.238361000 | 1.247285000  | 2.288909000  |
| H | -1.264658000 | 0.889132000  | 2.403870000  |
| H | 0.246672000  | 1.183135000  | 3.271700000  |
| H | -0.255084000 | 2.303524000  | 1.995209000  |
| C | -2.869310000 | 0.593045000  | -0.043204000 |
| C | -0.459021000 | 0.948365000  | -0.552122000 |
| C | -0.518459000 | -0.296060000 | -1.292271000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.623540000 | -1.065754000 | -1.281430000 |
| N | -2.778945000 | -0.658476000 | -0.636898000 |
| H | -1.808949000 | 2.312078000  | 0.183841000  |
| H | -1.655513000 | -2.022764000 | -1.787501000 |
| C | -3.826115000 | -1.635986000 | -0.340934000 |
| H | -4.747164000 | -1.098458000 | -0.121032000 |
| H | -3.535096000 | -2.238278000 | 0.526819000  |
| H | -3.971600000 | -2.282912000 | -1.210017000 |
| O | -3.848256000 | 1.002597000  | 0.555466000  |
| N | -1.729947000 | 1.388329000  | -0.225034000 |
| S | 0.739550000  | 2.217299000  | -0.971376000 |
| F | 0.590003000  | -0.714738000 | -1.927676000 |

IM2-A-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.972432000  | -0.910611000 | -0.011764000 |
| C | 0.900848000  | -0.978785000 | 1.395982000  |
| C | 0.595447000  | 0.464424000  | 1.019484000  |
| C | 1.683004000  | 1.210078000  | 0.209316000  |
| N | 2.740125000  | 0.401088000  | -0.339266000 |
| H | 2.284259000  | -2.450580000 | 1.129652000  |
| H | 2.125552000  | 2.051026000  | 0.754940000  |
| C | 3.640246000  | 1.061840000  | -1.275099000 |
| H | 4.423077000  | 0.360602000  | -1.558700000 |
| H | 4.089814000  | 1.945479000  | -0.804259000 |
| H | 3.086250000  | 1.377569000  | -2.166483000 |
| O | 3.882556000  | -1.586816000 | -0.462586000 |
| N | 2.101823000  | -1.470550000 | 0.943716000  |
| O | 0.125372000  | -1.649112000 | 2.054671000  |
| C | 0.255823000  | 1.224208000  | 2.307057000  |
| H | -0.592392000 | 0.753865000  | 2.807638000  |
| H | 1.115986000  | 1.200431000  | 2.984359000  |
| H | 0.026922000  | 2.273771000  | 2.092547000  |
| C | -3.120906000 | 0.535031000  | 0.185127000  |
| C | -0.578763000 | 0.551844000  | -0.060291000 |
| C | -0.814240000 | -0.677028000 | -0.850545000 |
| C | -2.021883000 | -1.199060000 | -1.078157000 |
| N | -3.182953000 | -0.622598000 | -0.577079000 |
| H | -1.852513000 | 1.895406000  | 0.915579000  |
| H | -2.138207000 | -2.099509000 | -1.668952000 |
| C | -4.476580000 | -1.242388000 | -0.843072000 |
| H | -5.243380000 | -0.622057000 | -0.381555000 |
| H | -4.514040000 | -2.249405000 | -0.413055000 |
| H | -4.656572000 | -1.302278000 | -1.922086000 |
| O | -4.102589000 | 1.107376000  | 0.635870000  |
| N | -1.839003000 | 1.015528000  | 0.418567000  |
| S | 0.438888000  | 1.861221000  | -1.029772000 |
| F | 0.291979000  | -1.265228000 | -1.358524000 |

## R-A-T1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.398750000  | 2.007190000  | 0.519278000  |
| C | -0.921000000 | 2.112766000  | -0.437834000 |
| C | -0.468337000 | 1.255013000  | -1.528427000 |
| C | 0.827805000  | 0.855169000  | -1.530771000 |
| N | 1.750163000  | 1.210160000  | -0.568566000 |
| H | -0.196762000 | 3.032777000  | 1.261243000  |
| H | 1.214536000  | 0.202097000  | -2.305877000 |
| C | 3.123475000  | 0.698439000  | -0.594058000 |
| H | 3.811409000  | 1.509051000  | -0.349595000 |
| H | 3.336725000  | 0.314005000  | -1.591965000 |
| H | 3.240661000  | -0.104463000 | 0.137296000  |
| O | 2.176132000  | 2.301933000  | 1.411360000  |
| N | 0.079983000  | 2.438233000  | 0.488601000  |
| O | -2.065813000 | 2.527058000  | -0.283780000 |
| C | -1.470939000 | 0.853200000  | -2.571283000 |
| H | -2.306778000 | 0.308256000  | -2.119168000 |
| H | -1.896102000 | 1.737183000  | -3.059849000 |
| H | -1.012902000 | 0.217433000  | -3.335517000 |
| C | -1.960220000 | -1.453358000 | 0.023470000  |
| C | 0.473826000  | -2.015867000 | 0.055275000  |
| C | 0.589876000  | -1.250717000 | 1.202108000  |
| C | -0.506934000 | -0.586300000 | 1.801420000  |
| N | -1.749486000 | -0.689112000 | 1.194801000  |
| H | -0.998662000 | -2.651082000 | -1.288045000 |
| H | -0.411747000 | -0.012095000 | 2.709751000  |
| C | -2.879348000 | 0.073451000  | 1.726056000  |
| H | -3.801055000 | -0.391854000 | 1.380989000  |
| H | -2.839495000 | 1.104961000  | 1.360359000  |
| H | -2.832713000 | 0.054691000  | 2.818383000  |
| O | -3.051234000 | -1.513705000 | -0.520388000 |
| N | -0.852621000 | -2.117870000 | -0.441533000 |
| S | 1.776302000  | -2.715586000 | -0.825129000 |
| F | 1.773487000  | -1.064185000 | 1.780222000  |

## TS1-I-T1

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.326152000 | -1.215940000 | 0.580927000  |
| C | 0.233255000 | -0.281463000 | 1.595924000  |
| C | 0.737735000 | 1.054596000  | 1.314941000  |
| C | 1.923673000 | 1.183220000  | 0.545033000  |
| N | 2.763476000 | 0.092746000  | 0.365773000  |
| H | 0.762672000 | -2.259121000 | 1.365335000  |
| H | 2.431665000 | 2.142336000  | 0.528728000  |
| C | 3.968914000 | 0.271655000  | -0.442610000 |
| H | 4.604174000 | -0.603095000 | -0.317431000 |
| H | 4.496778000 | 1.167574000  | -0.104139000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3.697834000  | 0.381512000  | -1.498697000 |
| O | 2.970513000  | -2.200149000 | 0.268954000  |
| N | 1.098921000  | -1.313747000 | 1.228171000  |
| O | -0.856022000 | -0.525576000 | 2.111041000  |
| C | -0.055324000 | 2.231235000  | 1.774442000  |
| H | -1.127163000 | 2.035978000  | 1.667228000  |
| H | 0.120949000  | 2.416975000  | 2.843550000  |
| H | 0.213285000  | 3.133958000  | 1.218781000  |
| C | -2.794340000 | 0.566680000  | -0.255846000 |
| C | -0.548997000 | 0.604850000  | -1.335462000 |
| C | -0.603301000 | -0.787801000 | -1.403990000 |
| C | -1.687961000 | -1.492877000 | -0.936291000 |
| N | -2.765821000 | -0.824549000 | -0.357860000 |
| H | -1.767856000 | 2.215350000  | -0.824916000 |
| H | -1.742264000 | -2.571261000 | -0.993136000 |
| C | -3.680323000 | -1.577525000 | 0.497056000  |
| H | -4.578592000 | -0.982488000 | 0.653548000  |
| H | -3.200168000 | -1.778466000 | 1.461910000  |
| H | -3.939296000 | -2.518996000 | 0.004476000  |
| O | -3.671147000 | 1.186282000  | 0.326960000  |
| N | -1.745218000 | 1.207328000  | -0.899436000 |
| S | 0.870682000  | 1.584200000  | -1.558976000 |
| F | 0.463769000  | -1.476014000 | -1.853172000 |

IM1-I-T1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251812000  | -1.159283000 | 0.715498000  |
| C | 0.168021000  | -0.132333000 | 1.654905000  |
| C | 0.653404000  | 1.166717000  | 1.216853000  |
| C | 1.789001000  | 1.219700000  | 0.282222000  |
| N | 2.677159000  | 0.106985000  | 0.343571000  |
| H | 0.696286000  | -2.122412000 | 1.621299000  |
| H | 2.351927000  | 2.154675000  | 0.346763000  |
| C | 3.914148000  | 0.195678000  | -0.427617000 |
| H | 4.550829000  | -0.645988000 | -0.160805000 |
| H | 4.419997000  | 1.135680000  | -0.185161000 |
| H | 3.704368000  | 0.163622000  | -1.503313000 |
| O | 2.906131000  | -2.174390000 | 0.552405000  |
| N | 1.012317000  | -1.197770000 | 1.357152000  |
| O | -0.904375000 | -0.312713000 | 2.232017000  |
| C | -0.107677000 | 2.390793000  | 1.591303000  |
| H | -1.177634000 | 2.169913000  | 1.659751000  |
| H | 0.206844000  | 2.750533000  | 2.582662000  |
| H | 0.060931000  | 3.199404000  | 0.873536000  |
| C | -2.730218000 | 0.545080000  | -0.327304000 |
| C | -0.481097000 | 0.496175000  | -1.402319000 |
| C | -0.553127000 | -0.899906000 | -1.395997000 |
| C | -1.647236000 | -1.559806000 | -0.897810000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -2.715187000 | -0.848789000 | -0.350826000 |
| H | -1.678663000 | 2.148359000  | -0.967906000 |
| H | -1.714695000 | -2.639117000 | -0.894181000 |
| C | -3.650776000 | -1.544535000 | 0.530716000  |
| H | -4.549494000 | -0.937879000 | 0.630592000  |
| H | -3.194229000 | -1.686000000 | 1.517059000  |
| H | -3.904081000 | -2.513421000 | 0.091655000  |
| O | -3.603224000 | 1.207200000  | 0.212302000  |
| N | -1.667440000 | 1.137840000  | -0.995810000 |
| S | 0.979609000  | 1.434057000  | -1.566688000 |
| F | 0.508904000  | -1.620066000 | -1.804448000 |

TS2-I-T1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.029727000  | -1.039237000 | -0.076010000 |
| C | 0.837319000  | -1.100932000 | 1.126481000  |
| C | 0.758114000  | 0.366788000  | 1.027933000  |
| C | 1.914345000  | 1.133975000  | 0.453487000  |
| N | 3.052974000  | 0.327084000  | 0.061737000  |
| H | 1.933593000  | -2.686206000 | 0.432238000  |
| H | 2.266547000  | 1.875727000  | 1.181591000  |
| C | 4.207837000  | 1.046557000  | -0.461102000 |
| H | 5.033488000  | 0.345181000  | -0.569674000 |
| H | 4.485592000  | 1.842367000  | 0.239700000  |
| H | 3.979939000  | 1.495637000  | -1.434847000 |
| O | 3.924604000  | -1.702538000 | -0.578392000 |
| N | 1.909555000  | -1.675122000 | 0.474435000  |
| O | 0.000288000  | -1.781677000 | 1.714367000  |
| C | -0.042504000 | 1.051983000  | 2.095765000  |
| H | -0.979989000 | 0.524222000  | 2.281101000  |
| H | 0.527853000  | 1.046016000  | 3.036477000  |
| H | -0.243566000 | 2.094883000  | 1.836271000  |
| C | -3.135538000 | 0.886361000  | -0.041193000 |
| C | -0.783916000 | 0.366397000  | -0.656847000 |
| C | -1.216000000 | -0.946008000 | -0.932898000 |
| C | -2.512391000 | -1.332372000 | -0.772629000 |
| N | -3.453301000 | -0.445649000 | -0.313261000 |
| H | -1.573024000 | 2.180530000  | -0.164395000 |
| H | -2.849712000 | -2.335074000 | -1.009977000 |
| C | -4.841401000 | -0.842943000 | -0.065376000 |
| H | -5.514373000 | -0.165696000 | -0.595182000 |
| H | -5.060396000 | -0.782396000 | 1.004008000  |
| H | -4.984034000 | -1.865900000 | -0.415562000 |
| O | -3.949098000 | 1.697332000  | 0.362832000  |
| N | -1.796645000 | 1.197427000  | -0.301100000 |
| S | 1.173504000  | 2.129091000  | -0.951518000 |
| F | -0.320663000 | -1.856587000 | -1.358473000 |

IM2-A-T1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.695523000  | -0.777495000 | -0.693445000 |
| C | 1.677081000  | -0.591445000 | 1.563522000  |
| C | 0.742099000  | 0.534572000  | 1.053775000  |
| C | 1.462330000  | 1.252329000  | -0.150000000 |
| N | 1.901686000  | 0.256231000  | -1.130989000 |
| H | 3.275254000  | -1.718548000 | 1.015492000  |
| H | 2.355016000  | 1.757275000  | 0.267520000  |
| C | 1.779489000  | 0.470316000  | -2.567768000 |
| H | 2.203290000  | -0.401291000 | -3.064255000 |
| H | 2.318381000  | 1.369879000  | -2.886466000 |
| H | 0.726745000  | 0.583947000  | -2.841290000 |
| O | 3.345294000  | -1.524343000 | -1.404244000 |
| N | 2.711305000  | -0.932164000 | 0.709788000  |
| O | 1.558352000  | -1.091891000 | 2.663082000  |
| C | 0.585895000  | 1.497725000  | 2.251933000  |
| H | 0.121026000  | 0.965809000  | 3.083404000  |
| H | 1.570303000  | 1.845810000  | 2.580257000  |
| H | -0.000195000 | 2.383166000  | 1.996663000  |
| C | -2.992206000 | 0.465624000  | 0.160178000  |
| C | -0.581485000 | -0.049873000 | 0.608913000  |
| C | -0.799219000 | -1.298134000 | 0.047704000  |
| C | -2.028359000 | -1.693463000 | -0.435715000 |
| N | -3.111116000 | -0.808659000 | -0.385432000 |
| H | -1.670076000 | 1.698629000  | 1.037553000  |
| H | -2.197852000 | -2.673621000 | -0.856711000 |
| C | -4.403975000 | -1.239717000 | -0.902388000 |
| H | -5.109656000 | -0.419907000 | -0.778706000 |
| H | -4.759134000 | -2.116852000 | -0.349306000 |
| H | -4.319221000 | -1.496087000 | -1.964643000 |
| O | -3.915286000 | 1.262685000  | 0.240507000  |
| N | -1.719547000 | 0.781768000  | 0.618226000  |
| S | 0.518415000  | 2.636950000  | -0.824786000 |
| F | 0.220585000  | -2.182653000 | -0.037680000 |

TS1-II-T1

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.381401000 | -1.416286000 | 0.255678000  |
| C | 0.243169000 | -0.706340000 | 1.366402000  |
| C | 0.592133000 | 0.738383000  | 1.054781000  |
| C | 2.013285000 | 0.915275000  | 0.778181000  |
| N | 2.773306000 | -0.093563000 | 0.213081000  |
| H | 0.924186000 | -2.608487000 | 1.049951000  |
| H | 2.494414000 | 1.878859000  | 0.877516000  |
| C | 3.981715000 | 0.250292000  | -0.534342000 |
| H | 4.559124000 | -0.657559000 | -0.700627000 |
| H | 4.573308000 | 0.966983000  | 0.043532000  |
| H | 3.706072000 | 0.696484000  | -1.495685000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | 3.005464000  | -2.347252000 | -0.228049000 |
| N | 1.180793000  | -1.632968000 | 0.951554000  |
| O | -0.794769000 | -1.046108000 | 1.910412000  |
| C | 0.052529000  | 1.678843000  | 2.129236000  |
| H | -0.992746000 | 1.454113000  | 2.346443000  |
| H | 0.619511000  | 1.532047000  | 3.054655000  |
| H | 0.154377000  | 2.723869000  | 1.823436000  |
| C | -2.847211000 | 0.327176000  | 0.039487000  |
| C | -0.463031000 | 1.016456000  | -0.458952000 |
| C | -0.423836000 | -0.213238000 | -1.280609000 |
| C | -1.438063000 | -1.086786000 | -1.319210000 |
| N | -2.634609000 | -0.862892000 | -0.648945000 |
| H | -2.019296000 | 2.127267000  | 0.387797000  |
| H | -1.360719000 | -2.004980000 | -1.889431000 |
| C | -3.566903000 | -1.964996000 | -0.435577000 |
| H | -4.533730000 | -1.545385000 | -0.161383000 |
| H | -3.215047000 | -2.617639000 | 0.372232000  |
| H | -3.664991000 | -2.542792000 | -1.359254000 |
| O | -3.874561000 | 0.584133000  | 0.645875000  |
| N | -1.816472000 | 1.252105000  | -0.076164000 |
| S | 0.366095000  | 2.466676000  | -1.136915000 |
| F | 0.726300000  | -0.474137000 | -1.936842000 |

IM1-II-T1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.578518000  | -1.312949000 | 0.262248000  |
| C | 0.510939000  | -0.598604000 | 1.506766000  |
| C | 0.654380000  | 0.818314000  | 0.933641000  |
| C | 2.022662000  | 1.041571000  | 0.381885000  |
| N | 2.821687000  | 0.004457000  | -0.064097000 |
| H | 1.343524000  | -2.461174000 | 1.414390000  |
| H | 2.324004000  | 2.034765000  | 0.075935000  |
| C | 3.891338000  | 0.290081000  | -1.019565000 |
| H | 4.544553000  | -0.578420000 | -1.082226000 |
| H | 4.459524000  | 1.159729000  | -0.676944000 |
| H | 3.459387000  | 0.498945000  | -2.004132000 |
| O | 3.244740000  | -2.262297000 | -0.121425000 |
| N | 1.480813000  | -1.501399000 | 1.117706000  |
| O | -0.417940000 | -0.932896000 | 2.220605000  |
| C | 0.370825000  | 1.838425000  | 2.055088000  |
| H | -0.549646000 | 1.585420000  | 2.586246000  |
| H | 1.188688000  | 1.817824000  | 2.780600000  |
| H | 0.298294000  | 2.848594000  | 1.641629000  |
| C | -2.856426000 | 0.046822000  | 0.232728000  |
| C | -0.475625000 | 0.918394000  | -0.213698000 |
| C | -0.426534000 | -0.232913000 | -1.162555000 |
| C | -1.426539000 | -1.099963000 | -1.339816000 |
| N | -2.630016000 | -0.999348000 | -0.648026000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2.014846000 | 1.696536000  | 1.001209000  |
| H | -1.339010000 | -1.913063000 | -2.050299000 |
| C | -3.618459000 | -2.067839000 | -0.748655000 |
| H | -4.544406000 | -1.713165000 | -0.298400000 |
| H | -3.279917000 | -2.964749000 | -0.216872000 |
| H | -3.791102000 | -2.313111000 | -1.801316000 |
| O | -3.883051000 | 0.187969000  | 0.877420000  |
| N | -1.820777000 | 0.972793000  | 0.322090000  |
| S | -0.398888000 | 2.523206000  | -1.170002000 |
| F | 0.713417000  | -0.355021000 | -1.876079000 |

TS2-II-T1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.695523000  | -0.777495000 | -0.693445000 |
| C | 1.677081000  | -0.591445000 | 1.563522000  |
| C | 0.742099000  | 0.534572000  | 1.053775000  |
| C | 1.462330000  | 1.252329000  | -0.150000000 |
| N | 1.901686000  | 0.256231000  | -1.130989000 |
| H | 3.275254000  | -1.718548000 | 1.015492000  |
| H | 2.355016000  | 1.757275000  | 0.267520000  |
| C | 1.779489000  | 0.470316000  | -2.567768000 |
| H | 2.203290000  | -0.401291000 | -3.064255000 |
| H | 2.318381000  | 1.369879000  | -2.886466000 |
| H | 0.726745000  | 0.583947000  | -2.841290000 |
| O | 3.345294000  | -1.524343000 | -1.404244000 |
| N | 2.711305000  | -0.932164000 | 0.709788000  |
| O | 1.558352000  | -1.091891000 | 2.663082000  |
| C | 0.585895000  | 1.497725000  | 2.251933000  |
| H | 0.121026000  | 0.965809000  | 3.083404000  |
| H | 1.570303000  | 1.845810000  | 2.580257000  |
| H | -0.000195000 | 2.383166000  | 1.996663000  |
| C | -2.992206000 | 0.465624000  | 0.160178000  |
| C | -0.581485000 | -0.049873000 | 0.608913000  |
| C | -0.799219000 | -1.298134000 | 0.047704000  |
| C | -2.028359000 | -1.693463000 | -0.435715000 |
| N | -3.111116000 | -0.808659000 | -0.385432000 |
| H | -1.670076000 | 1.698629000  | 1.037553000  |
| H | -2.197852000 | -2.673621000 | -0.856711000 |
| C | -4.403975000 | -1.239717000 | -0.902388000 |
| H | -5.109656000 | -0.419907000 | -0.778706000 |
| H | -4.759134000 | -2.116852000 | -0.349306000 |
| H | -4.319221000 | -1.496087000 | -1.964643000 |
| O | -3.915286000 | 1.262685000  | 0.240507000  |
| N | -1.719547000 | 0.781768000  | 0.618226000  |
| S | 0.518415000  | 2.636950000  | -0.824786000 |
| F | 0.220585000  | -2.182653000 | -0.037680000 |

TS1-I-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.872956000  | -0.597332000 | -0.552277000 |
| C | 1.512410000  | -0.866418000 | 1.510364000  |
| C | 0.685383000  | 0.377433000  | 1.114086000  |
| C | 1.430603000  | 1.298264000  | 0.075451000  |
| N | 2.061474000  | 0.424462000  | -0.955754000 |
| H | 3.206582000  | -1.865599000 | 1.014782000  |
| H | 2.243006000  | 1.797509000  | 0.625335000  |
| C | 2.336089000  | 0.961980000  | -2.291215000 |
| H | 2.652585000  | 0.137744000  | -2.930089000 |
| H | 3.132437000  | 1.716217000  | -2.262219000 |
| H | 1.427651000  | 1.425988000  | -2.671842000 |
| O | 3.713119000  | -1.167754000 | -1.231067000 |
| N | 2.658229000  | -1.044198000 | 0.781628000  |
| O | 1.192754000  | -1.585654000 | 2.441405000  |
| C | 0.456886000  | 1.153277000  | 2.431091000  |
| H | -0.141583000 | 0.565157000  | 3.130131000  |
| H | 1.428193000  | 1.342548000  | 2.896605000  |
| H | -0.003145000 | 2.124985000  | 2.233583000  |
| C | -3.026449000 | 0.365640000  | 0.251738000  |
| C | -0.613046000 | -0.070272000 | 0.482481000  |
| C | -0.769492000 | -1.186590000 | -0.352849000 |
| C | -1.997933000 | -1.506501000 | -0.870182000 |
| N | -3.095710000 | -0.760973000 | -0.584047000 |
| H | -1.646955000 | 1.520309000  | 1.185892000  |
| H | -2.119966000 | -2.361045000 | -1.524534000 |
| C | -4.414555000 | -1.048351000 | -1.162162000 |
| H | -5.143866000 | -1.159433000 | -0.357340000 |
| H | -4.351882000 | -1.966586000 | -1.746527000 |
| H | -4.721633000 | -0.214916000 | -1.798162000 |
| O | -3.984774000 | 1.067675000  | 0.491296000  |
| N | -1.756015000 | 0.589089000  | 0.784853000  |
| S | 0.269965000  | 2.527893000  | -0.596993000 |
| F | 0.270820000  | -1.974306000 | -0.651411000 |

IM3-I-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.355606000 | 0.302132000  | 0.068885000  |
| C | -1.204730000 | 1.440922000  | 0.675003000  |
| C | -0.543362000 | 0.064916000  | 0.759857000  |
| C | -1.275817000 | -0.984321000 | -0.120902000 |
| N | -2.702433000 | -0.913553000 | 0.074333000  |
| H | -3.014358000 | 2.303363000  | 0.279754000  |
| H | -0.934193000 | -1.972014000 | 0.194270000  |
| C | -3.484550000 | -2.122832000 | -0.172996000 |
| H | -4.531003000 | -1.902688000 | 0.032340000  |
| H | -3.135461000 | -2.918642000 | 0.492622000  |
| H | -3.378606000 | -2.450662000 | -1.213560000 |
| O | -4.560971000 | 0.443258000  | -0.039374000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -2.518617000 | 1.419459000  | 0.243583000  |
| O | -0.665172000 | 2.463504000  | 1.049389000  |
| C | -0.684959000 | -0.354136000 | 2.248921000  |
| H | -0.207118000 | 0.396874000  | 2.882773000  |
| H | -1.741539000 | -0.428249000 | 2.520336000  |
| H | -0.192939000 | -1.313680000 | 2.415290000  |
| C | 3.050765000  | -0.915365000 | 0.645647000  |
| C | 0.940388000  | 0.110229000  | 0.376314000  |
| C | 1.477461000  | 1.044511000  | -0.553284000 |
| C | 2.814952000  | 1.006559000  | -0.815946000 |
| N | 3.600305000  | 0.074563000  | -0.220937000 |
| H | 0.268351000  | -1.525844000 | -1.924902000 |
| H | 3.275067000  | 1.705584000  | -1.505010000 |
| C | 5.040129000  | -0.004035000 | -0.467167000 |
| H | 5.572301000  | 0.049414000  | 0.485371000  |
| H | 5.342116000  | 0.819920000  | -1.116195000 |
| H | 5.280686000  | -0.963058000 | -0.932923000 |
| O | 3.784382000  | -1.778020000 | 1.101485000  |
| N | 1.698022000  | -0.813442000 | 0.917039000  |
| S | -0.917388000 | -0.882735000 | -1.972855000 |
| F | 0.713337000  | 1.932538000  | -1.211178000 |

#### IM4-I-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.349970000  | 0.308932000  | -0.148818000 |
| C | 1.165137000  | 1.346160000  | -0.822565000 |
| C | 0.528845000  | -0.043728000 | -0.752661000 |
| C | 1.299364000  | -0.967018000 | 0.235177000  |
| N | 2.720267000  | -0.910795000 | -0.032702000 |
| H | 2.964710000  | 2.274993000  | -0.546083000 |
| H | 0.958039000  | -1.989225000 | 0.055605000  |
| C | 3.527873000  | -2.063106000 | 0.357780000  |
| H | 4.558181000  | -1.881986000 | 0.055325000  |
| H | 3.145008000  | -2.955472000 | -0.146751000 |
| H | 3.490325000  | -2.215815000 | 1.443227000  |
| O | 4.553107000  | 0.486322000  | -0.073711000 |
| N | 2.484471000  | 1.392960000  | -0.403122000 |
| O | 0.599053000  | 2.319277000  | -1.279643000 |
| C | 0.668273000  | -0.623275000 | -2.186633000 |
| H | 0.162564000  | 0.037404000  | -2.894814000 |
| H | 1.723209000  | -0.703174000 | -2.461145000 |
| H | 0.197745000  | -1.606326000 | -2.236680000 |
| C | -3.090393000 | -0.938110000 | -0.597988000 |
| C | -0.954159000 | 0.034631000  | -0.369734000 |
| C | -1.466559000 | 1.022608000  | 0.516047000  |
| C | -2.799582000 | 1.031137000  | 0.790317000  |
| N | -3.609666000 | 0.093488000  | 0.238079000  |
| H | 1.212264000  | 0.581837000  | 2.089360000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -3.238952000 | 1.768597000  | 1.452166000  |
| C | -5.048664000 | 0.056911000  | 0.496941000  |
| H | -5.588187000 | 0.098719000  | -0.452160000 |
| H | -5.324930000 | 0.904472000  | 1.126875000  |
| H | -5.307717000 | -0.883356000 | 0.989987000  |
| O | -3.849655000 | -1.792065000 | -1.026493000 |
| N | -1.735590000 | -0.884018000 | -0.877751000 |
| S | 0.908593000  | -0.731904000 | 2.055226000  |
| F | -0.667421000 | 1.926582000  | 1.122395000  |

TS2-I-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.285630000  | 0.199891000  | 0.382177000  |
| C | 1.073018000  | 1.125576000  | 1.126774000  |
| C | 0.527208000  | 0.874014000  | -0.291983000 |
| C | 1.312972000  | -0.272013000 | -0.992310000 |
| N | 2.736233000  | -0.096884000 | -0.849655000 |
| H | 2.791495000  | 0.942433000  | 2.220251000  |
| H | 1.080070000  | -0.236097000 | -2.058852000 |
| C | 3.596346000  | -0.762205000 | -1.826088000 |
| H | 4.625309000  | -0.452030000 | -1.650476000 |
| H | 3.287081000  | -0.467162000 | -2.833130000 |
| H | 3.529907000  | -1.853637000 | -1.732688000 |
| O | 4.463710000  | 0.070836000  | 0.663455000  |
| N | 2.378093000  | 0.713413000  | 1.322870000  |
| O | 0.438589000  | 1.697669000  | 1.987123000  |
| C | 0.682170000  | 2.190573000  | -1.075715000 |
| H | 0.144246000  | 2.987730000  | -0.559025000 |
| H | 1.739420000  | 2.456941000  | -1.161260000 |
| H | 0.253187000  | 2.086978000  | -2.075992000 |
| C | -3.219845000 | 0.802883000  | -0.531819000 |
| C | -0.921495000 | 0.447512000  | -0.173761000 |
| C | -1.185769000 | -0.847085000 | 0.321665000  |
| C | -2.458688000 | -1.282510000 | 0.482490000  |
| N | -3.468913000 | -0.481213000 | 0.031232000  |
| H | 0.527245000  | -1.715640000 | 1.098924000  |
| H | -2.717504000 | -2.234866000 | 0.927033000  |
| C | -4.870738000 | -0.893180000 | 0.106611000  |
| H | -5.432555000 | -0.160072000 | 0.690319000  |
| H | -4.933983000 | -1.877549000 | 0.573846000  |
| H | -5.297831000 | -0.923284000 | -0.899032000 |
| O | -4.160261000 | 1.472806000  | -0.926935000 |
| N | -1.891859000 | 1.210010000  | -0.599652000 |
| S | 0.732248000  | -1.990264000 | -0.462484000 |
| F | -0.272009000 | -1.284227000 | 1.840987000  |

TS1-II-S0

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.282578000 | 0.050682000 | 0.335831000 |
|---|-------------|-------------|-------------|

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.237443000  | 1.376211000  | 0.898235000  |
| C | 0.566792000  | 0.883595000  | -0.407049000 |
| C | 1.240084000  | -0.432833000 | -0.959871000 |
| N | 2.688206000  | -0.353719000 | -0.837214000 |
| H | 2.935698000  | 1.179394000  | 2.006354000  |
| H | 1.030799000  | -0.462265000 | -2.032486000 |
| C | 3.453529000  | -1.282795000 | -1.667210000 |
| H | 4.511107000  | -1.032690000 | -1.592329000 |
| H | 3.121593000  | -1.183620000 | -2.705062000 |
| H | 3.303475000  | -2.318605000 | -1.337990000 |
| O | 4.436687000  | -0.181363000 | 0.651716000  |
| N | 2.475741000  | 0.853376000  | 1.163731000  |
| O | 0.711189000  | 2.221821000  | 1.595764000  |
| C | 0.695321000  | 2.029438000  | -1.426491000 |
| H | 0.298730000  | 2.962527000  | -1.013316000 |
| H | 1.751391000  | 2.186375000  | -1.663103000 |
| H | 0.178432000  | 1.787688000  | -2.362347000 |
| C | -3.226774000 | 0.625868000  | -0.582816000 |
| C | -0.832241000 | 0.487744000  | -0.068638000 |
| C | -0.967861000 | -0.710599000 | 0.711030000  |
| C | -2.318245000 | -1.158466000 | 0.795922000  |
| N | -3.350167000 | -0.545706000 | 0.156748000  |
| H | -1.795575000 | 1.910939000  | -1.186079000 |
| H | -2.559001000 | -2.062328000 | 1.340471000  |
| C | -4.716990000 | -1.077163000 | 0.238864000  |
| H | -4.701273000 | -2.014965000 | 0.793832000  |
| H | -5.100059000 | -1.238114000 | -0.770745000 |
| H | -5.359871000 | -0.348812000 | 0.738217000  |
| O | -4.162868000 | 1.203111000  | -1.128628000 |
| N | -1.910577000 | 1.061520000  | -0.642997000 |
| S | 0.497972000  | -1.955138000 | -0.200303000 |
| F | -0.363032000 | -0.654473000 | 1.994433000  |

#### IM3-II-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.870365000 | 0.641534000  | -0.783558000 |
| C | -1.116736000 | 1.808848000  | 0.572660000  |
| C | -0.560165000 | 0.461043000  | 1.043146000  |
| C | -1.545677000 | -0.727406000 | 0.821963000  |
| N | -2.444019000 | -0.577219000 | -0.315572000 |
| H | -2.536379000 | 2.649790000  | -0.620792000 |
| H | -2.133889000 | -0.907487000 | 1.731950000  |
| C | -3.239796000 | -1.747628000 | -0.692892000 |
| H | -4.018182000 | -1.421773000 | -1.379853000 |
| H | -3.700524000 | -2.193843000 | 0.198123000  |
| H | -2.607600000 | -2.495728000 | -1.175744000 |
| O | -3.757893000 | 0.808296000  | -1.602772000 |
| N | -2.205663000 | 1.763513000  | -0.254533000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -0.583139000 | 2.864634000  | 0.875679000  |
| C | -0.221238000 | 0.600274000  | 2.539045000  |
| H | 0.537329000  | 1.374323000  | 2.668329000  |
| H | -1.108275000 | 0.889248000  | 3.112048000  |
| H | 0.153981000  | -0.347506000 | 2.933875000  |
| C | 2.683349000  | 0.983243000  | -0.744781000 |
| C | 0.705569000  | 0.146118000  | 0.201750000  |
| C | 0.816636000  | -1.299359000 | -0.212444000 |
| C | 1.902038000  | -0.712118000 | 0.669958000  |
| N | 3.023944000  | -0.112359000 | 0.040391000  |
| H | 0.915024000  | 2.046189000  | -0.745901000 |
| H | 2.038391000  | -1.091076000 | 1.680374000  |
| C | 4.327469000  | -0.738783000 | -0.030445000 |
| H | 4.996486000  | -0.042869000 | -0.540342000 |
| H | 4.287545000  | -1.680454000 | -0.592369000 |
| H | 4.711524000  | -0.939117000 | 0.976402000  |
| O | 3.443551000  | 1.684103000  | -1.384074000 |
| N | 1.291595000  | 1.110382000  | -0.679568000 |
| S | -0.454852000 | -2.234054000 | 0.642374000  |
| F | 1.108280000  | -1.637324000 | -1.497354000 |

TS2-II-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.600079000 | 0.355989000  | -1.108844000 |
| C | -1.081337000 | 1.921417000  | 0.091106000  |
| C | -0.669413000 | 0.772115000  | 1.028300000  |
| C | -1.624312000 | -0.464916000 | 1.034985000  |
| N | -2.580092000 | -0.511534000 | -0.050491000 |
| H | -2.095640000 | 2.273697000  | -1.634577000 |
| H | -2.178935000 | -0.494629000 | 1.977887000  |
| C | -3.305538000 | -1.765934000 | -0.242805000 |
| H | -4.228081000 | -1.559381000 | -0.784344000 |
| H | -3.540830000 | -2.193023000 | 0.736443000  |
| H | -2.695864000 | -2.472883000 | -0.813734000 |
| O | -3.236027000 | 0.189312000  | -2.131848000 |
| N | -1.954694000 | 1.596692000  | -0.892921000 |
| O | -0.544748000 | 3.019173000  | 0.184600000  |
| C | -0.481639000 | 1.310467000  | 2.462797000  |
| H | 0.230081000  | 2.137900000  | 2.467154000  |
| H | -1.435243000 | 1.679102000  | 2.853537000  |
| H | -0.114429000 | 0.510901000  | 3.112453000  |
| C | 2.909321000  | 0.720464000  | -0.327644000 |
| C | 0.648315000  | 0.292312000  | 0.456854000  |
| C | 0.741720000  | -1.091465000 | 0.168992000  |
| C | 2.061601000  | -1.541734000 | 0.024322000  |
| N | 3.063021000  | -0.655107000 | -0.312988000 |
| H | 1.507765000  | 2.125636000  | 0.219384000  |
| H | 2.336780000  | -2.587011000 | 0.051386000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 4.376768000  | -1.154429000 | -0.729837000 |
| H | 5.145823000  | -0.468511000 | -0.374517000 |
| H | 4.427510000  | -1.206214000 | -1.821839000 |
| H | 4.528349000  | -2.149246000 | -0.306836000 |
| O | 3.766224000  | 1.524809000  | -0.672812000 |
| N | 1.656667000  | 1.118081000  | 0.161868000  |
| S | -0.498855000 | -1.970248000 | 1.130646000  |
| F | -0.103997000 | -0.989041000 | -1.366654000 |

IM4-II-S0

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.058671000 | 0.416573000  | -0.711744000 |
| C | -1.287013000 | 1.771977000  | 0.407772000  |
| C | -0.612594000 | 0.492766000  | 0.899036000  |
| C | -1.508695000 | -0.770448000 | 0.827980000  |
| N | -2.521879000 | -0.744471000 | -0.212969000 |
| H | -2.863248000 | 2.447152000  | -0.686159000 |
| H | -1.994315000 | -0.945351000 | 1.796248000  |
| C | -3.256112000 | -1.984361000 | -0.457012000 |
| H | -4.121561000 | -1.752799000 | -1.075037000 |
| H | -3.591178000 | -2.418125000 | 0.494913000  |
| H | -2.619148000 | -2.708278000 | -0.971748000 |
| O | -4.007409000 | 0.472388000  | -1.476292000 |
| N | -2.465374000 | 1.614114000  | -0.265975000 |
| O | -0.769150000 | 2.866078000  | 0.575575000  |
| C | -0.107520000 | 0.702930000  | 2.335482000  |
| H | 0.520288000  | 1.592552000  | 2.383915000  |
| H | -0.955711000 | 0.840824000  | 3.013840000  |
| H | 0.472090000  | -0.161555000 | 2.669480000  |
| C | 2.961337000  | 0.838319000  | -0.312749000 |
| C | 0.567637000  | 0.221644000  | -0.080279000 |
| C | 1.016129000  | -1.179812000 | 0.129662000  |
| C | 2.311032000  | -1.491099000 | -0.031956000 |
| N | 3.262176000  | -0.523252000 | -0.346835000 |
| H | 1.417946000  | 2.113269000  | 0.020995000  |
| H | 2.697798000  | -2.498462000 | 0.079900000  |
| C | 4.619963000  | -0.936891000 | -0.689713000 |
| H | 5.226706000  | -0.038715000 | -0.793508000 |
| H | 4.627384000  | -1.492692000 | -1.633782000 |
| H | 5.035295000  | -1.567712000 | 0.104005000  |
| O | 3.784326000  | 1.716765000  | -0.518116000 |
| N | 1.647437000  | 1.124299000  | 0.036299000  |
| S | -0.323057000 | -2.221963000 | 0.628810000  |
| F | -0.008339000 | 0.323892000  | -1.387319000 |

TS3-II-S0

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.833091000 | -0.319824000 | -0.893849000 |
| C | 1.391679000 | -1.648055000 | 0.595154000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.685153000  | -0.362749000 | 1.062843000  |
| C | 1.500559000  | 0.921706000  | 0.761477000  |
| N | 2.216293000  | 0.856255000  | -0.495365000 |
| H | 2.963076000  | -2.290096000 | -0.491359000 |
| H | 2.178658000  | 1.155242000  | 1.593689000  |
| C | 2.739087000  | 2.099860000  | -1.054941000 |
| H | 3.426749000  | 1.839057000  | -1.857215000 |
| H | 3.277000000  | 2.676863000  | -0.288814000 |
| H | 1.926378000  | 2.712540000  | -1.451820000 |
| O | 3.618187000  | -0.394117000 | -1.821991000 |
| N | 2.571027000  | -1.442311000 | -0.094535000 |
| O | 1.034420000  | -2.743584000 | 0.981228000  |
| C | 0.413973000  | -0.499051000 | 2.582184000  |
| H | -0.166187000 | -1.406556000 | 2.755632000  |
| H | 1.365240000  | -0.590206000 | 3.115869000  |
| H | -0.124356000 | 0.369536000  | 2.971341000  |
| C | -2.814438000 | -0.904427000 | -0.350747000 |
| C | -0.647348000 | -0.158872000 | 0.373684000  |
| C | -1.043956000 | 1.189920000  | 0.311297000  |
| C | -2.332842000 | 1.463855000  | -0.069355000 |
| N | -3.204519000 | 0.462412000  | -0.349884000 |
| H | -0.953611000 | -1.842588000 | -0.447002000 |
| H | -2.717746000 | 2.474939000  | -0.151703000 |
| C | -4.565800000 | 0.729673000  | -0.825959000 |
| H | -5.271978000 | 0.132487000  | -0.246499000 |
| H | -4.653826000 | 0.442810000  | -1.876831000 |
| H | -4.782184000 | 1.792197000  | -0.705448000 |
| O | -3.568966000 | -1.767650000 | -0.746125000 |
| N | -1.535085000 | -1.147059000 | 0.134470000  |
| S | 0.235218000  | 2.318200000  | 0.786933000  |
| F | 0.201245000  | -1.276879000 | -1.347689000 |

P-3a

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.364977000 | 0.313988000  | -1.355902000 |
| C | -1.316277000 | 1.827007000  | 0.328212000  |
| C | -0.745398000 | 0.597799000  | 1.042409000  |
| C | -1.593393000 | -0.679948000 | 0.814592000  |
| N | -2.218276000 | -0.751772000 | -0.490632000 |
| H | -2.140722000 | 2.336208000  | -1.477689000 |
| H | -2.347988000 | -0.802358000 | 1.600576000  |
| C | -2.929601000 | -1.986508000 | -0.816709000 |
| H | -3.560731000 | -1.801422000 | -1.683883000 |
| H | -3.551440000 | -2.288875000 | 0.035409000  |
| H | -2.225708000 | -2.793231000 | -1.040405000 |
| O | -2.917505000 | 0.239763000  | -2.441139000 |
| N | -1.878290000 | 1.545629000  | -0.900128000 |
| O | -1.225368000 | 2.955915000  | 0.760308000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.588055000 | 0.907938000  | 2.543267000  |
| H | 0.050341000  | 1.785190000  | 2.657049000  |
| H | -1.562768000 | 1.132945000  | 2.987100000  |
| H | -0.143746000 | 0.058544000  | 3.068797000  |
| C | 2.707412000  | 0.875275000  | -0.409533000 |
| C | 0.637141000  | 0.284011000  | 0.456193000  |
| C | 0.924459000  | -1.113392000 | 0.442793000  |
| C | 2.148989000  | -1.480818000 | -0.035962000 |
| N | 3.021477000  | -0.521451000 | -0.448327000 |
| H | 2.481379000  | -2.511039000 | -0.109782000 |
| C | 4.348066000  | -0.859070000 | -0.964561000 |
| H | 5.113613000  | -0.384774000 | -0.345682000 |
| H | 4.453419000  | -0.474643000 | -1.981886000 |
| H | 4.473931000  | -1.943564000 | -0.955679000 |
| O | 3.543807000  | 1.675255000  | -0.790856000 |
| N | 1.447150000  | 1.220791000  | 0.062755000  |
| S | -0.388855000 | -2.115658000 | 1.074069000  |

HF

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 0.000000000 | 0.000000000 | -0.840422000 |
| F | 0.000000000 | 0.000000000 | 0.093380000  |

LIIC path connecting IM1-I-T1S0 and TS-A-S0

Coord\_1

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251897000  | -1.159267000 | 0.715587000  |
| C | 0.167471000  | -0.133127000 | 1.655189000  |
| C | 0.652127000  | 1.167298000  | 1.216750000  |
| C | 1.789570000  | 1.220246000  | 0.278911000  |
| N | 2.677100000  | 0.106700000  | 0.344007000  |
| H | 0.695921000  | -2.122114000 | 1.621734000  |
| H | 2.352064000  | 2.154562000  | 0.346703000  |
| C | 3.914128000  | 0.195347000  | -0.427477000 |
| H | 4.550726000  | -0.646306000 | -0.160398000 |
| H | 4.419985000  | 1.135362000  | -0.185186000 |
| H | 3.704392000  | 0.163030000  | -1.503144000 |
| O | 2.905725000  | -2.174292000 | 0.553143000  |
| N | 1.011735000  | -1.197396000 | 1.357670000  |
| O | -0.904145000 | -0.311904000 | 2.231722000  |
| C | -0.107718000 | 2.391127000  | 1.590529000  |
| H | -1.177717000 | 2.170249000  | 1.659033000  |
| H | 0.206751000  | 2.751000000  | 2.581941000  |
| H | 0.060973000  | 3.199496000  | 0.872707000  |
| C | -2.729873000 | 0.544801000  | -0.327921000 |
| C | -0.481278000 | 0.494643000  | -1.402096000 |
| C | -0.553203000 | -0.899822000 | -1.395879000 |
| C | -1.646913000 | -1.560619000 | -0.897747000 |
| N | -2.715990000 | -0.848282000 | -0.350728000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.678658000 | 2.148083000  | -0.968704000 |
| H | -1.714888000 | -2.639276000 | -0.893876000 |
| C | -3.650815000 | -1.544126000 | 0.530602000  |
| H | -4.549683000 | -0.937549000 | 0.630387000  |
| H | -3.194534000 | -1.685585000 | 1.517180000  |
| H | -3.904306000 | -2.513266000 | 0.091871000  |
| O | -3.603466000 | 1.207555000  | 0.211801000  |
| N | -1.668253000 | 1.138221000  | -0.996203000 |
| S | 0.981125000  | 1.433991000  | -1.565501000 |
| F | 0.509061000  | -1.620681000 | -1.804163000 |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.284856000  | -1.209526000 | 0.609944000  |
| C | 0.183042000  | -0.303508000 | 1.634309000  |
| C | 0.632686000  | 1.033713000  | 1.281456000  |
| C | 1.790561000  | 1.190860000  | 0.384370000  |
| N | 2.687924000  | 0.092902000  | 0.340300000  |
| H | 0.756022000  | -2.272479000 | 1.446844000  |
| H | 2.331459000  | 2.128670000  | 0.524868000  |
| C | 3.920929000  | 0.267153000  | -0.423443000 |
| H | 4.568933000  | -0.587376000 | -0.237232000 |
| H | 4.415980000  | 1.187619000  | -0.098497000 |
| H | 3.703276000  | 0.331400000  | -1.496116000 |
| O | 2.956453000  | -2.194372000 | 0.360166000  |
| N | 1.051463000  | -1.323679000 | 1.254012000  |
| O | -0.881402000 | -0.550933000 | 2.198126000  |
| C | -0.128056000 | 2.216224000  | 1.776298000  |
| H | -1.195218000 | 1.982549000  | 1.843876000  |
| H | 0.203170000  | 2.492865000  | 2.788414000  |
| H | 0.021796000  | 3.084434000  | 1.127172000  |
| C | -2.752804000 | 0.570812000  | -0.280304000 |
| C | -0.480302000 | 0.618192000  | -1.299448000 |
| C | -0.549299000 | -0.776854000 | -1.425162000 |
| C | -1.648619000 | -1.475678000 | -1.003893000 |
| N | -2.729778000 | -0.815468000 | -0.417762000 |
| H | -1.697428000 | 2.223978000  | -0.770444000 |
| H | -1.715616000 | -2.550823000 | -1.094725000 |
| C | -3.681400000 | -1.586588000 | 0.379233000  |
| H | -4.583757000 | -0.991688000 | 0.512187000  |
| H | -3.245717000 | -1.813543000 | 1.359075000  |
| H | -3.922817000 | -2.513975000 | -0.147584000 |
| O | -3.641040000 | 1.183966000  | 0.292184000  |
| N | -1.679828000 | 1.219077000  | -0.876381000 |
| S | 0.966797000  | 1.586241000  | -1.466939000 |
| F | 0.520116000  | -1.452156000 | -1.887996000 |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.316118000  | -1.245183000 | 0.513310000  |
| C | 0.197397000  | -0.454973000 | 1.599230000  |
| C | 0.612430000  | 0.910064000  | 1.323126000  |
| C | 1.789573000  | 1.156423000  | 0.476330000  |
| N | 2.696726000  | 0.083440000  | 0.337068000  |
| H | 0.814015000  | -2.394672000 | 1.279886000  |
| H | 2.308861000  | 2.093191000  | 0.682201000  |
| C | 3.925871000  | 0.335489000  | -0.411466000 |
| H | 4.585163000  | -0.523031000 | -0.297820000 |
| H | 4.409758000  | 1.232776000  | -0.013536000 |
| H | 3.700865000  | 0.485351000  | -1.474046000 |
| O | 3.005667000  | -2.195026000 | 0.189437000  |
| N | 1.089433000  | -1.429012000 | 1.151607000  |
| O | -0.860051000 | -0.764395000 | 2.144883000  |
| C | -0.149201000 | 2.044784000  | 1.924132000  |
| H | -1.213126000 | 1.797305000  | 1.990814000  |
| H | 0.198241000  | 2.246733000  | 2.948067000  |
| H | -0.018256000 | 2.961621000  | 1.340760000  |
| C | -2.772792000 | 0.589431000  | -0.235936000 |
| C | -0.478370000 | 0.717260000  | -1.194619000 |
| C | -0.544532000 | -0.668095000 | -1.439417000 |
| C | -1.648591000 | -1.393984000 | -1.088887000 |
| N | -2.740824000 | -0.782590000 | -0.473254000 |
| H | -1.714500000 | 2.275960000  | -0.588413000 |
| H | -1.714353000 | -2.459098000 | -1.263307000 |
| C | -3.707719000 | -1.612896000 | 0.242049000  |
| H | -4.613145000 | -1.029522000 | 0.402308000  |
| H | -3.291622000 | -1.915640000 | 1.209782000  |
| H | -3.937370000 | -2.496566000 | -0.359734000 |
| O | -3.674533000 | 1.157908000  | 0.360155000  |
| N | -1.689503000 | 1.280511000  | -0.763012000 |
| S | 0.950084000  | 1.718212000  | -1.369171000 |
| F | 0.531505000  | -1.298896000 | -1.946667000 |

Coord\_4

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.346025000 | -1.268422000 | 0.428806000  |
| C | 0.211291000 | -0.584614000 | 1.556016000  |
| C | 0.592068000 | 0.800789000  | 1.344340000  |
| C | 1.787088000 | 1.120421000  | 0.553098000  |
| N | 2.703840000 | 0.078230000  | 0.333906000  |
| H | 0.870455000 | -2.490659000 | 1.129557000  |
| H | 2.285006000 | 2.053602000  | 0.814926000  |
| C | 3.928973000 | 0.398699000  | -0.395214000 |
| H | 4.599450000 | -0.457061000 | -0.344136000 |
| H | 4.401547000 | 1.271915000  | 0.064658000  |
| H | 3.696727000 | 0.621406000  | -1.443385000 |
| O | 3.053515000 | -2.181536000 | 0.044756000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 1.126221000  | -1.513833000 | 1.056604000  |
| O | -0.839088000 | -0.948433000 | 2.081014000  |
| C | -0.170040000 | 1.885543000  | 2.035839000  |
| H | -1.230330000 | 1.623688000  | 2.102621000  |
| H | 0.193560000  | 2.023515000  | 3.064443000  |
| H | -0.058212000 | 2.840432000  | 1.512177000  |
| C | -2.790417000 | 0.601601000  | -0.196460000 |
| C | -0.475761000 | 0.792867000  | -1.091937000 |
| C | -0.539331000 | -0.576339000 | -1.440543000 |
| C | -1.647405000 | -1.320153000 | -1.152974000 |
| N | -2.749830000 | -0.752258000 | -0.517123000 |
| H | -1.730112000 | 2.308398000  | -0.428054000 |
| H | -1.711708000 | -2.371499000 | -1.398519000 |
| C | -3.730793000 | -1.627023000 | 0.122389000  |
| H | -4.638893000 | -1.054051000 | 0.303596000  |
| H | -3.333490000 | -1.994513000 | 1.075425000  |
| H | -3.948976000 | -2.468311000 | -0.541143000 |
| O | -3.704675000 | 1.131948000  | 0.414655000  |
| N | -1.697610000 | 1.324627000  | -0.660086000 |
| S | 0.930826000  | 1.829558000  | -1.279180000 |
| F | 0.542800000  | -1.165911000 | -1.982440000 |

Coord\_5

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.374861000  | -1.282131000 | 0.356817000  |
| C | 0.225431000  | -0.693200000 | 1.509662000  |
| C | 0.572193000  | 0.707120000  | 1.349307000  |
| C | 1.783534000  | 1.085355000  | 0.615363000  |
| N | 2.709522000  | 0.076830000  | 0.330366000  |
| H | 0.925864000  | -2.564992000 | 0.999524000  |
| H | 2.260585000  | 2.014041000  | 0.923501000  |
| C | 3.930174000  | 0.456604000  | -0.377916000 |
| H | 4.611740000  | -0.391789000 | -0.379624000 |
| H | 4.391508000  | 1.306809000  | 0.133293000  |
| H | 3.690342000  | 0.739744000  | -1.409685000 |
| O | 3.100084000  | -2.158940000 | -0.074841000 |
| N | 1.162359000  | -1.580938000 | 0.972087000  |
| O | -0.817516000 | -1.104307000 | 2.013845000  |
| C | -0.189549000 | 1.742592000  | 2.117317000  |
| H | -1.245781000 | 1.465961000  | 2.185875000  |
| H | 0.190630000  | 1.827377000  | 3.145359000  |
| H | -0.097215000 | 2.726734000  | 1.646164000  |
| C | -2.806193000 | 0.608584000  | -0.162191000 |
| C | -0.472737000 | 0.848415000  | -0.993622000 |
| C | -0.534084000 | -0.501341000 | -1.431276000 |
| C | -1.645439000 | -1.256279000 | -1.199040000 |
| N | -2.757332000 | -0.725955000 | -0.550824000 |
| H | -1.744526000 | 2.326429000  | -0.289841000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.707924000 | -2.292280000 | -1.504153000 |
| C | -3.751400000 | -1.633179000 | 0.019935000  |
| H | -4.661838000 | -1.068990000 | 0.216274000  |
| H | -3.372318000 | -2.055070000 | 0.957675000  |
| H | -3.958314000 | -2.435219000 | -0.693825000 |
| O | -3.732151000 | 1.107576000  | 0.456823000  |
| N | -1.704473000 | 1.354802000  | -0.568602000 |
| S | 0.908749000  | 1.922724000  | -1.200512000 |
| F | 0.553628000  | -1.053932000 | -1.999588000 |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.402826000  | -1.288924000 | 0.296071000  |
| C | 0.240466000  | -0.783269000 | 1.463628000  |
| C | 0.553278000  | 0.628263000  | 1.342305000  |
| C | 1.779290000  | 1.052628000  | 0.664890000  |
| N | 2.713951000  | 0.078664000  | 0.325913000  |
| H | 0.980693000  | -2.622520000 | 0.890028000  |
| H | 2.236278000  | 1.976964000  | 1.010433000  |
| C | 3.929332000  | 0.509814000  | -0.362153000 |
| H | 4.621874000  | -0.328288000 | -0.408135000 |
| H | 4.379747000  | 1.339155000  | 0.191046000  |
| H | 3.681105000  | 0.842405000  | -1.377060000 |
| O | 3.145369000  | -2.130994000 | -0.172857000 |
| N | 1.198312000  | -1.633718000 | 0.898853000  |
| O | -0.794359000 | -1.235731000 | 1.948454000  |
| C | -0.206783000 | 1.616558000  | 2.175555000  |
| H | -1.258478000 | 1.324773000  | 2.248031000  |
| H | 0.190877000  | 1.657864000  | 3.199314000  |
| H | -0.134491000 | 2.623124000  | 1.749892000  |
| C | -2.820559000 | 0.611488000  | -0.132616000 |
| C | -0.469550000 | 0.887927000  | -0.900065000 |
| C | -0.529151000 | -0.441113000 | -1.414047000 |
| C | -1.642866000 | -1.202537000 | -1.230858000 |
| N | -2.763696000 | -0.704205000 | -0.576430000 |
| H | -1.758036000 | 2.334401000  | -0.171241000 |
| H | -1.702856000 | -2.222867000 | -1.586053000 |
| C | -3.770059000 | -1.634830000 | -0.067832000 |
| H | -4.682585000 | -1.077771000 | 0.138829000  |
| H | -3.408825000 | -2.102498000 | 0.855059000  |
| H | -3.965723000 | -2.401237000 | -0.822657000 |
| O | -3.757596000 | 1.085200000  | 0.488758000  |
| N | -1.710406000 | 1.374337000  | -0.487550000 |
| S | 0.883483000  | 2.001007000  | -1.134091000 |
| F | 0.563655000  | -0.960998000 | -2.002403000 |

Coord\_7

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.430029000 | -1.290796000 | 0.244601000 |
|---|-------------|--------------|-------------|



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.256975000  | -0.857767000 | 1.420113000  |
| C | 0.535672000  | 0.562538000  | 1.327001000  |
| C | 1.774678000  | 1.022845000  | 0.703645000  |
| N | 2.717221000  | 0.083181000  | 0.319958000  |
| H | 1.035310000  | -2.667325000 | 0.799610000  |
| H | 2.212742000  | 1.943537000  | 1.078740000  |
| C | 3.926222000  | 0.559205000  | -0.349941000 |
| H | 4.629584000  | -0.266814000 | -0.433316000 |
| H | 4.366309000  | 1.370303000  | 0.237298000  |
| H | 3.668320000  | 0.931961000  | -1.348362000 |
| O | 3.189263000  | -2.100113000 | -0.253605000 |
| N | 1.234461000  | -1.675224000 | 0.836444000  |
| O | -0.768677000 | -1.347006000 | 1.888106000  |
| C | -0.220887000 | 1.506188000  | 2.217008000  |
| H | -1.267475000 | 1.198811000  | 2.295884000  |
| H | 0.195622000  | 1.512234000  | 3.233735000  |
| H | -0.169352000 | 2.530038000  | 1.830685000  |
| C | -2.833865000 | 0.611083000  | -0.106855000 |
| C | -0.466429000 | 0.915080000  | -0.810503000 |
| C | -0.524867000 | -0.393005000 | -1.390595000 |
| C | -1.639651000 | -1.158027000 | -1.252106000 |
| N | -2.769099000 | -0.686954000 | -0.596073000 |
| H | -1.770965000 | 2.335424000  | -0.068454000 |
| H | -1.695970000 | -2.162835000 | -1.650309000 |
| C | -3.786995000 | -1.634512000 | -0.144368000 |
| H | -4.701487000 | -1.083216000 | 0.068889000  |
| H | -3.443405000 | -2.141334000 | 0.764415000  |
| H | -3.971173000 | -2.368514000 | -0.933441000 |
| O | -3.781562000 | 1.064440000  | 0.512712000  |
| N | -1.715703000 | 1.385888000  | -0.414926000 |
| S | 0.854574000  | 2.067462000  | -1.079356000 |
| F | 0.572567000  | -0.883940000 | -1.994355000 |

Coord\_8

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.456509000 | -1.289127000 | 0.200328000  |
| C | 0.275454000 | -0.919418000 | 1.380450000  |
| C | 0.519564000 | 0.508054000  | 1.306323000  |
| C | 1.769936000 | 0.996146000  | 0.733418000  |
| N | 2.719334000 | 0.089938000  | 0.311917000  |
| H | 1.090031000 | -2.702500000 | 0.726191000  |
| H | 2.190552000 | 1.914136000  | 1.131244000  |
| C | 3.920528000 | 0.605705000  | -0.342840000 |
| H | 4.634510000 | -0.207129000 | -0.458355000 |
| H | 4.351142000 | 1.401294000  | 0.271744000  |
| H | 3.651227000 | 1.010911000  | -1.325501000 |
| O | 3.231596000 | -2.067653000 | -0.321291000 |
| N | 1.271125000 | -1.707874000 | 0.783856000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -0.739578000 | -1.442142000 | 1.834830000  |
| C | -0.231145000 | 1.409429000  | 2.247053000  |
| H | -1.271929000 | 1.085922000  | 2.335063000  |
| H | 0.206001000  | 1.386964000  | 3.254516000  |
| H | -0.201243000 | 2.446729000  | 1.895050000  |
| C | -2.846351000 | 0.607798000  | -0.083950000 |
| C | -0.463568000 | 0.932861000  | -0.723611000 |
| C | -0.521522000 | -0.354318000 | -1.362037000 |
| C | -1.635571000 | -1.121381000 | -1.265986000 |
| N | -2.773533000 | -0.673873000 | -0.611685000 |
| H | -1.783634000 | 2.331473000  | 0.022562000  |
| H | -1.686401000 | -2.110748000 | -1.702435000 |
| C | -3.802147000 | -1.633969000 | -0.213294000 |
| H | -4.718631000 | -1.087534000 | 0.003831000  |
| H | -3.476108000 | -2.175232000 | 0.681927000  |
| H | -3.974307000 | -2.337940000 | -1.031825000 |
| O | -3.804487000 | 1.044443000  | 0.530723000  |
| N | -1.720619000 | 1.391370000  | -0.348413000 |
| S | 0.821473000  | 2.124534000  | -1.035053000 |
| F | 0.580079000  | -0.819297000 | -1.978012000 |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.482326000  | -1.284748000 | 0.161302000  |
| C | 0.296353000  | -0.970567000 | 1.345370000  |
| C | 0.504973000  | 0.462977000  | 1.282537000  |
| C | 1.765169000  | 0.972431000  | 0.755739000  |
| N | 2.720218000  | 0.098668000  | 0.301277000  |
| H | 1.145272000  | -2.730272000 | 0.667545000  |
| H | 2.170077000  | 1.888731000  | 1.170411000  |
| C | 3.911857000  | 0.650320000  | -0.341985000 |
| H | 4.636243000  | -0.148564000 | -0.485853000 |
| H | 4.334038000  | 1.433069000  | 0.294306000  |
| H | 3.629019000  | 1.081586000  | -1.309656000 |
| O | 3.272279000  | -2.034139000 | -0.379677000 |
| N | 1.308644000  | -1.733479000 | 0.739874000  |
| O | -0.706167000 | -1.524669000 | 1.789782000  |
| C | -0.237058000 | 1.323952000  | 2.269943000  |
| H | -1.271162000 | 0.983610000  | 2.369971000  |
| H | 0.222851000  | 1.278435000  | 3.266099000  |
| H | -0.229831000 | 2.371824000  | 1.948425000  |
| C | -2.858146000 | 0.601791000  | -0.062997000 |
| C | -0.461091000 | 0.943487000  | -0.637927000 |
| C | -0.519342000 | -0.322636000 | -1.329088000 |
| C | -1.630294000 | -1.091101000 | -1.275108000 |
| N | -2.776859000 | -0.664532000 | -0.624885000 |
| H | -1.796282000 | 2.323599000  | 0.105577000  |
| H | -1.673162000 | -2.064715000 | -1.747016000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.815262000 | -1.634296000 | -0.277921000 |
| H | -4.733904000 | -1.092321000 | -0.058806000 |
| H | -3.506732000 | -2.206940000 | 0.603812000  |
| H | -3.974585000 | -2.309578000 | -1.122732000 |
| O | -3.826666000 | 1.024160000  | 0.544509000  |
| N | -1.725337000 | 1.392000000  | -0.285768000 |
| S | 0.783468000  | 2.174047000  | -0.999631000 |
| F | 0.585950000  | -0.763809000 | -1.955286000 |

Coord\_10

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.507710000  | -1.277961000 | 0.125753000  |
| C | 0.320188000  | -1.013252000 | 1.315130000  |
| C | 0.491789000  | 0.425557000  | 1.257340000  |
| C | 1.760323000  | 0.951522000  | 0.771897000  |
| N | 2.719778000  | 0.109393000  | 0.287629000  |
| H | 1.201808000  | -2.752183000 | 0.621396000  |
| H | 2.151329000  | 1.867140000  | 1.198384000  |
| C | 3.899734000  | 0.694327000  | -0.348102000 |
| H | 4.634394000  | -0.089864000 | -0.517811000 |
| H | 4.314546000  | 1.466770000  | 0.305166000  |
| H | 3.600834000  | 1.146333000  | -1.301390000 |
| O | 3.311510000  | -1.999327000 | -0.432049000 |
| N | 1.347570000  | -1.753332000 | 0.703166000  |
| O | -0.667401000 | -1.597737000 | 1.753412000  |
| C | -0.238361000 | 1.247285000  | 2.288909000  |
| H | -1.264658000 | 0.889132000  | 2.403870000  |
| H | 0.246672000  | 1.183135000  | 3.271700000  |
| H | -0.255084000 | 2.303524000  | 1.995209000  |
| C | -2.869310000 | 0.593045000  | -0.043204000 |
| C | -0.459021000 | 0.948365000  | -0.552122000 |
| C | -0.518459000 | -0.296060000 | -1.292271000 |
| C | -1.623540000 | -1.065754000 | -1.281430000 |
| N | -2.778945000 | -0.658476000 | -0.636898000 |
| H | -1.808949000 | 2.312078000  | 0.183841000  |
| H | -1.655513000 | -2.022764000 | -1.787501000 |
| C | -3.826115000 | -1.635986000 | -0.340934000 |
| H | -4.747164000 | -1.098458000 | -0.121032000 |
| H | -3.535096000 | -2.238278000 | 0.526819000  |
| H | -3.971600000 | -2.282912000 | -1.210017000 |
| O | -3.848256000 | 1.002597000  | 0.555466000  |
| N | -1.729947000 | 1.388329000  | -0.225034000 |
| S | 0.739550000  | 2.217299000  | -0.971376000 |
| F | 0.590003000  | -0.714738000 | -1.927676000 |

LIIC path connecting IM1-II-T1S0 and IM2-A-S0

Coord\_1

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.582993700 | -1.313703400 | 0.261548100 |
|---|-------------|--------------|-------------|

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.509982100  | -0.599239200 | 1.505653400  |
| C | 0.654993200  | 0.818900200  | 0.933467300  |
| C | 2.039118600  | 1.044249300  | 0.409302100  |
| N | 2.823835800  | -0.000135000 | -0.065563000 |
| H | 1.345148400  | -2.458792700 | 1.414400400  |
| H | 2.323869700  | 2.031268600  | 0.069267000  |
| C | 3.891749100  | 0.288945100  | -1.021208300 |
| H | 4.546375300  | -0.578915200 | -1.084624300 |
| H | 4.458566200  | 1.158044300  | -0.676487200 |
| H | 3.461127000  | 0.499090100  | -2.006015600 |
| O | 3.242946900  | -2.267980600 | -0.120648000 |
| N | 1.481704400  | -1.499302400 | 1.118210300  |
| O | -0.419424100 | -0.932556300 | 2.219832600  |
| C | 0.367413100  | 1.837522500  | 2.054354600  |
| H | -0.551789200 | 1.586813400  | 2.588355700  |
| H | 1.187360300  | 1.815402500  | 2.776326800  |
| H | 0.297808100  | 2.849388800  | 1.644037500  |
| C | -2.856026800 | 0.050282000  | 0.228070100  |
| C | -0.468352100 | 0.915844300  | -0.211564100 |
| C | -0.424082100 | -0.234490100 | -1.161884300 |
| C | -1.426230400 | -1.097967300 | -1.341382400 |
| N | -2.629745700 | -0.997536300 | -0.648460200 |
| H | -2.012120600 | 1.693121500  | 1.007778300  |
| H | -1.338736400 | -1.913016500 | -2.049655600 |
| C | -3.618298000 | -2.067495600 | -0.748373200 |
| H | -4.544643300 | -1.713474500 | -0.298370100 |
| H | -3.279534900 | -2.964444800 | -0.216613100 |
| H | -3.790867100 | -2.312955600 | -1.801196500 |
| O | -3.879427100 | 0.189715100  | 0.877539200  |
| N | -1.821853500 | 0.983214300  | 0.313016100  |
| S | -0.433825100 | 2.520620700  | -1.175325300 |
| F | 0.714078200  | -0.353485100 | -1.877707500 |

Coord\_2

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.643802500 | -1.274627600 | 0.269236800  |
| C | 0.561046000 | -0.628019200 | 1.515583600  |
| C | 0.656705600 | 0.783462700  | 0.938155200  |
| C | 2.012524900 | 1.054347100  | 0.378196300  |
| N | 2.832581400 | 0.030529200  | -0.082144100 |
| H | 1.461012900 | -2.443328500 | 1.441139400  |
| H | 2.309314400 | 2.034671400  | 0.124033700  |
| C | 3.887618600 | 0.346049300  | -1.039244900 |
| H | 4.559482800 | -0.505148800 | -1.108706300 |
| H | 4.436407000 | 1.224951300  | -0.693623600 |
| H | 3.449634100 | 0.550413100  | -2.021738700 |
| O | 3.335727300 | -2.202472900 | -0.101420200 |
| N | 1.562067500 | -1.486683000 | 1.138939400  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -0.354964700 | -0.988417100 | 2.228769400  |
| C | 0.352616200  | 1.793827900  | 2.059641500  |
| H | -0.561507900 | 1.525838600  | 2.591317800  |
| H | 1.171763500  | 1.785709000  | 2.782119200  |
| H | 0.265373800  | 2.804032900  | 1.651310000  |
| C | -2.870001600 | 0.083395500  | 0.191939300  |
| C | -0.464020100 | 0.857195300  | -0.207804600 |
| C | -0.442965300 | -0.314566900 | -1.119090500 |
| C | -1.465122300 | -1.146599600 | -1.303016700 |
| N | -2.668254300 | -0.988468800 | -0.650697700 |
| H | -1.986823300 | 1.709105700  | 0.950104500  |
| H | -1.394436500 | -1.980498200 | -1.982244700 |
| C | -3.687419700 | -2.015667000 | -0.766977500 |
| H | -4.600245000 | -1.626938600 | -0.332866500 |
| H | -3.392131900 | -2.916009700 | -0.229761100 |
| H | -3.852584700 | -2.259758900 | -1.821177300 |
| O | -3.892763000 | 0.275347400  | 0.801480200  |
| N | -1.811126500 | 0.972911700  | 0.293720400  |
| S | -0.315261100 | 2.413104000  | -1.186383900 |
| F | 0.696063000  | -0.490755100 | -1.792707500 |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.704611300  | -1.235551800 | 0.276925400  |
| C | 0.612109900  | -0.656799300 | 1.525513800  |
| C | 0.658418000  | 0.748025100  | 0.942843100  |
| C | 1.985931200  | 1.064444900  | 0.347090500  |
| N | 2.841327100  | 0.061193400  | -0.098725200 |
| H | 1.576877400  | -2.427864300 | 1.467878500  |
| H | 2.294759100  | 2.038074300  | 0.178800400  |
| C | 3.883488100  | 0.403153500  | -1.057281500 |
| H | 4.572590400  | -0.431382400 | -1.132788300 |
| H | 4.414247700  | 1.291858300  | -0.710760100 |
| H | 3.438141300  | 0.601736100  | -2.037461800 |
| O | 3.428507700  | -2.136965100 | -0.082192300 |
| N | 1.642430600  | -1.474063500 | 1.159668500  |
| O | -0.290505400 | -1.044277900 | 2.237706200  |
| C | 0.337819400  | 1.750133300  | 2.064928500  |
| H | -0.571226700 | 1.464863800  | 2.594280000  |
| H | 1.156166600  | 1.756015400  | 2.787911600  |
| H | 0.232939600  | 2.758677000  | 1.658582400  |
| C | -2.883976300 | 0.116508900  | 0.155808500  |
| C | -0.459688000 | 0.798546400  | -0.204045100 |
| C | -0.461848500 | -0.394643800 | -1.076296800 |
| C | -1.504014200 | -1.195231800 | -1.264651000 |
| N | -2.706762800 | -0.979401300 | -0.652935200 |
| H | -1.961526000 | 1.725090000  | 0.892430700  |
| H | -1.450136600 | -2.047979800 | -1.914833900 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.756541300 | -1.963838500 | -0.785581700 |
| H | -4.655846800 | -1.540402800 | -0.367362900 |
| H | -3.504728900 | -2.867574600 | -0.242909100 |
| H | -3.914302300 | -2.206562100 | -1.841158100 |
| O | -3.906099000 | 0.360979800  | 0.725421100  |
| N | -1.800399500 | 0.962609100  | 0.274424800  |
| S | -0.196697100 | 2.305587300  | -1.197442500 |
| F | 0.678047700  | -0.628025200 | -1.707707600 |

Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.764582000  | -1.197551000 | 0.285175700  |
| C | 0.662938300  | -0.685048700 | 1.535514700  |
| C | 0.660158100  | 0.712429600  | 0.948083300  |
| C | 1.958905900  | 1.072187900  | 0.315078000  |
| N | 2.849360700  | 0.094228400  | -0.115259500 |
| H | 1.692712000  | -2.412850400 | 1.494734600  |
| H | 2.280834300  | 2.043269500  | 0.233532600  |
| C | 3.879587500  | 0.460399400  | -1.075488800 |
| H | 4.585784600  | -0.357718800 | -1.156857900 |
| H | 4.392126000  | 1.358805900  | -0.727899500 |
| H | 3.426566000  | 0.653046600  | -2.053129000 |
| O | 3.521719100  | -2.071867000 | -0.063141500 |
| N | 1.723346900  | -1.461739500 | 1.180116200  |
| O | -0.226344700 | -1.100279500 | 2.246848500  |
| C | 0.323135700  | 1.706597700  | 2.070229400  |
| H | -0.580995700 | 1.403817200  | 2.597233000  |
| H | 1.140615700  | 1.726344000  | 2.793792500  |
| H | 0.200499700  | 2.713370100  | 1.665789500  |
| C | -2.896769700 | 0.149346400  | 0.119394600  |
| C | -0.455834600 | 0.740344900  | -0.200521800 |
| C | -0.481129500 | -0.474639500 | -1.033068000 |
| C | -1.542415900 | -1.244049000 | -1.226493000 |
| N | -2.745578800 | -0.970380900 | -0.655153900 |
| H | -1.936501600 | 1.741730200  | 0.835091800  |
| H | -1.505691900 | -2.115677500 | -1.847736400 |
| C | -3.825766100 | -1.911964300 | -0.804387300 |
| H | -4.711802800 | -1.453775100 | -0.401747100 |
| H | -3.617229700 | -2.819555500 | -0.255850300 |
| H | -3.976027600 | -2.153374200 | -1.861158700 |
| O | -3.921706100 | 0.447176100  | 0.650464200  |
| N | -1.789184600 | 0.951516500  | 0.255035700  |
| S | -0.077083400 | 2.198467500  | -1.208724200 |
| F | 0.661303800  | -0.765674700 | -1.623416500 |

Coord\_5

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.825393600 | -1.158401400 | 0.292848800 |
| C | 0.713986300 | -0.713804200 | 1.545418800 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.661702800  | 0.676991700  | 0.952719000  |
| C | 1.932230600  | 1.082332000  | 0.283799800  |
| N | 2.858042600  | 0.124815000  | -0.131950200 |
| H | 1.808556400  | -2.397432100 | 1.521483600  |
| H | 2.266417800  | 2.046859300  | 0.288479000  |
| C | 3.875427400  | 0.517495400  | -1.093522200 |
| H | 4.598901500  | -0.283986900 | -1.180933700 |
| H | 4.369978000  | 1.425700400  | -0.745029100 |
| H | 3.415079800  | 0.704357100  | -2.068851400 |
| O | 3.614564500  | -2.006501100 | -0.043934400 |
| N | 1.803694600  | -1.449127000 | 1.200865700  |
| O | -0.161966800 | -1.156158800 | 2.255835500  |
| C | 0.308334000  | 1.662893900  | 2.075507300  |
| H | -0.590717900 | 1.342867400  | 2.600202100  |
| H | 1.125029700  | 1.696662800  | 2.799576500  |
| H | 0.168077600  | 2.668045800  | 1.673069300  |
| C | -2.910610500 | 0.182353800  | 0.083231100  |
| C | -0.451353200 | 0.681624200  | -0.196547600 |
| C | -0.500075300 | -0.554681900 | -0.990324000 |
| C | -1.581230400 | -1.292689100 | -1.188153800 |
| N | -2.784125800 | -0.961300000 | -0.657383900 |
| H | -1.911231800 | 1.757790300  | 0.777480700  |
| H | -1.561354800 | -2.183186500 | -1.780355900 |
| C | -3.894880400 | -1.860149800 | -0.823014900 |
| H | -4.767426900 | -1.367240200 | -0.436227000 |
| H | -3.729802400 | -2.771184000 | -0.268967500 |
| H | -4.037727200 | -2.100194000 | -1.881137100 |
| O | -3.935301300 | 0.532978000  | 0.574475400  |
| N | -1.778490500 | 0.941252900  | 0.235713300  |
| S | 0.041549200  | 2.090940100  | -1.219827200 |
| F | 0.643442800  | -0.902991000 | -1.538465200 |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.886251500  | -1.119205500 | 0.300480600  |
| C | 0.765043700  | -0.742603100 | 1.555325100  |
| C | 0.663291200  | 0.641558900  | 0.957352600  |
| C | 1.905533900  | 1.092775800  | 0.252487500  |
| N | 2.866783800  | 0.155227600  | -0.148623600 |
| H | 1.924390600  | -2.381965800 | 1.548215100  |
| H | 2.251914200  | 2.050185200  | 0.343443300  |
| C | 3.871253500  | 0.574572700  | -1.111538100 |
| H | 4.612006500  | -0.210250800 | -1.205007900 |
| H | 4.347827400  | 1.492582500  | -0.762157100 |
| H | 3.403597200  | 0.755661100  | -2.084574200 |
| O | 3.707344500  | -1.941057700 | -0.024703800 |
| N | 1.883994100  | -1.436484800 | 1.221629400  |
| O | -0.097548500 | -1.212015700 | 2.264787300  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.293529300  | 1.619188400  | 2.080784900  |
| H | -0.600433000 | 1.281927400  | 2.603168100  |
| H | 1.109440400  | 1.666982800  | 2.805355500  |
| H | 0.135658800  | 2.622717300  | 1.680347700  |
| C | -2.924596100 | 0.215398100  | 0.047133000  |
| C | -0.446905900 | 0.622922200  | -0.192643400 |
| C | -0.518967000 | -0.634721800 | -0.947617100 |
| C | -1.620103000 | -1.341307400 | -1.149788500 |
| N | -2.822626000 | -0.952218500 | -0.659621600 |
| H | -1.885934700 | 1.773776500  | 0.719820000  |
| H | -1.617031800 | -2.250659500 | -1.712949500 |
| C | -3.963970200 | -1.808341100 | -0.841616900 |
| H | -4.823002200 | -1.280725400 | -0.470716400 |
| H | -3.842374000 | -2.722769000 | -0.282107900 |
| H | -4.099419100 | -2.047019100 | -1.901111200 |
| O | -3.948611600 | 0.618696500  | 0.498352200  |
| N | -1.767829900 | 0.931026700  | 0.216431800  |
| S | 0.160171500  | 1.983325600  | -1.230815300 |
| F | 0.625434600  | -1.040247900 | -1.453440700 |

Coord\_7

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.947846300  | -1.079248700 | 0.307680200  |
| C | 0.816365300  | -0.771919600 | 1.565234700  |
| C | 0.665267700  | 0.606274800  | 0.961594700  |
| C | 1.879556300  | 1.104836200  | 0.222667200  |
| N | 2.876309700  | 0.183850100  | -0.165049600 |
| H | 2.040335400  | -2.366007400 | 1.574834600  |
| H | 2.236538000  | 2.051685600  | 0.397867100  |
| C | 3.866966200  | 0.631570400  | -1.129427900 |
| H | 4.625020500  | -0.136316900 | -1.229116400 |
| H | 4.325610700  | 1.559486200  | -0.779306000 |
| H | 3.392169800  | 0.807028100  | -2.100354400 |
| O | 3.799629200  | -1.874934100 | -0.005280800 |
| N | 1.963882800  | -1.423585800 | 1.242585000  |
| O | -0.032667800 | -1.267721100 | 2.273453300  |
| C | 0.278631800  | 1.575354700  | 2.086076300  |
| H | -0.610101800 | 1.220964600  | 2.606128500  |
| H | 1.093779100  | 1.637241200  | 2.811081200  |
| H | 0.103202600  | 2.577253300  | 1.687672400  |
| C | -2.939875400 | 0.248962700  | 0.011285400  |
| C | -0.442359700 | 0.563950700  | -0.189007200 |
| C | -0.537381100 | -0.714951300 | -0.905121600 |
| C | -1.659581800 | -1.389760900 | -1.111188300 |
| N | -2.860797000 | -0.943131300 | -0.661885300 |
| H | -1.860336800 | 1.789026900  | 0.661735500  |
| H | -1.672937000 | -2.317906400 | -1.645190400 |
| C | -4.033028000 | -1.756524300 | -0.859998800 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -4.878253700 | -1.194259500 | -0.505348700 |
| H | -3.955116900 | -2.673834300 | -0.295501300 |
| H | -4.161172700 | -1.993775100 | -1.921081300 |
| O | -3.959442800 | 0.703509200  | 0.421184900  |
| N | -1.757491400 | 0.921398800  | 0.197242100  |
| S | 0.277559100  | 1.875520500  | -1.241676800 |
| F | 0.605986800  | -1.177105300 | -1.367707600 |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.008655100  | -1.040172900 | 0.315368900  |
| C | 0.867429200  | -0.800699700 | 1.575164900  |
| C | 0.666980100  | 0.570837200  | 0.966282600  |
| C | 1.852962600  | 1.114934000  | 0.191561300  |
| N | 2.885055300  | 0.214514300  | -0.181630700 |
| H | 2.156199900  | -2.350543200 | 1.601573700  |
| H | 2.221982700  | 2.055088500  | 0.452633700  |
| C | 3.862835700  | 0.688674700  | -1.147464500 |
| H | 4.638128100  | -0.062550500 | -1.253198400 |
| H | 4.303451500  | 1.626393200  | -0.796442400 |
| H | 3.380677000  | 0.858351100  | -2.116077600 |
| O | 3.892409600  | -1.809426400 | 0.013947000  |
| N | 2.044245900  | -1.410966400 | 1.263314100  |
| O | 0.031791500  | -1.323581900 | 2.282390100  |
| C | 0.263835000  | 1.531660100  | 2.091363200  |
| H | -0.619820600 | 1.159989800  | 2.609090600  |
| H | 1.078182200  | 1.607547700  | 2.816873600  |
| H | 0.070768400  | 2.531897300  | 1.694944900  |
| C | -2.953850200 | 0.282076100  | -0.024845300 |
| C | -0.438027600 | 0.505301800  | -0.185247700 |
| C | -0.556264300 | -0.795028200 | -0.862327900 |
| C | -1.698473700 | -1.438393200 | -1.072822600 |
| N | -2.899305500 | -0.934063800 | -0.664122800 |
| H | -1.835039500 | 1.805011200  | 0.604061700  |
| H | -1.728637000 | -2.385388000 | -1.577779500 |
| C | -4.102149600 | -1.704695700 | -0.878603100 |
| H | -4.933855500 | -1.107723600 | -0.539845100 |
| H | -4.067713800 | -2.625399200 | -0.308649300 |
| H | -4.222890300 | -1.940578400 | -1.941062100 |
| O | -3.972778800 | 0.789141600  | 0.345125900  |
| N | -1.746764300 | 0.911096200  | 0.177946500  |
| S | 0.396123100  | 1.768003800  | -1.252735300 |
| F | 0.587971500  | -1.314375400 | -1.282707700 |

Coord\_9

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 3.069463900 | -1.001097100 | 0.323057600 |
| C | 0.918493100 | -0.829479800 | 1.585095100 |
| C | 0.668692500 | 0.535399600  | 0.970970500 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.826368900  | 1.125031800  | 0.160455500  |
| N | 2.893800900  | 0.245178500  | -0.198211800 |
| H | 2.272064400  | -2.335079000 | 1.628312700  |
| H | 2.207427400  | 2.058491300  | 0.507400400  |
| C | 3.858705200  | 0.745778900  | -1.165501100 |
| H | 4.651235600  | 0.011215900  | -1.277280400 |
| H | 4.281292200  | 1.693300200  | -0.813578900 |
| H | 3.369184100  | 0.909674100  | -2.131800700 |
| O | 3.985190000  | -1.743918600 | 0.033174900  |
| N | 2.124609000  | -1.398346900 | 1.284043200  |
| O | 0.096250900  | -1.379442700 | 2.291326900  |
| C | 0.249038100  | 1.487965500  | 2.096650200  |
| H | -0.629539400 | 1.099015000  | 2.612052700  |
| H | 1.062585300  | 1.577854100  | 2.822666100  |
| H | 0.038334100  | 2.486541400  | 1.702217400  |
| C | -2.967825000 | 0.315189500  | -0.060976100 |
| C | -0.433695500 | 0.446652900  | -0.181488200 |
| C | -0.575147500 | -0.875105100 | -0.819534100 |
| C | -1.737365600 | -1.487025400 | -1.034456900 |
| N | -2.937814100 | -0.924996300 | -0.666360300 |
| H | -1.809742200 | 1.820995400  | 0.546387900  |
| H | -1.784337100 | -2.452869600 | -1.510368700 |
| C | -4.171271300 | -1.652867200 | -0.897207300 |
| H | -4.989457200 | -1.021187800 | -0.574341500 |
| H | -4.180310800 | -2.576964100 | -0.321797300 |
| H | -4.284607900 | -1.887381700 | -1.961043000 |
| O | -3.986114700 | 0.874774000  | 0.269066800  |
| N | -1.736037300 | 0.900793600  | 0.158650800  |
| S | 0.514687200  | 1.660487100  | -1.263793900 |
| F | 0.569956300  | -1.451645400 | -1.197707700 |

Coord\_10

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 3.130272600 | -0.962021300 | 0.330746200  |
| C | 0.969556900 | -0.858259900 | 1.595025300  |
| C | 0.670404900 | 0.499962000  | 0.975658400  |
| C | 1.799775200 | 1.135129700  | 0.129349700  |
| N | 2.902546600 | 0.275842700  | -0.214792900 |
| H | 2.387928900 | -2.319614800 | 1.655051800  |
| H | 2.192872100 | 2.061894200  | 0.562167100  |
| C | 3.854574700 | 0.802883100  | -1.183537700 |
| H | 4.664343200 | 0.084982300  | -1.301362400 |
| H | 4.259133000 | 1.760207100  | -0.830715300 |
| H | 3.357691300 | 0.960997100  | -2.147523800 |
| O | 4.077970400 | -1.678410900 | 0.052402800  |
| N | 2.204972000 | -1.385727500 | 1.304772300  |
| O | 0.160710300 | -1.435303500 | 2.300263600  |
| C | 0.234241200 | 1.444270900  | 2.101937100  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.639258200 | 1.038040200  | 2.615014800  |
| H | 1.046988500  | 1.548160600  | 2.828458500  |
| H | 0.005899900  | 2.441185500  | 1.709489900  |
| C | -2.981799800 | 0.348303000  | -0.097106900 |
| C | -0.429363400 | 0.388003900  | -0.177728700 |
| C | -0.594030600 | -0.955181900 | -0.776740300 |
| C | -1.776257500 | -1.535657700 | -0.996091200 |
| N | -2.976322600 | -0.915928800 | -0.668597800 |
| H | -1.784444900 | 1.836979700  | 0.488714100  |
| H | -1.840037200 | -2.520351300 | -1.442957800 |
| C | -4.240392900 | -1.601038600 | -0.915811600 |
| H | -5.045058900 | -0.934652000 | -0.608837900 |
| H | -4.292907800 | -2.528529000 | -0.334945400 |
| H | -4.346325500 | -1.834184900 | -1.981023800 |
| O | -3.999450700 | 0.960406300  | 0.193007800  |
| N | -1.725310300 | 0.890491100  | 0.139355200  |
| S | 0.633251200  | 1.552970400  | -1.274852500 |
| F | 0.551941100  | -1.588915500 | -1.112707700 |

LIIC path connecting IM1-I-T1 and IM1-I-T1S0

| Coord_1 |              |              |              |
|---------|--------------|--------------|--------------|
| C       | 2.251813000  | -1.159284000 | 0.715498000  |
| C       | 0.168021000  | -0.132333000 | 1.654905000  |
| C       | 0.653404000  | 1.166717000  | 1.216853000  |
| C       | 1.789002000  | 1.219700000  | 0.282222000  |
| N       | 2.677160000  | 0.106985000  | 0.343571000  |
| H       | 0.696286000  | -2.122413000 | 1.621299000  |
| H       | 2.351928000  | 2.154675000  | 0.346763000  |
| C       | 3.914149000  | 0.195678000  | -0.427617000 |
| H       | 4.550830000  | -0.645989000 | -0.160805000 |
| H       | 4.419998000  | 1.135680000  | -0.185161000 |
| H       | 3.704369000  | 0.163622000  | -1.503313000 |
| O       | 2.906132000  | -2.174391000 | 0.552405000  |
| N       | 1.012317000  | -1.197770000 | 1.357152000  |
| O       | -0.904375000 | -0.312713000 | 2.232018000  |
| C       | -0.107677000 | 2.390794000  | 1.591303000  |
| H       | -1.177634000 | 2.169914000  | 1.659751000  |
| H       | 0.206844000  | 2.750534000  | 2.582663000  |
| H       | 0.060931000  | 3.199405000  | 0.873536000  |
| C       | -2.730219000 | 0.545080000  | -0.327304000 |
| C       | -0.481097000 | 0.496175000  | -1.402319000 |
| C       | -0.553127000 | -0.899906000 | -1.395997000 |
| C       | -1.647237000 | -1.559806000 | -0.897810000 |
| N       | -2.715188000 | -0.848789000 | -0.350826000 |
| H       | -1.678663000 | 2.148360000  | -0.967906000 |
| H       | -1.714696000 | -2.639118000 | -0.894181000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.650777000 | -1.544535000 | 0.530716000  |
| H | -4.549495000 | -0.937879000 | 0.630592000  |
| H | -3.194230000 | -1.686000000 | 1.517059000  |
| H | -3.904082000 | -2.513421000 | 0.091655000  |
| O | -3.603225000 | 1.207201000  | 0.212302000  |
| N | -1.667440000 | 1.137840000  | -0.995810000 |
| S | 0.979609000  | 1.434057000  | -1.566688000 |
| F | 0.508904000  | -1.620067000 | -1.804449000 |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251828000  | -1.159301000 | 0.715458000  |
| C | 0.167974000  | -0.132465000 | 1.654931000  |
| C | 0.653272000  | 1.166750000  | 1.216867000  |
| C | 1.789067000  | 1.219754000  | 0.281871000  |
| N | 2.677156000  | 0.106944000  | 0.343600000  |
| H | 0.696259000  | -2.122422000 | 1.621285000  |
| H | 2.351946000  | 2.154654000  | 0.346794000  |
| C | 3.914144000  | 0.195652000  | -0.427629000 |
| H | 4.550818000  | -0.646020000 | -0.160815000 |
| H | 4.419996000  | 1.135649000  | -0.185171000 |
| H | 3.704360000  | 0.163596000  | -1.503321000 |
| O | 2.906091000  | -2.174395000 | 0.552405000  |
| N | 1.012264000  | -1.197765000 | 1.357169000  |
| O | -0.904331000 | -0.312682000 | 2.231983000  |
| C | -0.107668000 | 2.390789000  | 1.591281000  |
| H | -1.177630000 | 2.169907000  | 1.659738000  |
| H | 0.206855000  | 2.750517000  | 2.582653000  |
| H | 0.060943000  | 3.199392000  | 0.873528000  |
| C | -2.730183000 | 0.545058000  | -0.327335000 |
| C | -0.481129000 | 0.496042000  | -1.402277000 |
| C | -0.553147000 | -0.899860000 | -1.396003000 |
| C | -1.647208000 | -1.559873000 | -0.897830000 |
| N | -2.715280000 | -0.848724000 | -0.350814000 |
| H | -1.678671000 | 2.148355000  | -0.967924000 |
| H | -1.714724000 | -2.639112000 | -0.894202000 |
| C | -3.650777000 | -1.544504000 | 0.530694000  |
| H | -4.549511000 | -0.937859000 | 0.630583000  |
| H | -3.194251000 | -1.685994000 | 1.517056000  |
| H | -3.904106000 | -2.513407000 | 0.091646000  |
| O | -3.603250000 | 1.207234000  | 0.212309000  |
| N | -1.667539000 | 1.137909000  | -0.995810000 |
| S | 0.979765000  | 1.434091000  | -1.566527000 |
| F | 0.508907000  | -1.620087000 | -1.804464000 |

Coord\_3

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.251843000 | -1.159318000 | 0.715418000 |
| C | 0.167926000 | -0.132597000 | 1.654957000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.653140000  | 1.166782000  | 1.216880000  |
| C | 1.789133000  | 1.219807000  | 0.281521000  |
| N | 2.677153000  | 0.106903000  | 0.343629000  |
| H | 0.696231000  | -2.122432000 | 1.621271000  |
| H | 2.351965000  | 2.154633000  | 0.346824000  |
| C | 3.914138000  | 0.195627000  | -0.427641000 |
| H | 4.550805000  | -0.646051000 | -0.160825000 |
| H | 4.419993000  | 1.135619000  | -0.185180000 |
| H | 3.704350000  | 0.163570000  | -1.503329000 |
| O | 2.906050000  | -2.174399000 | 0.552405000  |
| N | 1.012210000  | -1.197759000 | 1.357186000  |
| O | -0.904287000 | -0.312651000 | 2.231949000  |
| C | -0.107659000 | 2.390784000  | 1.591258000  |
| H | -1.177625000 | 2.169901000  | 1.659725000  |
| H | 0.206866000  | 2.750501000  | 2.582643000  |
| H | 0.060955000  | 3.199379000  | 0.873519000  |
| C | -2.730147000 | 0.545035000  | -0.327366000 |
| C | -0.481161000 | 0.495909000  | -1.402235000 |
| C | -0.553167000 | -0.899813000 | -1.396009000 |
| C | -1.647179000 | -1.559939000 | -0.897850000 |
| N | -2.715372000 | -0.848658000 | -0.350803000 |
| H | -1.678679000 | 2.148350000  | -0.967942000 |
| H | -1.714753000 | -2.639106000 | -0.894223000 |
| C | -3.650776000 | -1.544473000 | 0.530671000  |
| H | -4.549526000 | -0.937840000 | 0.630574000  |
| H | -3.194272000 | -1.685988000 | 1.517052000  |
| H | -3.904130000 | -2.513392000 | 0.091637000  |
| O | -3.603275000 | 1.207268000  | 0.212315000  |
| N | -1.667638000 | 1.137978000  | -0.995809000 |
| S | 0.979920000  | 1.434126000  | -1.566365000 |
| F | 0.508909000  | -1.620107000 | -1.804479000 |

#### Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251859000  | -1.159335000 | 0.715378000  |
| C | 0.167879000  | -0.132729000 | 1.654983000  |
| C | 0.653009000  | 1.166815000  | 1.216894000  |
| C | 1.789199000  | 1.219860000  | 0.281170000  |
| N | 2.677150000  | 0.106862000  | 0.343657000  |
| H | 0.696204000  | -2.122442000 | 1.621257000  |
| H | 2.351983000  | 2.154611000  | 0.346855000  |
| C | 3.914133000  | 0.195601000  | -0.427653000 |
| H | 4.550793000  | -0.646082000 | -0.160835000 |
| H | 4.419990000  | 1.135588000  | -0.185190000 |
| H | 3.704341000  | 0.163544000  | -1.503337000 |
| O | 2.906010000  | -2.174402000 | 0.552404000  |
| N | 1.012157000  | -1.197753000 | 1.357203000  |
| O | -0.904243000 | -0.312620000 | 2.231915000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.107651000 | 2.390779000  | 1.591236000  |
| H | -1.177620000 | 2.169894000  | 1.659712000  |
| H | 0.206877000  | 2.750485000  | 2.582634000  |
| H | 0.060967000  | 3.199367000  | 0.873511000  |
| C | -2.730112000 | 0.545013000  | -0.327397000 |
| C | -0.481193000 | 0.495776000  | -1.402193000 |
| C | -0.553187000 | -0.899767000 | -1.396015000 |
| C | -1.647151000 | -1.560006000 | -0.897870000 |
| N | -2.715464000 | -0.848593000 | -0.350791000 |
| H | -1.678686000 | 2.148344000  | -0.967959000 |
| H | -1.714782000 | -2.639100000 | -0.894244000 |
| C | -3.650776000 | -1.544441000 | 0.530649000  |
| H | -4.549542000 | -0.937820000 | 0.630565000  |
| H | -3.194293000 | -1.685982000 | 1.517048000  |
| H | -3.904154000 | -2.513378000 | 0.091628000  |
| O | -3.603300000 | 1.207301000  | 0.212322000  |
| N | -1.667737000 | 1.138046000  | -0.995808000 |
| S | 0.980075000  | 1.434160000  | -1.566204000 |
| F | 0.508911000  | -1.620128000 | -1.804494000 |

Coord\_5

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251874000  | -1.159352000 | 0.715339000  |
| C | 0.167832000  | -0.132861000 | 1.655010000  |
| C | 0.652877000  | 1.166847000  | 1.216908000  |
| C | 1.789264000  | 1.219914000  | 0.280819000  |
| N | 2.677146000  | 0.106821000  | 0.343686000  |
| H | 0.696177000  | -2.122451000 | 1.621243000  |
| H | 2.352001000  | 2.154590000  | 0.346885000  |
| C | 3.914127000  | 0.195576000  | -0.427665000 |
| H | 4.550780000  | -0.646113000 | -0.160845000 |
| H | 4.419988000  | 1.135558000  | -0.185200000 |
| H | 3.704331000  | 0.163518000  | -1.503345000 |
| O | 2.905969000  | -2.174406000 | 0.552405000  |
| N | 1.012104000  | -1.197747000 | 1.357220000  |
| O | -0.904199000 | -0.312589000 | 2.231881000  |
| C | -0.107642000 | 2.390774000  | 1.591214000  |
| H | -1.177616000 | 2.169888000  | 1.659699000  |
| H | 0.206889000  | 2.750469000  | 2.582624000  |
| H | 0.060979000  | 3.199354000  | 0.873502000  |
| C | -2.730076000 | 0.544990000  | -0.327428000 |
| C | -0.481225000 | 0.495643000  | -1.402151000 |
| C | -0.553208000 | -0.899721000 | -1.396020000 |
| C | -1.647122000 | -1.560073000 | -0.897891000 |
| N | -2.715556000 | -0.848527000 | -0.350780000 |
| H | -1.678694000 | 2.148339000  | -0.967977000 |
| H | -1.714811000 | -2.639094000 | -0.894266000 |
| C | -3.650776000 | -1.544410000 | 0.530626000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -4.549558000 | -0.937800000 | 0.630556000  |
| H | -3.194313000 | -1.685976000 | 1.517044000  |
| H | -3.904178000 | -2.513363000 | 0.091619000  |
| O | -3.603326000 | 1.207335000  | 0.212329000  |
| N | -1.667835000 | 1.138115000  | -0.995808000 |
| S | 0.980230000  | 1.434193000  | -1.566042000 |
| F | 0.508914000  | -1.620148000 | -1.804509000 |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251890000  | -1.159369000 | 0.715299000  |
| C | 0.167784000  | -0.132992000 | 1.655036000  |
| C | 0.652745000  | 1.166879000  | 1.216922000  |
| C | 1.789329000  | 1.219967000  | 0.280468000  |
| N | 2.677142000  | 0.106781000  | 0.343715000  |
| H | 0.696150000  | -2.122461000 | 1.621230000  |
| H | 2.352020000  | 2.154568000  | 0.346916000  |
| C | 3.914121000  | 0.195550000  | -0.427678000 |
| H | 4.550767000  | -0.646144000 | -0.160855000 |
| H | 4.419985000  | 1.135528000  | -0.185210000 |
| H | 3.704321000  | 0.163492000  | -1.503353000 |
| O | 2.905929000  | -2.174410000 | 0.552405000  |
| N | 1.012050000  | -1.197742000 | 1.357238000  |
| O | -0.904155000 | -0.312558000 | 2.231848000  |
| C | -0.107633000 | 2.390769000  | 1.591192000  |
| H | -1.177611000 | 2.169881000  | 1.659686000  |
| H | 0.206900000  | 2.750452000  | 2.582615000  |
| H | 0.060991000  | 3.199341000  | 0.873494000  |
| C | -2.730040000 | 0.544968000  | -0.327459000 |
| C | -0.481257000 | 0.495509000  | -1.402109000 |
| C | -0.553228000 | -0.899675000 | -1.396026000 |
| C | -1.647094000 | -1.560139000 | -0.897911000 |
| N | -2.715648000 | -0.848461000 | -0.350768000 |
| H | -1.678702000 | 2.148334000  | -0.967995000 |
| H | -1.714839000 | -2.639088000 | -0.894287000 |
| C | -3.650775000 | -1.544378000 | 0.530604000  |
| H | -4.549573000 | -0.937780000 | 0.630547000  |
| H | -3.194334000 | -1.685970000 | 1.517040000  |
| H | -3.904202000 | -2.513348000 | 0.091609000  |
| O | -3.603351000 | 1.207369000  | 0.212335000  |
| N | -1.667934000 | 1.138183000  | -0.995807000 |
| S | 0.980386000  | 1.434227000  | -1.565880000 |
| F | 0.508916000  | -1.620169000 | -1.804524000 |

Coord\_7

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.251905000 | -1.159386000 | 0.715260000 |
| C | 0.167737000 | -0.133124000 | 1.655063000 |
| C | 0.652613000 | 1.166912000  | 1.216936000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.789395000  | 1.220021000  | 0.280117000  |
| N | 2.677138000  | 0.106740000  | 0.343744000  |
| H | 0.696124000  | -2.122470000 | 1.621216000  |
| H | 2.352037000  | 2.154546000  | 0.346946000  |
| C | 3.914115000  | 0.195525000  | -0.427690000 |
| H | 4.550754000  | -0.646175000 | -0.160865000 |
| H | 4.419981000  | 1.135497000  | -0.185220000 |
| H | 3.704310000  | 0.163466000  | -1.503361000 |
| O | 2.905888000  | -2.174413000 | 0.552405000  |
| N | 1.011997000  | -1.197736000 | 1.357255000  |
| O | -0.904110000 | -0.312527000 | 2.231815000  |
| C | -0.107624000 | 2.390764000  | 1.591170000  |
| H | -1.177606000 | 2.169875000  | 1.659674000  |
| H | 0.206911000  | 2.750436000  | 2.582606000  |
| H | 0.061003000  | 3.199328000  | 0.873486000  |
| C | -2.730005000 | 0.544946000  | -0.327491000 |
| C | -0.481289000 | 0.495376000  | -1.402067000 |
| C | -0.553248000 | -0.899628000 | -1.396032000 |
| C | -1.647066000 | -1.560206000 | -0.897931000 |
| N | -2.715740000 | -0.848396000 | -0.350757000 |
| H | -1.678709000 | 2.148329000  | -0.968013000 |
| H | -1.714868000 | -2.639082000 | -0.894308000 |
| C | -3.650775000 | -1.544347000 | 0.530581000  |
| H | -4.549589000 | -0.937760000 | 0.630538000  |
| H | -3.194355000 | -1.685964000 | 1.517036000  |
| H | -3.904226000 | -2.513333000 | 0.091600000  |
| O | -3.603376000 | 1.207403000  | 0.212341000  |
| N | -1.668033000 | 1.138252000  | -0.995807000 |
| S | 0.980541000  | 1.434261000  | -1.565719000 |
| F | 0.508918000  | -1.620190000 | -1.804539000 |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251920000  | -1.159403000 | 0.715220000  |
| C | 0.167690000  | -0.133256000 | 1.655090000  |
| C | 0.652482000  | 1.166944000  | 1.216950000  |
| C | 1.789460000  | 1.220074000  | 0.279767000  |
| N | 2.677135000  | 0.106699000  | 0.343772000  |
| H | 0.696097000  | -2.122480000 | 1.621203000  |
| H | 2.352055000  | 2.154524000  | 0.346976000  |
| C | 3.914108000  | 0.195499000  | -0.427702000 |
| H | 4.550741000  | -0.646206000 | -0.160875000 |
| H | 4.419978000  | 1.135467000  | -0.185230000 |
| H | 3.704300000  | 0.163439000  | -1.503369000 |
| O | 2.905848000  | -2.174417000 | 0.552406000  |
| N | 1.011944000  | -1.197730000 | 1.357273000  |
| O | -0.904066000 | -0.312496000 | 2.231782000  |
| C | -0.107615000 | 2.390760000  | 1.591148000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.177601000 | 2.169868000  | 1.659661000  |
| H | 0.206923000  | 2.750420000  | 2.582597000  |
| H | 0.061016000  | 3.199315000  | 0.873478000  |
| C | -2.729969000 | 0.544923000  | -0.327522000 |
| C | -0.481320000 | 0.495242000  | -1.402025000 |
| C | -0.553268000 | -0.899582000 | -1.396038000 |
| C | -1.647037000 | -1.560273000 | -0.897952000 |
| N | -2.715832000 | -0.848330000 | -0.350746000 |
| H | -1.678716000 | 2.148323000  | -0.968031000 |
| H | -1.714897000 | -2.639076000 | -0.894330000 |
| C | -3.650775000 | -1.544315000 | 0.530558000  |
| H | -4.549604000 | -0.937740000 | 0.630528000  |
| H | -3.194377000 | -1.685958000 | 1.517031000  |
| H | -3.904250000 | -2.513318000 | 0.091590000  |
| O | -3.603401000 | 1.207437000  | 0.212348000  |
| N | -1.668131000 | 1.138320000  | -0.995807000 |
| S | 0.980696000  | 1.434295000  | -1.565557000 |
| F | 0.508920000  | -1.620210000 | -1.804555000 |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251887000  | -1.159269000 | 0.715577000  |
| C | 0.167532000  | -0.133039000 | 1.655156000  |
| C | 0.652268000  | 1.167233000  | 1.216762000  |
| C | 1.789507000  | 1.220186000  | 0.279279000  |
| N | 2.677107000  | 0.106731000  | 0.343959000  |
| H | 0.695961000  | -2.122148000 | 1.621685000  |
| H | 2.352049000  | 2.154575000  | 0.346711000  |
| C | 3.914131000  | 0.195384000  | -0.427492000 |
| H | 4.550738000  | -0.646271000 | -0.160443000 |
| H | 4.419987000  | 1.135398000  | -0.185182000 |
| H | 3.704390000  | 0.163097000  | -1.503162000 |
| O | 2.905770000  | -2.174304000 | 0.553060000  |
| N | 1.011799000  | -1.197438000 | 1.357611000  |
| O | -0.904171000 | -0.311994000 | 2.231754000  |
| C | -0.107714000 | 2.391090000  | 1.590615000  |
| H | -1.177708000 | 2.170211000  | 1.659113000  |
| H | 0.206761000  | 2.750948000  | 2.582022000  |
| H | 0.060969000  | 3.199486000  | 0.872800000  |
| C | -2.729911000 | 0.544832000  | -0.327853000 |
| C | -0.481258000 | 0.494814000  | -1.402120000 |
| C | -0.553194000 | -0.899830000 | -1.395892000 |
| C | -1.646949000 | -1.560528000 | -0.897754000 |
| N | -2.715901000 | -0.848338000 | -0.350739000 |
| H | -1.678659000 | 2.148114000  | -0.968615000 |
| H | -1.714866000 | -2.639258000 | -0.893911000 |
| C | -3.650811000 | -1.544172000 | 0.530614000  |
| H | -4.549662000 | -0.937586000 | 0.630409000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -3.194500000 | -1.685632000 | 1.517166000  |
| H | -3.904281000 | -2.513284000 | 0.091847000  |
| O | -3.603440000 | 1.207516000  | 0.211856000  |
| N | -1.668163000 | 1.138179000  | -0.996159000 |
| S | 0.980957000  | 1.433999000  | -1.565632000 |
| F | 0.509044000  | -1.620611000 | -1.804195000 |

Coord\_10

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.251897000  | -1.159267000 | 0.715587000  |
| C | 0.167471000  | -0.133127000 | 1.655188000  |
| C | 0.652127000  | 1.167298000  | 1.216750000  |
| C | 1.789570000  | 1.220246000  | 0.278911000  |
| N | 2.677100000  | 0.106700000  | 0.344007000  |
| H | 0.695921000  | -2.122114000 | 1.621734000  |
| H | 2.352064000  | 2.154562000  | 0.346703000  |
| C | 3.914128000  | 0.195347000  | -0.427477000 |
| H | 4.550726000  | -0.646306000 | -0.160399000 |
| H | 4.419985000  | 1.135362000  | -0.185186000 |
| H | 3.704392000  | 0.163030000  | -1.503144000 |
| O | 2.905725000  | -2.174292000 | 0.553143000  |
| N | 1.011735000  | -1.197396000 | 1.357670000  |
| O | -0.904145000 | -0.311904000 | 2.231722000  |
| C | -0.107718000 | 2.391127000  | 1.590529000  |
| H | -1.177717000 | 2.170248000  | 1.659033000  |
| H | 0.206751000  | 2.751000000  | 2.581942000  |
| H | 0.060973000  | 3.199496000  | 0.872708000  |
| C | -2.729873000 | 0.544801000  | -0.327921000 |
| C | -0.481278000 | 0.494643000  | -1.402095000 |
| C | -0.553203000 | -0.899821000 | -1.395879000 |
| C | -1.646913000 | -1.560619000 | -0.897747000 |
| N | -2.715990000 | -0.848282000 | -0.350728000 |
| H | -1.678658000 | 2.148083000  | -0.968704000 |
| H | -1.714888000 | -2.639276000 | -0.893876000 |
| C | -3.650815000 | -1.544126000 | 0.530602000  |
| H | -4.549683000 | -0.937549000 | 0.630387000  |
| H | -3.194534000 | -1.685585000 | 1.517180000  |
| H | -3.904306000 | -2.513266000 | 0.091871000  |
| O | -3.603466000 | 1.207555000  | 0.211800000  |
| N | -1.668253000 | 1.138221000  | -0.996203000 |
| S | 0.981125000  | 1.433991000  | -1.565501000 |
| F | 0.509061000  | -1.620680000 | -1.804163000 |

LIIC path connecting IM1-II-T1 and IM1-II-T1S0

Coord\_1

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.578519000 | -1.312949000 | 0.262248000 |
| C | 0.510939000 | -0.598604000 | 1.506766000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.654380000  | 0.818314000  | 0.933641000  |
| C | 2.022663000  | 1.041571000  | 0.381885000  |
| N | 2.821688000  | 0.004457000  | -0.064097000 |
| H | 1.343524000  | -2.461175000 | 1.414390000  |
| H | 2.324005000  | 2.034766000  | 0.075935000  |
| C | 3.891339000  | 0.290081000  | -1.019565000 |
| H | 4.544554000  | -0.578420000 | -1.082226000 |
| H | 4.459525000  | 1.159729000  | -0.676944000 |
| H | 3.459388000  | 0.498945000  | -2.004133000 |
| O | 3.244741000  | -2.262298000 | -0.121425000 |
| N | 1.480813000  | -1.501399000 | 1.117706000  |
| O | -0.417940000 | -0.932896000 | 2.220606000  |
| C | 0.370825000  | 1.838425000  | 2.055089000  |
| H | -0.549646000 | 1.585420000  | 2.586247000  |
| H | 1.188688000  | 1.817824000  | 2.780601000  |
| H | 0.298294000  | 2.848595000  | 1.641630000  |
| C | -2.856427000 | 0.046822000  | 0.232728000  |
| C | -0.475625000 | 0.918394000  | -0.213698000 |
| C | -0.426534000 | -0.232913000 | -1.162555000 |
| C | -1.426539000 | -1.099963000 | -1.339816000 |
| N | -2.630017000 | -0.999348000 | -0.648026000 |
| H | -2.014847000 | 1.696537000  | 1.001209000  |
| H | -1.339011000 | -1.913063000 | -2.050300000 |
| C | -3.618460000 | -2.067840000 | -0.748655000 |
| H | -4.544407000 | -1.713165000 | -0.298400000 |
| H | -3.279918000 | -2.964750000 | -0.216872000 |
| H | -3.791103000 | -2.313112000 | -1.801316000 |
| O | -3.883052000 | 0.187969000  | 0.877420000  |
| N | -1.820778000 | 0.972793000  | 0.322090000  |
| S | -0.398888000 | 2.523207000  | -1.170002000 |
| F | 0.713417000  | -0.355021000 | -1.876079000 |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.579911000  | -1.311919000 | 0.261641000  |
| C | 0.511682000  | -0.598494000 | 1.506561000  |
| C | 0.654533000  | 0.818646000  | 0.933559000  |
| C | 2.024394000  | 1.042791000  | 0.384537000  |
| N | 2.822190000  | 0.005167000  | -0.064821000 |
| H | 1.345345000  | -2.460357000 | 1.414091000  |
| H | 2.323310000  | 2.035548000  | 0.074814000  |
| C | 3.891324000  | 0.291649000  | -1.020530000 |
| H | 4.545055000  | -0.576500000 | -1.083427000 |
| H | 4.459058000  | 1.161474000  | -0.677780000 |
| H | 3.459224000  | 0.500487000  | -2.005029000 |
| O | 3.245762000  | -2.261527000 | -0.122027000 |
| N | 1.482074000  | -1.500548000 | 1.117455000  |
| O | -0.416954000 | -0.933125000 | 2.220621000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.370278000  | 1.838420000  | 2.055024000  |
| H | -0.549829000 | 1.585224000  | 2.586675000  |
| H | 1.188527000  | 1.818010000  | 2.779980000  |
| H | 0.297518000  | 2.848757000  | 1.641959000  |
| C | -2.856096000 | 0.045886000  | 0.232856000  |
| C | -0.475019000 | 0.917904000  | -0.213287000 |
| C | -0.426140000 | -0.233234000 | -1.162366000 |
| C | -1.426025000 | -1.100337000 | -1.339699000 |
| N | -2.629406000 | -1.000324000 | -0.647524000 |
| H | -2.014884000 | 1.695199000  | 1.002507000  |
| H | -1.338278000 | -1.913584000 | -2.049991000 |
| C | -3.617394000 | -2.069425000 | -0.747915000 |
| H | -4.543453000 | -1.715268000 | -0.297477000 |
| H | -3.278305000 | -2.966210000 | -0.216247000 |
| H | -3.790138000 | -2.314749000 | -1.800569000 |
| O | -3.882295000 | 0.186341000  | 0.878300000  |
| N | -1.821018000 | 0.973105000  | 0.321560000  |
| S | -0.403904000 | 2.522834000  | -1.170379000 |
| F | 0.713516000  | -0.354445000 | -1.876395000 |

Coord\_3

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.581303000  | -1.310886000 | 0.261031000  |
| C | 0.512423000  | -0.598383000 | 1.506356000  |
| C | 0.654688000  | 0.818976000  | 0.933471000  |
| C | 2.026120000  | 1.044000000  | 0.387194000  |
| N | 2.822687000  | 0.005881000  | -0.065545000 |
| H | 1.347167000  | -2.459539000 | 1.413792000  |
| H | 2.322629000  | 2.036291000  | 0.073685000  |
| C | 3.891302000  | 0.293225000  | -1.021494000 |
| H | 4.545551000  | -0.574570000 | -1.084629000 |
| H | 4.458581000  | 1.163228000  | -0.678615000 |
| H | 3.459052000  | 0.502036000  | -2.005926000 |
| O | 3.246786000  | -2.260750000 | -0.122631000 |
| N | 1.483334000  | -1.499695000 | 1.117203000  |
| O | -0.415971000 | -0.933348000 | 2.220638000  |
| C | 0.369744000  | 1.838417000  | 2.054956000  |
| H | -0.549998000 | 1.585038000  | 2.587101000  |
| H | 1.188381000  | 1.818195000  | 2.779352000  |
| H | 0.296759000  | 2.848922000  | 1.642282000  |
| C | -2.855766000 | 0.044963000  | 0.232984000  |
| C | -0.474411000 | 0.917412000  | -0.212879000 |
| C | -0.425747000 | -0.233562000 | -1.162175000 |
| C | -1.425516000 | -1.100714000 | -1.339576000 |
| N | -2.628800000 | -1.001294000 | -0.647016000 |
| H | -2.014904000 | 1.693871000  | 1.003788000  |
| H | -1.337555000 | -1.914111000 | -2.049671000 |
| C | -3.616336000 | -2.071002000 | -0.747161000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -4.542504000 | -1.717355000 | -0.296541000 |
| H | -3.276704000 | -2.967658000 | -0.215603000 |
| H | -3.789183000 | -2.316383000 | -1.799807000 |
| O | -3.881535000 | 0.184734000  | 0.879179000  |
| N | -1.821255000 | 0.973424000  | 0.321021000  |
| S | -0.408912000 | 2.522438000  | -1.170763000 |
| F | 0.713612000  | -0.353883000 | -1.876708000 |

Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.582693000  | -1.309851000 | 0.260421000  |
| C | 0.513162000  | -0.598270000 | 1.506150000  |
| C | 0.654846000  | 0.819305000  | 0.933378000  |
| C | 2.027841000  | 1.045199000  | 0.389856000  |
| N | 2.823178000  | 0.006599000  | -0.066269000 |
| H | 1.348988000  | -2.458719000 | 1.413495000  |
| H | 2.321962000  | 2.036995000  | 0.072547000  |
| C | 3.891273000  | 0.294809000  | -1.022458000 |
| H | 4.546042000  | -0.572629000 | -1.085831000 |
| H | 4.458094000  | 1.164991000  | -0.679450000 |
| H | 3.458871000  | 0.503592000  | -2.006821000 |
| O | 3.247812000  | -2.259968000 | -0.123236000 |
| N | 1.484592000  | -1.498841000 | 1.116952000  |
| O | -0.414989000 | -0.933562000 | 2.220657000  |
| C | 0.369222000  | 1.838419000  | 2.054881000  |
| H | -0.550154000 | 1.584864000  | 2.587526000  |
| H | 1.188250000  | 1.818382000  | 2.778716000  |
| H | 0.296019000  | 2.849090000  | 1.642597000  |
| C | -2.855435000 | 0.044051000  | 0.233112000  |
| C | -0.473799000 | 0.916919000  | -0.212477000 |
| C | -0.425356000 | -0.233896000 | -1.161981000 |
| C | -1.425013000 | -1.101096000 | -1.339445000 |
| N | -2.628198000 | -1.002258000 | -0.646501000 |
| H | -2.014907000 | 1.692553000  | 1.005052000  |
| H | -1.336840000 | -1.914647000 | -2.049340000 |
| C | -3.615287000 | -2.072570000 | -0.746393000 |
| H | -4.541563000 | -1.719425000 | -0.295594000 |
| H | -3.275116000 | -2.969094000 | -0.214939000 |
| H | -3.788239000 | -2.318015000 | -1.799028000 |
| O | -3.880773000 | 0.183148000  | 0.880059000  |
| N | -1.821489000 | 0.973749000  | 0.320475000  |
| S | -0.413913000 | 2.522018000  | -1.171155000 |
| F | 0.713704000  | -0.353338000 | -1.877017000 |

Coord\_5

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.584082000 | -1.308812000 | 0.259810000 |
| C | 0.513899000 | -0.598155000 | 1.505945000 |
| C | 0.655006000 | 0.819632000  | 0.933279000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.029557000  | 1.046388000  | 0.392524000  |
| N | 2.823664000  | 0.007321000  | -0.066992000 |
| H | 1.350809000  | -2.457897000 | 1.413200000  |
| H | 2.321309000  | 2.037658000  | 0.071401000  |
| C | 3.891236000  | 0.296399000  | -1.023422000 |
| H | 4.546528000  | -0.570679000 | -1.087033000 |
| H | 4.457597000  | 1.166762000  | -0.680284000 |
| H | 3.458682000  | 0.505154000  | -2.007717000 |
| O | 3.248840000  | -2.259180000 | -0.123842000 |
| N | 1.485848000  | -1.497986000 | 1.116703000  |
| O | -0.414011000 | -0.933768000 | 2.220678000  |
| C | 0.368714000  | 1.838426000  | 2.054801000  |
| H | -0.550296000 | 1.584703000  | 2.587949000  |
| H | 1.188134000  | 1.818570000  | 2.778071000  |
| H | 0.295298000  | 2.849263000  | 1.642904000  |
| C | -2.855104000 | 0.043151000  | 0.233240000  |
| C | -0.473184000 | 0.916425000  | -0.212079000 |
| C | -0.424967000 | -0.234238000 | -1.161785000 |
| C | -1.424515000 | -1.101481000 | -1.339307000 |
| N | -2.627601000 | -1.003217000 | -0.645980000 |
| H | -2.014893000 | 1.691246000  | 1.006298000  |
| H | -1.336135000 | -1.915191000 | -2.048996000 |
| C | -3.614247000 | -2.074128000 | -0.745611000 |
| H | -4.540628000 | -1.721480000 | -0.294634000 |
| H | -3.273540000 | -2.970519000 | -0.214254000 |
| H | -3.787304000 | -2.319643000 | -1.798233000 |
| O | -3.880008000 | 0.181585000  | 0.880938000  |
| N | -1.821719000 | 0.974081000  | 0.319920000  |
| S | -0.418905000 | 2.521574000  | -1.171557000 |
| F | 0.713794000  | -0.352809000 | -1.877321000 |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.585469000  | -1.307771000 | 0.259198000  |
| C | 0.514634000  | -0.598037000 | 1.505740000  |
| C | 0.655168000  | 0.819959000  | 0.933175000  |
| C | 2.031268000  | 1.047566000  | 0.395196000  |
| N | 2.824144000  | 0.008047000  | -0.067715000 |
| H | 1.352630000  | -2.457073000 | 1.412907000  |
| H | 2.320670000  | 2.038281000  | 0.070245000  |
| C | 3.891192000  | 0.297997000  | -1.024385000 |
| H | 4.547009000  | -0.568720000 | -1.088236000 |
| H | 4.457090000  | 1.168541000  | -0.681118000 |
| H | 3.458484000  | 0.506722000  | -2.008611000 |
| O | 3.249870000  | -2.258388000 | -0.124448000 |
| N | 1.487101000  | -1.497128000 | 1.116454000  |
| O | -0.413035000 | -0.933964000 | 2.220701000  |
| C | 0.368219000  | 1.838438000  | 2.054716000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.550426000 | 1.584555000  | 2.588369000  |
| H | 1.188032000  | 1.818762000  | 2.777417000  |
| H | 0.294595000  | 2.849439000  | 1.643202000  |
| C | -2.854772000 | 0.042264000  | 0.233368000  |
| C | -0.472566000 | 0.915930000  | -0.211686000 |
| C | -0.424580000 | -0.234587000 | -1.161586000 |
| C | -1.424023000 | -1.101870000 | -1.339161000 |
| N | -2.627009000 | -1.004170000 | -0.645450000 |
| H | -2.014862000 | 1.689951000  | 1.007526000  |
| H | -1.335437000 | -1.915744000 | -2.048638000 |
| C | -3.613216000 | -2.075677000 | -0.744813000 |
| H | -4.539700000 | -1.723518000 | -0.293661000 |
| H | -3.271976000 | -2.971933000 | -0.213549000 |
| H | -3.786380000 | -2.321269000 | -1.797422000 |
| O | -3.879240000 | 0.180044000  | 0.881817000  |
| N | -1.821946000 | 0.974421000  | 0.319356000  |
| S | -0.423889000 | 2.521106000  | -1.171968000 |
| F | 0.713882000  | -0.352297000 | -1.877622000 |

Coord\_7

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.586855000  | -1.306727000 | 0.258586000  |
| C | 0.515366000  | -0.597918000 | 1.505535000  |
| C | 0.655334000  | 0.820284000  | 0.933066000  |
| C | 2.032974000  | 1.048734000  | 0.397874000  |
| N | 2.824618000  | 0.008776000  | -0.068437000 |
| H | 1.354450000  | -2.456247000 | 1.412617000  |
| H | 2.320045000  | 2.038864000  | 0.069081000  |
| C | 3.891140000  | 0.299601000  | -1.025348000 |
| H | 4.547484000  | -0.566752000 | -1.089438000 |
| H | 4.456574000  | 1.170328000  | -0.681951000 |
| H | 3.458278000  | 0.508295000  | -2.009505000 |
| O | 3.250900000  | -2.257591000 | -0.125054000 |
| N | 1.488353000  | -1.496270000 | 1.116207000  |
| O | -0.412063000 | -0.934152000 | 2.220727000  |
| C | 0.367737000  | 1.838456000  | 2.054624000  |
| H | -0.550542000 | 1.584422000  | 2.588787000  |
| H | 1.187946000  | 1.818956000  | 2.776755000  |
| H | 0.293911000  | 2.849621000  | 1.643491000  |
| C | -2.854440000 | 0.041389000  | 0.233496000  |
| C | -0.471945000 | 0.915433000  | -0.211298000 |
| C | -0.424194000 | -0.234943000 | -1.161385000 |
| C | -1.423536000 | -1.102264000 | -1.339007000 |
| N | -2.626421000 | -1.005118000 | -0.644914000 |
| H | -2.014813000 | 1.688667000  | 1.008737000  |
| H | -1.334749000 | -1.916307000 | -2.048268000 |
| C | -3.612193000 | -2.077216000 | -0.744001000 |
| H | -4.538779000 | -1.725540000 | -0.292675000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -3.270425000 | -2.973334000 | -0.212823000 |
| H | -3.785465000 | -2.322892000 | -1.796594000 |
| O | -3.878470000 | 0.178527000  | 0.882695000  |
| N | -1.822169000 | 0.974768000  | 0.318784000  |
| S | -0.428864000 | 2.520614000  | -1.172389000 |
| F | 0.713967000  | -0.351803000 | -1.877918000 |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.588238000  | -1.305681000 | 0.257972000  |
| C | 0.516096000  | -0.597795000 | 1.505331000  |
| C | 0.655501000  | 0.820608000  | 0.932951000  |
| C | 2.034676000  | 1.049891000  | 0.400557000  |
| N | 2.825086000  | 0.009509000  | -0.069159000 |
| H | 1.356269000  | -2.455419000 | 1.412329000  |
| H | 2.319433000  | 2.039406000  | 0.067906000  |
| C | 3.891081000  | 0.301211000  | -1.026310000 |
| H | 4.547954000  | -0.564776000 | -1.090641000 |
| H | 4.456047000  | 1.172123000  | -0.682784000 |
| H | 3.458064000  | 0.509874000  | -2.010398000 |
| O | 3.251931000  | -2.256790000 | -0.125660000 |
| N | 1.489601000  | -1.495409000 | 1.115961000  |
| O | -0.411093000 | -0.934330000 | 2.220755000  |
| C | 0.367268000  | 1.838480000  | 2.054527000  |
| H | -0.550644000 | 1.584303000  | 2.589202000  |
| H | 1.187874000  | 1.819153000  | 2.776084000  |
| H | 0.293246000  | 2.849807000  | 1.643771000  |
| C | -2.854108000 | 0.040528000  | 0.233624000  |
| C | -0.471320000 | 0.914934000  | -0.210915000 |
| C | -0.423810000 | -0.235308000 | -1.161180000 |
| C | -1.423053000 | -1.102663000 | -1.338845000 |
| N | -2.625837000 | -1.006060000 | -0.644371000 |
| H | -2.014748000 | 1.687395000  | 1.009928000  |
| H | -1.334069000 | -1.916880000 | -2.047884000 |
| C | -3.611179000 | -2.078747000 | -0.743173000 |
| H | -4.537865000 | -1.727546000 | -0.291676000 |
| H | -3.268886000 | -2.974723000 | -0.212074000 |
| H | -3.784561000 | -2.324514000 | -1.795748000 |
| O | -3.877697000 | 0.177032000  | 0.883572000  |
| N | -1.822387000 | 0.975122000  | 0.318202000  |
| S | -0.433829000 | 2.520097000  | -1.172820000 |
| F | 0.714050000  | -0.351327000 | -1.878209000 |

Coord\_9

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.589618000 | -1.304632000 | 0.257359000 |
| C | 0.516823000 | -0.597670000 | 1.505128000 |
| C | 0.655672000 | 0.820932000  | 0.932831000 |
| C | 2.036372000 | 1.051037000  | 0.403245000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 2.825549000  | 0.010245000  | -0.069881000 |
| H | 1.358086000  | -2.454588000 | 1.412044000  |
| H | 2.318836000  | 2.039908000  | 0.066722000  |
| C | 3.891014000  | 0.302828000  | -1.027272000 |
| H | 4.548418000  | -0.562791000 | -1.091844000 |
| H | 4.455511000  | 1.173924000  | -0.683615000 |
| H | 3.457840000  | 0.511458000  | -2.011290000 |
| O | 3.252963000  | -2.255984000 | -0.126267000 |
| N | 1.490846000  | -1.494547000 | 1.115717000  |
| O | -0.410128000 | -0.934498000 | 2.220786000  |
| C | 0.366813000  | 1.838510000  | 2.054423000  |
| H | -0.550734000 | 1.584198000  | 2.589615000  |
| H | 1.187818000  | 1.819354000  | 2.775404000  |
| H | 0.292600000  | 2.849999000  | 1.644041000  |
| C | -2.853775000 | 0.039679000  | 0.233751000  |
| C | -0.470691000 | 0.914434000  | -0.210537000 |
| C | -0.423427000 | -0.235681000 | -1.160973000 |
| C | -1.422576000 | -1.103066000 | -1.338675000 |
| N | -2.625258000 | -1.006996000 | -0.643820000 |
| H | -2.014665000 | 1.686135000  | 1.011101000  |
| H | -1.333397000 | -1.917462000 | -2.047486000 |
| C | -3.610173000 | -2.080268000 | -0.742330000 |
| H | -4.536958000 | -1.729534000 | -0.290665000 |
| H | -3.267361000 | -2.976101000 | -0.211304000 |
| H | -3.783666000 | -2.326133000 | -1.794885000 |
| O | -3.876922000 | 0.175561000  | 0.884448000  |
| N | -1.822602000 | 0.975484000  | 0.317610000  |
| S | -0.438785000 | 2.519556000  | -1.173263000 |
| F | 0.714130000  | -0.350868000 | -1.878496000 |

Coord\_10

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.590995000  | -1.303582000 | 0.256745000  |
| C | 0.517548000  | -0.597541000 | 1.504925000  |
| C | 0.655845000  | 0.821255000  | 0.932705000  |
| C | 2.038064000  | 1.052173000  | 0.405938000  |
| N | 2.826006000  | 0.010984000  | -0.070601000 |
| H | 1.359900000  | -2.453755000 | 1.411762000  |
| H | 2.318252000  | 2.040368000  | 0.065529000  |
| C | 3.890939000  | 0.304450000  | -1.028233000 |
| H | 4.548877000  | -0.560799000 | -1.093046000 |
| H | 4.454965000  | 1.175733000  | -0.684446000 |
| H | 3.457608000  | 0.513047000  | -2.012181000 |
| O | 3.253994000  | -2.255174000 | -0.126873000 |
| N | 1.492088000  | -1.493683000 | 1.115475000  |
| O | -0.409166000 | -0.934655000 | 2.220820000  |
| C | 0.366371000  | 1.838547000  | 2.054313000  |
| H | -0.550810000 | 1.584110000  | 2.590024000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1.187776000  | 1.819559000  | 2.774715000  |
| H | 0.291974000  | 2.850196000  | 1.644302000  |
| C | -2.853441000 | 0.038843000  | 0.233878000  |
| C | -0.470059000 | 0.913933000  | -0.210164000 |
| C | -0.423045000 | -0.236062000 | -1.160763000 |
| C | -1.422104000 | -1.103475000 | -1.338496000 |
| N | -2.624683000 | -1.007927000 | -0.643261000 |
| H | -2.014565000 | 1.684887000  | 1.012254000  |
| H | -1.332733000 | -1.918055000 | -2.047074000 |
| C | -3.609177000 | -2.081779000 | -0.741470000 |
| H | -4.536057000 | -1.731506000 | -0.289640000 |
| H | -3.265848000 | -2.977466000 | -0.210511000 |
| H | -3.782781000 | -2.327750000 | -1.794004000 |
| O | -3.876145000 | 0.174114000  | 0.885322000  |
| N | -1.822813000 | 0.975853000  | 0.317009000  |
| S | -0.443731000 | 2.518991000  | -1.173716000 |
| F | 0.714210000  | -0.350429000 | -1.878777000 |

LIIC path connecting IM1-I-T1S0 and R-A-S0

| Coord_1 |              |              |              |
|---------|--------------|--------------|--------------|
| C       | 2.251813000  | -1.159284000 | 0.715498000  |
| C       | 0.168021000  | -0.132333000 | 1.654905000  |
| C       | 0.653404000  | 1.166717000  | 1.216853000  |
| C       | 1.789002000  | 1.219700000  | 0.282222000  |
| N       | 2.677160000  | 0.106985000  | 0.343571000  |
| H       | 0.696286000  | -2.122413000 | 1.621299000  |
| H       | 2.351928000  | 2.154675000  | 0.346763000  |
| C       | 3.914149000  | 0.195678000  | -0.427617000 |
| H       | 4.550830000  | -0.645989000 | -0.160805000 |
| H       | 4.419998000  | 1.135680000  | -0.185161000 |
| H       | 3.704369000  | 0.163622000  | -1.503313000 |
| O       | 2.906132000  | -2.174391000 | 0.552405000  |
| N       | 1.012317000  | -1.197770000 | 1.357152000  |
| O       | -0.904375000 | -0.312713000 | 2.232018000  |
| C       | -0.107677000 | 2.390794000  | 1.591303000  |
| H       | -1.177634000 | 2.169914000  | 1.659751000  |
| H       | 0.206844000  | 2.750534000  | 2.582663000  |
| H       | 0.060931000  | 3.199405000  | 0.873536000  |
| C       | -2.730219000 | 0.545080000  | -0.327304000 |
| C       | -0.481097000 | 0.496175000  | -1.402319000 |
| C       | -0.553127000 | -0.899906000 | -1.395997000 |
| C       | -1.647237000 | -1.559806000 | -0.897810000 |
| N       | -2.715188000 | -0.848789000 | -0.350826000 |
| H       | -1.678663000 | 2.148360000  | -0.967906000 |
| H       | -1.714696000 | -2.639118000 | -0.894181000 |
| C       | -3.650777000 | -1.544535000 | 0.530716000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -4.549495000 | -0.937879000 | 0.630592000  |
| H | -3.194230000 | -1.686000000 | 1.517059000  |
| H | -3.904082000 | -2.513421000 | 0.091655000  |
| O | -3.603225000 | 1.207201000  | 0.212302000  |
| N | -1.667440000 | 1.137840000  | -0.995810000 |
| S | 0.979609000  | 1.434057000  | -1.566688000 |
| F | 0.508904000  | -1.620067000 | -1.804449000 |

Coord\_2

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.242887000  | -1.254425000 | 0.559007000  |
| C | 0.159010000  | -0.405664000 | 1.668246000  |
| C | 0.625890000  | 0.952324000  | 1.426441000  |
| C | 1.761089000  | 1.156693000  | 0.530810000  |
| N | 2.649295000  | 0.059376000  | 0.378457000  |
| H | 0.712203000  | -2.361043000 | 1.333936000  |
| H | 2.297179000  | 2.096039000  | 0.682858000  |
| C | 3.875825000  | 0.280528000  | -0.384661000 |
| H | 4.541355000  | -0.566752000 | -0.227618000 |
| H | 4.354041000  | 1.199568000  | -0.032597000 |
| H | 3.654309000  | 0.373646000  | -1.453898000 |
| O | 2.903623000  | -2.224080000 | 0.229837000  |
| N | 1.013821000  | -1.403394000 | 1.204167000  |
| O | -0.904973000 | -0.686243000 | 2.222399000  |
| C | -0.153677000 | 2.097391000  | 1.977288000  |
| H | -1.224864000 | 1.871673000  | 1.968860000  |
| H | 0.123415000  | 2.282842000  | 3.025575000  |
| H | 0.035777000  | 3.015494000  | 1.412730000  |
| C | -2.720882000 | 0.566513000  | -0.264721000 |
| C | -0.480198000 | 0.728860000  | -1.349496000 |
| C | -0.511886000 | -0.661332000 | -1.526264000 |
| C | -1.579196000 | -1.409685000 | -1.110343000 |
| N | -2.662204000 | -0.810318000 | -0.473937000 |
| H | -1.715154000 | 2.269404000  | -0.683584000 |
| H | -1.612547000 | -2.482480000 | -1.244017000 |
| C | -3.584485000 | -1.647306000 | 0.289339000  |
| H | -4.512160000 | -1.096011000 | 0.448509000  |
| H | -3.140310000 | -1.890261000 | 1.260089000  |
| H | -3.788114000 | -2.559068000 | -0.276619000 |
| O | -3.612667000 | 1.122358000  | 0.356987000  |
| N | -1.675424000 | 1.271708000  | -0.844573000 |
| S | 0.939153000  | 1.718369000  | -1.442943000 |
| F | 0.563987000  | -1.287580000 | -2.038179000 |

Coord\_3

|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 2.231820000 | -1.364082000 | 0.237700000 |
| C | 0.146720000 | -0.871769000 | 1.547268000 |
| C | 0.591943000 | 0.510981000  | 1.668676000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.725621000  | 0.950651000  | 0.881402000  |
| N | 2.615606000  | -0.041479000 | 0.406825000  |
| H | 0.729370000  | -2.662264000 | 0.712378000  |
| H | 2.230872000  | 1.852489000  | 1.230564000  |
| C | 3.830630000  | 0.395168000  | -0.279766000 |
| H | 4.526470000  | -0.441369000 | -0.324600000 |
| H | 4.277541000  | 1.222085000  | 0.279479000  |
| H | 3.598794000  | 0.728891000  | -1.296987000 |
| O | 2.901336000  | -2.198393000 | -0.346146000 |
| N | 1.013970000  | -1.697986000 | 0.832226000  |
| O | -0.907981000 | -1.307112000 | 2.013194000  |
| C | -0.208735000 | 1.461328000  | 2.494862000  |
| H | -1.279056000 | 1.258026000  | 2.386606000  |
| H | 0.030346000  | 1.341047000  | 3.561351000  |
| H | -0.001753000 | 2.499697000  | 2.218198000  |
| C | -2.706427000 | 0.599594000  | -0.136361000 |
| C | -0.475590000 | 1.096410000  | -1.140559000 |
| C | -0.465452000 | -0.212126000 | -1.653769000 |
| C | -1.504761000 | -1.070155000 | -1.434111000 |
| N | -2.603283000 | -0.680030000 | -0.678849000 |
| H | -1.748880000 | 2.380212000  | -0.110891000 |
| H | -1.502281000 | -2.079530000 | -1.823240000 |
| C | -3.512033000 | -1.704284000 | -0.171362000 |
| H | -4.466187000 | -1.239774000 | 0.087781000  |
| H | -3.083143000 | -2.156700000 | 0.727291000  |
| H | -3.665457000 | -2.455572000 | -0.947877000 |
| O | -3.616829000 | 0.956327000  | 0.594213000  |
| N | -1.679347000 | 1.454011000  | -0.512202000 |
| S | 0.898408000  | 2.129107000  | -1.028435000 |
| F | 0.623954000  | -0.656826000 | -2.306116000 |

Coord\_4

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.218663000  | -1.387815000 | -0.154141000 |
| C | 0.130942000  | -1.352122000 | 1.243849000  |
| C | 0.551294000  | -0.060010000 | 1.774836000  |
| C | 1.682543000  | 0.596570000  | 1.181157000  |
| N | 2.576032000  | -0.168329000 | 0.404266000  |
| H | 0.747812000  | -2.801647000 | -0.083674000 |
| H | 2.152853000  | 1.397222000  | 1.752020000  |
| C | 3.778631000  | 0.480038000  | -0.119458000 |
| H | 4.505948000  | -0.288027000 | -0.379467000 |
| H | 4.190249000  | 1.138663000  | 0.649997000  |
| H | 3.538587000  | 1.069322000  | -1.010430000 |
| O | 2.899407000  | -1.989800000 | -0.966242000 |
| N | 1.012724000  | -1.909424000 | 0.315379000  |
| O | -0.913637000 | -1.927745000 | 1.554836000  |
| C | -0.273305000 | 0.589576000  | 2.837556000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.340670000 | 0.450456000  | 2.637067000  |
| H | -0.072948000 | 0.131138000  | 3.816160000  |
| H | -0.052131000 | 1.658702000  | 2.913109000  |
| C | -2.686703000 | 0.605193000  | 0.013669000  |
| C | -0.467269000 | 1.435982000  | -0.776593000 |
| C | -0.413758000 | 0.323956000  | -1.641129000 |
| C | -1.423868000 | -0.590313000 | -1.683980000 |
| N | -2.538266000 | -0.462710000 | -0.869311000 |
| H | -1.779749000 | 2.326865000  | 0.564967000  |
| H | -1.383878000 | -1.449685000 | -2.340136000 |
| C | -3.433288000 | -1.605176000 | -0.707164000 |
| H | -4.411294000 | -1.253069000 | -0.367163000 |
| H | -3.022511000 | -2.280243000 | 0.047515000  |
| H | -3.536022000 | -2.109119000 | -1.668830000 |
| O | -3.615591000 | 0.713643000  | 0.797443000  |
| N | -1.679115000 | 1.555070000  | -0.082163000 |
| S | 0.857425000  | 2.453364000  | -0.397557000 |
| F | 0.688957000  | 0.118808000  | -2.383036000 |

Coord\_5

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.203369000  | -1.353925000 | -0.389313000 |
| C | 0.111268000  | -1.629705000 | 0.977519000  |
| C | 0.503511000  | -0.454447000 | 1.749012000  |
| C | 1.631677000  | 0.300821000  | 1.319641000  |
| N | 2.530444000  | -0.255746000 | 0.395140000  |
| H | 0.767355000  | -2.789946000 | -0.593927000 |
| H | 2.062951000  | 1.025293000  | 2.008770000  |
| C | 3.719898000  | 0.507574000  | 0.013225000  |
| H | 4.479463000  | -0.183678000 | -0.350470000 |
| H | 4.091964000  | 1.044693000  | 0.889210000  |
| H | 3.474576000  | 1.225894000  | -0.775060000 |
| O | 2.897899000  | -1.768386000 | -1.301071000 |
| N | 1.009875000  | -1.981819000 | -0.033670000 |
| O | -0.922411000 | -2.274547000 | 1.162701000  |
| C | -0.348030000 | -0.029553000 | 2.902312000  |
| H | -1.410274000 | -0.099788000 | 2.645992000  |
| H | -0.187341000 | -0.689525000 | 3.765758000  |
| H | -0.116008000 | 0.994820000  | 3.209790000  |
| C | -2.661491000 | 0.590921000  | 0.089709000  |
| C | -0.455067000 | 1.611061000  | -0.493957000 |
| C | -0.356593000 | 0.667187000  | -1.541674000 |
| C | -1.336362000 | -0.251526000 | -1.761674000 |
| N | -2.466946000 | -0.298512000 | -0.965336000 |
| H | -1.807542000 | 2.204680000  | 0.961929000  |
| H | -1.257245000 | -0.982904000 | -2.555326000 |
| C | -3.348146000 | -1.460961000 | -1.044204000 |
| H | -4.347193000 | -1.184759000 | -0.692706000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2.958298000 | -2.250635000 | -0.398765000 |
| H | -3.399716000 | -1.789843000 | -2.082182000 |
| O | -3.608807000 | 0.536694000  | 0.856276000  |
| N | -1.674516000 | 1.562352000  | 0.190481000  |
| S | 0.816481000  | 2.605589000  | 0.050313000  |
| F | 0.759328000  | 0.629731000  | -2.290127000 |

Coord\_6

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.185707000  | -1.333548000 | -0.495245000 |
| C | 0.086962000  | -1.788634000 | 0.813984000  |
| C | 0.447930000  | -0.689574000 | 1.704490000  |
| C | 1.572680000  | 0.099873000  | 1.383621000  |
| N | 2.478612000  | -0.312738000 | 0.400478000  |
| H | 0.787458000  | -2.775967000 | -0.854293000 |
| H | 1.960990000  | 0.798710000  | 2.121375000  |
| C | 3.654529000  | 0.511440000  | 0.111449000  |
| H | 4.446568000  | -0.128176000 | -0.277306000 |
| H | 3.982582000  | 0.994352000  | 1.034737000  |
| H | 3.407839000  | 1.276952000  | -0.629866000 |
| O | 2.896721000  | -1.632139000 | -1.439137000 |
| N | 1.004926000  | -2.019897000 | -0.216226000 |
| O | -0.935171000 | -2.468224000 | 0.917720000  |
| C | -0.433801000 | -0.392515000 | 2.876887000  |
| H | -1.488592000 | -0.405751000 | 2.582920000  |
| H | -0.314106000 | -1.157495000 | 3.655573000  |
| H | -0.194245000 | 0.581173000  | 3.315435000  |
| C | -2.630465000 | 0.583836000  | 0.106423000  |
| C | -0.438533000 | 1.708473000  | -0.328712000 |
| C | -0.293525000 | 0.858327000  | -1.453984000 |
| C | -1.241984000 | -0.061444000 | -1.773451000 |
| N | -2.389066000 | -0.204000000 | -1.017531000 |
| H | -1.831792000 | 2.128222000  | 1.143596000  |
| H | -1.122241000 | -0.721382000 | -2.622918000 |
| C | -3.256588000 | -1.360073000 | -1.235735000 |
| H | -4.273623000 | -1.119230000 | -0.909565000 |
| H | -2.890612000 | -2.198862000 | -0.641302000 |
| H | -3.256503000 | -1.599226000 | -2.298988000 |
| O | -3.596275000 | 0.443080000  | 0.837489000  |
| N | -1.665123000 | 1.559279000  | 0.322147000  |
| S | 0.776262000  | 2.709664000  | 0.299322000  |
| F | 0.835662000  | 0.917206000  | -2.179727000 |

Coord\_7

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.165075000 | -1.334564000 | -0.537498000 |
| C | 0.056689000 | -1.902275000 | 0.711903000  |
| C | 0.383502000 | -0.847918000 | 1.667168000  |
| C | 1.504974000 | -0.049490000 | 1.423734000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 2.420128000  | -0.358644000 | 0.418883000  |
| H | 0.806842000  | -2.787350000 | -0.992726000 |
| H | 1.846848000  | 0.653435000  | 2.178865000  |
| C | 3.582680000  | 0.505151000  | 0.195145000  |
| H | 4.406643000  | -0.101107000 | -0.181183000 |
| H | 3.862219000  | 0.971358000  | 1.142138000  |
| H | 3.339769000  | 1.283037000  | -0.533658000 |
| O | 2.895424000  | -1.558537000 | -1.487369000 |
| N | 0.996797000  | -2.059797000 | -0.313801000 |
| O | -0.953539000 | -2.604387000 | 0.757187000  |
| C | -0.531881000 | -0.625360000 | 2.832154000  |
| H | -1.576572000 | -0.589250000 | 2.505551000  |
| H | -0.455143000 | -1.452368000 | 3.549785000  |
| H | -0.287959000 | 0.305091000  | 3.354268000  |
| C | -2.593112000 | 0.587589000  | 0.093220000  |
| C | -0.416681000 | 1.782208000  | -0.228547000 |
| C | -0.223752000 | 0.980311000  | -1.386893000 |
| C | -1.140338000 | 0.053984000  | -1.768341000 |
| N | -2.304321000 | -0.144944000 | -1.056828000 |
| H | -1.851502000 | 2.095872000  | 1.224252000  |
| H | -0.978724000 | -0.568690000 | -2.638975000 |
| C | -3.158822000 | -1.292180000 | -1.363925000 |
| H | -4.190429000 | -1.063475000 | -1.077884000 |
| H | -2.820038000 | -2.154633000 | -0.788001000 |
| H | -3.106572000 | -1.487312000 | -2.434896000 |
| O | -3.577686000 | 0.398171000  | 0.786679000  |
| N | -1.650086000 | 1.566792000  | 0.383658000  |
| S | 0.738272000  | 2.809892000  | 0.445630000  |
| F | 0.919004000  | 1.098506000  | -2.082410000 |

Coord\_8

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.140025000  | -1.353793000 | -0.545799000 |
| C | 0.017823000  | -1.997094000 | 0.642390000  |
| C | 0.308424000  | -0.968998000 | 1.636443000  |
| C | 1.427583000  | -0.174060000 | 1.455467000  |
| N | 2.354223000  | -0.403883000 | 0.447195000  |
| H | 0.822542000  | -2.820172000 | -1.069503000 |
| H | 1.720588000  | 0.548347000  | 2.211352000  |
| C | 3.504671000  | 0.488704000  | 0.275417000  |
| H | 4.358815000  | -0.095414000 | -0.067880000 |
| H | 3.731500000  | 0.957561000  | 1.234589000  |
| H | 3.272381000  | 1.262848000  | -0.460015000 |
| O | 2.892699000  | -1.526502000 | -1.489033000 |
| N | 0.983113000  | -2.107483000 | -0.367408000 |
| O | -0.980806000 | -2.715476000 | 0.639423000  |
| C | -0.644211000 | -0.791439000 | 2.781017000  |
| H | -1.675616000 | -0.708945000 | 2.421947000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.613551000 | -1.659839000 | 3.450880000  |
| H | -0.398593000 | 0.101667000  | 3.364058000  |
| C | -2.548514000 | 0.602581000  | 0.063401000  |
| C | -0.387347000 | 1.849157000  | -0.162776000 |
| C | -0.145712000 | 1.070177000  | -1.332887000 |
| C | -1.030824000 | 0.133969000  | -1.758092000 |
| N | -2.212370000 | -0.100364000 | -1.092499000 |
| H | -1.864466000 | 2.094161000  | 1.254035000  |
| H | -0.826677000 | -0.470129000 | -2.633095000 |
| C | -3.055621000 | -1.239154000 | -1.463766000 |
| H | -4.097788000 | -1.007981000 | -1.225205000 |
| H | -2.748257000 | -2.115158000 | -0.890313000 |
| H | -2.950741000 | -1.414347000 | -2.534659000 |
| O | -3.552481000 | 0.384851000  | 0.719058000  |
| N | -1.627603000 | 1.586516000  | 0.408974000  |
| S | 0.705850000  | 2.912321000  | 0.539164000  |
| F | 1.011292000  | 1.227054000  | -1.995236000 |

Coord\_9

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.106864000  | -1.392199000 | -0.532542000 |
| C | -0.035580000 | -2.082418000 | 0.590837000  |
| C | 0.219034000  | -1.069894000 | 1.609081000  |
| C | 1.338647000  | -0.288694000 | 1.483694000  |
| N | 2.279222000  | -0.457113000 | 0.483528000  |
| H | 0.827149000  | -2.870740000 | -1.110406000 |
| H | 1.582793000  | 0.461189000  | 2.228809000  |
| C | 3.421268000  | 0.454766000  | 0.357554000  |
| H | 4.301725000  | -0.116343000 | 0.061309000  |
| H | 3.592375000  | 0.936777000  | 1.321236000  |
| H | 3.209196000  | 1.216780000  | -0.395659000 |
| O | 2.884875000  | -1.530168000 | -1.460932000 |
| N | 0.958094000  | -2.164857000 | -0.395200000 |
| O | -1.024617000 | -2.810653000 | 0.543628000  |
| C | -0.774346000 | -0.916712000 | 2.724095000  |
| H | -1.788260000 | -0.786399000 | 2.330766000  |
| H | -0.795387000 | -1.814719000 | 3.353274000  |
| H | -0.528180000 | -0.057721000 | 3.356157000  |
| C | -2.494688000 | 0.633134000  | 0.022638000  |
| C | -0.345318000 | 1.915306000  | -0.116887000 |
| C | -0.055956000 | 1.143064000  | -1.286048000 |
| C | -0.912386000 | 0.197330000  | -1.745105000 |
| N | -2.112823000 | -0.056823000 | -1.127241000 |
| H | -1.865231000 | 2.118281000  | 1.253652000  |
| H | -0.666531000 | -0.399900000 | -2.614305000 |
| C | -2.949301000 | -1.185595000 | -1.549472000 |
| H | -3.996858000 | -0.939075000 | -1.363162000 |
| H | -2.679812000 | -2.071410000 | -0.970589000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2.791629000 | -1.355541000 | -2.615376000 |
| O | -3.519386000 | 0.402058000  | 0.639839000  |
| N | -1.593355000 | 1.620344000  | 0.412867000  |
| S | 0.687145000  | 3.015285000  | 0.602242000  |
| F | 1.116663000  | 1.322777000  | -1.912956000 |

Coord\_10

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.054119000  | -1.461909000 | -0.503288000 |
| C | -0.120636000 | -2.160499000 | 0.549566000  |
| C | 0.105432000  | -1.157908000 | 1.582261000  |
| C | 1.233355000  | -0.406919000 | 1.509894000  |
| N | 2.190229000  | -0.534817000 | 0.526684000  |
| H | 0.798146000  | -2.941156000 | -1.127159000 |
| H | 1.435521000  | 0.374002000  | 2.234230000  |
| C | 3.334501000  | 0.380217000  | 0.444091000  |
| H | 4.232358000  | -0.191540000 | 0.206182000  |
| H | 3.450893000  | 0.881431000  | 1.405619000  |
| H | 3.158391000  | 1.125862000  | -0.333613000 |
| O | 2.859982000  | -1.583623000 | -1.410046000 |
| N | 0.904364000  | -2.237243000 | -0.405735000 |
| O | -1.107296000 | -2.885876000 | 0.459044000  |
| C | -0.931193000 | -1.005866000 | 2.659415000  |
| H | -1.920911000 | -0.818292000 | 2.229106000  |
| H | -1.016580000 | -1.924548000 | 3.251370000  |
| H | -0.680443000 | -0.180843000 | 3.333572000  |
| C | -2.425810000 | 0.695313000  | -0.026266000 |
| C | -0.275077000 | 1.984008000  | -0.083666000 |
| C | 0.055265000  | 1.204224000  | -1.242488000 |
| C | -0.782430000 | 0.256156000  | -1.729260000 |
| N | -2.004957000 | 0.003086000  | -1.161574000 |
| H | -1.837145000 | 2.176571000  | 1.232384000  |
| H | -0.500240000 | -0.344686000 | -2.585057000 |
| C | -2.847147000 | -1.107640000 | -1.627108000 |
| H | -3.891938000 | -0.827223000 | -1.496817000 |
| H | -2.628631000 | -2.003318000 | -1.039104000 |
| H | -2.637843000 | -1.284422000 | -2.683959000 |
| O | -3.474308000 | 0.470146000  | 0.551129000  |
| N | -1.534351000 | 1.677631000  | 0.402328000  |
| S | 0.706507000  | 3.112937000  | 0.645297000  |
| F | 1.246445000  | 1.385591000  | -1.831483000 |

Thymine monomer

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.252811000 | -0.755886000 | 0.000010000  |
| C | 1.259789000  | -0.799359000 | 0.000009000  |
| C | 1.240553000  | 0.663705000  | -0.000005000 |
| C | 0.041732000  | 1.292088000  | 0.000022000  |
| N | -1.174136000 | 0.636614000  | 0.000092000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.049169000 | -2.398386000 | 0.000006000  |
| H | -0.027488000 | 2.375366000  | -0.000007000 |
| C | -2.448498000 | 1.355012000  | -0.000020000 |
| H | -3.030947000 | 1.088921000  | -0.885891000 |
| H | -2.248322000 | 2.427753000  | 0.000759000  |
| H | -3.031671000 | 1.087761000  | 0.885010000  |
| O | -2.316660000 | -1.353974000 | -0.000064000 |
| N | -0.018655000 | -1.385176000 | 0.000041000  |
| O | 2.265197000  | -1.494841000 | -0.000005000 |
| C | 2.561148000  | 1.376929000  | -0.000037000 |
| H | 3.153682000  | 1.095371000  | 0.877957000  |
| H | 3.153782000  | 1.095074000  | -0.877867000 |
| H | 2.429902000  | 2.463664000  | -0.000222000 |

5-Fluoro-4-Thiouridine monomer

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.295531000  | -0.941180000 | -0.000085000 |
| C | -1.132471000 | -0.303058000 | -0.000051000 |
| C | -0.680356000 | 1.064761000  | -0.000031000 |
| C | 0.636353000  | 1.382078000  | -0.000105000 |
| N | 1.616674000  | 0.415946000  | -0.000301000 |
| H | -0.311300000 | -2.186147000 | -0.000103000 |
| H | 0.960524000  | 2.415694000  | -0.000069000 |
| C | 3.042667000  | 0.748352000  | 0.000196000  |
| H | 3.523827000  | 0.324180000  | -0.884523000 |
| H | 3.522504000  | 0.328412000  | 0.887692000  |
| H | 3.151383000  | 1.833659000  | -0.002308000 |
| O | 2.139766000  | -1.819599000 | 0.000147000  |
| N | -0.071774000 | -1.199982000 | -0.000198000 |
| S | -2.714709000 | -0.798775000 | 0.000086000  |
| F | -1.590486000 | 2.044881000  | 0.000079000  |