Deciphering the curly arrows representation and electron flow for the 1,3-dipolar rearrangement between acetonitrile oxide and (1S,2R,4S)-2-cyano-7-oxabicyclo[2.2.1]hept-5-en-2-yl acetate derivatives

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Table S1: Electronic energies (a.u.) of species with \( \omega \)B97X-D/6311G(d).

| Species | 2a, R=H | 2b, R=Cl | 2c, R=Br | 2a, R=H | 2a, R=Cl | 2a, R=Br |
|---------|---------|---------|---------|---------|---------|---------|
|         | In vacuo |         |         | In benzene |         |         |
| 1       | -207.87438 | -207.87438 | -207.87438 | -207.87802 | -207.87802 | -207.87802 |
| 2       | -628.67994 | -1088.28794 | -3202.25515 | -628.68596 | -1088.29364 | -3202.26088 |
| TS-PS   | -836.54177 | -1296.14790 | -3410.11485 | -836.54939 | -1296.15551 | -3410.12244 |
| TS-PA   | -836.52943 | -1296.13292 | -3410.09944 | -836.53766 | -1296.14133 | -3410.10787 |
| TS-MS   | -836.53922 | -1296.14618 | -3410.11349 | -836.54746 | -1296.15357 | -3410.12086 |
| TS-MA   | -836.52938 | -1296.13179 | -3410.09892 | -836.53720 | -1296.13903 | -3410.10612 |
| 3       | -836.64659 | -1296.25560 | -3410.22114 | -836.65485 | -1296.26330 | -3410.22870 |
| 4       | -836.64161 | -1296.25191 | -3410.21714 | -836.64912 | -1296.25916 | -3410.22435 |
| 5       | -836.64399 | -1296.25074 | -3410.21702 | -836.65264 | -1296.25813 | -3410.22440 |
| 6       | -836.64275 | -1296.24906 | -3410.21535 | -836.65024 | -1296.25586 | -3410.22213 |

Table S2: Electronic thermodynamic parameters (H, G in a.u.; S in cal/mol·K) of species computed at 25°C in benzene with \( \omega \)B97X-D/6311G(d).

| Species | Case a, R=H | Case b, R=Cl | Case c, R=Br |
|---------|-------------|-------------|-------------|
|         | H           | G           | S           | H           | G           | S           |
| 1       | -207.82227  | -207.85410  | 66.988      | -207.82227  | -207.85410  | 66.988      |
| 2       | -628.50311  | -628.55271  | 104.392     | -628.50311  | -628.55271  | 104.392     |
| TS-PS   | -836.31026  | -836.37110  | 128.036     | -836.31026  | -836.37110  | 128.036     |
| TS-PA   | -836.29827  | -836.35641  | 122.363     | -836.29827  | -836.35641  | 122.363     |
| TS-MS   | -836.30837  | -836.36963  | 126.642     | -836.30837  | -836.36963  | 126.642     |
| TS-MA   | -836.29809  | -836.35827  | 126.642     | -836.29809  | -836.35827  | 126.642     |
| 3       | -836.41132  | -836.46929  | 122.021     | -836.41132  | -836.46929  | 122.021     |
| 4       | -836.40525  | -836.46209  | 119.638     | -836.40525  | -836.46209  | 119.638     |
| 5       | -836.40920  | -836.46728  | 122.249     | -836.40920  | -836.46728  | 122.249     |
| 6       | -836.40655  | -836.46324  | 119.314     | -836.40655  | -836.46324  | 119.314     |
Table S3: Relative (to the separate reactants) enthalpy ($\Delta H^\circ$, in kcal/mol), Gibbs energy ($\Delta G^\circ$, in kcal/mol) and entropy ($\Delta S^\circ$, in cal/mol.K) of species computed at 25°C in benzene with $\omega$B97X-D/6311G(d). In parentheses are given syn-to-anti differences.

| Species | Case a, R=H | Case b, R=Cl | Case c, R=Br |
|---------|-------------|--------------|--------------|
| TS-PS   | $\Delta H^\circ$ | $\Delta G^\circ$ | $\Delta S^\circ$ | $\Delta H^\circ$ | $\Delta G^\circ$ | $\Delta S^\circ$ | $\Delta H^\circ$ | $\Delta G^\circ$ | $\Delta S^\circ$ |
| TS-PA   | 17.01       | 31.62        | -49.02       | 19.3          | 33.62          | -48.03          | 19.68          | 33.72          | -47.08          |
|         | (7.53)      | (9.21)       | (-5.68)      | (7.76)        | (8.90)         | (-3.80)         | (9.09)         | (10.49)        | (-4.68)         |
| TS-MS   | 10.67       | 23.33        | -42.44       | 10.39         | 23.37          | -43.55          | 11.47          | 23.88          | -41.63          |
|         | (6.45)      | (7.13)       | (-2.30)      | (10.30)       | (11.45)        | (-3.87)         | (9.24)         | (10.53)        | (-4.31)         |
| TS-MA   | 17.12       | 30.46        | 44.74        | 20.69         | 34.82          | -47.42          | 20.71          | 34.41          | -45.94          |
|         | (6.45)      | (7.13)       | (-2.30)      | (10.30)       | (11.45)        | (-3.87)         | (9.24)         | (10.53)        | (-4.31)         |
|         | 3           | -53.93       | -39.21       | -49.36        | -54.80         | -39.37          | -51.74         | -53.85         | -38.9           |
|         | 4           | -50.12       | -34.69       | -51.74        | -52.3          | -36.94          | -51.51         | -51.05         | -35.98          |
|         |             | (3.81)       | (4.52)       | (-2.38)       | (2.50)         | (2.43)          | (0.23)         | (2.80)         | (2.92)          |
|         | 5           | -52.60       | -37.95       | -49.13        | -51.39         | -35.92          | -51.90         | -51.01         | -36.18          |
|         |             | (1.67)       | (2.54)       | (-2.94)       | (1.36)         | (1.81)          | (-1.49)        | (1.53)         | (2.43)          |

Table S4: Basin Populations in $|e|$ and IRC coordinates (RX, amu$^{1/2}$ Bohr) along the TS-PSa reaction pathway.

| SSD-I   | SSD-II  | SSD-III | SSD-IV | SSD-V |
|---------|---------|---------|---------|-------|
| V(N2,C3)| 6.12    | 6.26    | 4.71    | 4.53  |
| V(C4,C5)| 3.41    | 3.32    | 3.32    | 3.22  |
| V(O1)   | 5.77    | 5.76    | 5.72    | 5.72  |
| V(N2)   | -       | -       | 1.62    | 1.98  |
| V(C3)   | -       | -       | -       | 0.37  |
| V(C4)   | -       | -       | 0.31    | 0.63  |
| V(C5)   | -       | -       | -       | -     |
| V(C3,C4)| -       | -       | -       | -     |
| V(O1,C4)| -       | -       | -       | -     |
| IRC     | -24.604 | -1.263  | -0.947  | 0.000 |

S3
Table S5: Basin Populations in $|e|$ and IRC coordinates (RX, amu$^{1/2}$ Bohr) along the **TS-PSb** reaction pathway.

|       | SSD-I   | SSD-II  | SSD-III | SSD-IV  | SSD-V   | SSD-VI  | SSD-VII | SSD-VIII |
|-------|---------|---------|---------|---------|---------|---------|---------|----------|
| V(N2,C3) | 6.09   | 6.24   | 4.71   | 4.58   | 4.30   | 4.12   | 3.80   | 3.72     | 3.66     | 3.45     | 3.41     | 3.32     | 3.29     | 3.21     |
| V(C4,C5) | 3.59   | 3.50   | 3.48   | 3.45   | 3.47   | 3.13   | 2.90   | 2.54     | 2.44     | 2.21     | 2.17     | 2.09     | 2.08     | 2.01     |
| V(O1)    | 5.72   | 5.67   | 5.66   | 5.65   | 5.63   | 5.59   | 5.56   | 5.58     | 5.58     | 5.60     | 5.34     | 5.17     | 5.13     | 4.88     |
| V(N2)    | -      | -      | 1.59   | 1.82   | 1.93   | 2.02   | 2.29   | 2.36     | 2.41     | 2.60     | 2.65     | 2.74     | 2.77     | 2.86     |
| V(C3)    | -      | -      | -      | -      | 0.23   | 0.36   | 0.60   | 0.66     | -        | -        | -        | -        | -        | -        |
| V(C4)    | -      | -      | -      | -      | -      | 0.37   | 0.63   | 0.69     | -        | -        | -        | -        | -        | -        |
| V(C5)    | -      | -      | -      | -      | -      | -      | 0.31   | 0.36     | 0.47     | 0.48     | 0.52     | -        | -        | -        |
| V'(O1)   | -      | -      | -      | -      | -      | -      | -      | -        | 0.26     | 0.47     | -        | -        | -        | -        |
| V(C3,C4) | -      | -      | -      | -      | -      | -      | -      | 1.45     | 1.76     | 1.81     | 1.93     | 1.93     | 2.04     | -        |
| V(O1,C5) | -      | -      | -      | -      | -      | -      | -      | -        | -        | -        | 1.02     | 1.42     | -        | -        |
| IRC      | -15.134| -1.263 | -0.947 | -0.316 | 0.00   | 0.316  | 1.263  | 1.578    | 1.894    | 3.156    | 3.472    | 4.418    | 4.734    | 10.713   |

Table S6: Basin Populations in $|e|$ and IRC coordinates (RX, amu$^{1/2}$ Bohr) along the **TS-PSc** reaction pathway.

|       | SSD-I   | SSD-II  | SSD-III | SSD-IV  | SSD-V   | SSD-VI  | SSD-VII | SSD-VIII |
|-------|---------|---------|---------|---------|---------|---------|---------|----------|
| V(N2,C3) | 6.15   | 6.27   | 4.75   | 4.53   | 4.25   | 4.10   | 3.81   | 3.72     | 3.67     | 3.46     | 3.45     | 3.30     | 3.28     | 3.21     |
| V(C4,C5) | 3.53   | 3.46   | 3.46   | 3.41   | 3.44   | 3.13   | 2.89   | 2.53     | 2.43     | 2.21     | 2.16     | 2.06     | 2.05     | 2.00     |
| V(O1)    | 5.71   | 5.72   | 5.70   | 5.67   | 5.65   | 5.64   | 5.64   | 5.60     | 5.65     | 5.64     | 5.36     | 5.17     | 5.13     | 4.88     |
| V(N2)    | -      | -      | 1.58   | 1.84   | 1.93   | 2.02   | 2.30   | 2.36     | 2.42     | 2.60     | 2.64     | 2.76     | 2.78     | 2.87     |
| V(C3)    | -      | -      | -      | -      | 0.27   | 0.38   | 0.62   | 0.68     | -        | -        | -        | -        | -        | -        |
| V(C4)    | -      | -      | -      | -      | 0.35   | 0.62   | 0.68   | 0.68     | -        | -        | -        | -        | -        | -        |
| V(C5)    | -      | -      | -      | -      | -      | -      | 0.31   | 0.35     | 0.45     | 0.47     | 0.52     | -        | -        | -        |
| V'(O1)   | -      | -      | -      | -      | -      | -      | -      | -        | 0.24     | 0.47     | -        | -        | -        | -        |
| V(C3,C4) | -      | -      | -      | -      | -      | -      | -      | 1.45     | 1.77     | 1.82     | 1.96     | 1.98     | 2.05     | -        |
| V(O1,C5) | -      | -      | -      | -      | -      | -      | -      | -        | -        | -        | -        | -        | 1.09     | 1.41     |
| IRC      | -15.443| -1.261 | -0.946 | -0.315 | 0.000  | 0.315  | 1.261  | 1.576    | 1.892    | 3.152    | 3.467    | 4.727    | 5.043    | 10.698   |
Table S7: Basin Populations in $|e|$ and IRC coordinates (RX, amu$^{1/2}$ Bohr) along the **TS-MSa** reaction pathway.

|        | SSD-I | SSD-II | SSD-III | SSD-IV | SSD-V | SSD-VI |
|--------|-------|--------|---------|--------|-------|--------|
| V(N2,C3) | 6.12  | 6.32   | 4.80    | 4.61   | 4.23  | 3.74   |
| V(C4,C5) | 3.43  | 3.30   | 3.32    | 3.27   | 3.23  | 2.97   |
| V(O1)    | 5.76  | 5.69   | 5.70    | 5.64   | 5.63  | 5.60   |
| V(N2)    | -     | -      | 1.59    | 1.84   | 1.95  | 2.02   |
| V(C3)    | -     | -      | -       | -      | 0.31  | 0.43   |
| V(C4)    | -     | -      | -       | -      | -     | 0.19   |
| V(C5)    | -     | -      | -       | -      | -     | 0.31   |
| V(O1,C4) | -     | -      | -       | -      | -     | 1.44   |
| IRC      | -22.249 | -1.254 | -0.940  | -0.314 | 0.000 | 0.314  |

Table S8: Basin Populations in $|e|$ and IRC coordinates (RX, amu$^{1/2}$ Bohr) along the **TS-MSb** reaction pathway.

|        | SSD-I | SSD-II | SSD-III | SSD-IV | SSD-V | SSD-VI |
|--------|-------|--------|---------|--------|-------|--------|
| V(N2,C3) | 6.07  | 6.29   | 4.63    | 4.58   | 4.19  | 3.74   |
| V(C4,C5) | 3.60  | 3.59   | 3.60    | 3.56   | 3.07  | 2.67   |
| V(O1)    | 5.66  | 5.71   | 5.71    | 5.71   | 5.66  | 5.62   |
| V(N2)    | -     | -      | 1.73    | 1.84   | 1.95  | 2.34   |
| V(C3)    | -     | -      | -       | -      | 0.33  | 0.61   |
| V(C4)    | -     | -      | -       | -      | -     | 0.20   |
| V(C5)    | -     | -      | 0.50    | 0.88   | 0.88  | -      |
| V(O1,C4) | -     | -      | -       | -      | -     | 1.61   |
| IRC      | -10.975 | -0.969 | -0.646  | -0.323 | 0.000 | 1.292  |
Table S9: Basin Populations in |e| and IRC coordinates (RX, amu$^{1/2}$ Bohr) along the TS-MSe reaction pathway.

| Species | SSD-I | SSD-II | SSD-III | SSD-IV | SSD-V | SSD-VI |
|---------|-------|--------|---------|--------|-------|--------|
| V(N2,C3) | 6.09  | 6.25   | 4.72    | 4.55   | 4.19  | 3.75   | 3.68   | 3.61   | 3.43   | 3.40   | 3.23   |
| V(C4,C5) | 3.57  | 3.56   | 3.56    | 3.54   | 3.03  | 2.71   | 2.47   | 2.39   | 2.18   | 2.14   | 2.00   |
| V(O1)   | 5.72  | 5.67   | 5.65    | 5.64   | 5.64  | 5.60   | 5.59   | 5.60   | 5.30   | 5.19   | 4.87   |
| V(N2)   | -     | -      | 1.59    | 1.86   | 1.96  | 2.33   | 2.39   | 2.46   | 2.65   | 2.69   | 2.82   |
| V(C3)   | -     | -      | -       | -      | 0.30  | 0.60   | 0.64   | -      | -      | -      | -      |
| V(C4)   | -     | -      | -       | -      | -    | 0.20   | 0.25   | 0.25   | -      | -      | -      |
| V(C5)   | -     | -      | -       | -      | 0.51  | 0.84   | 0.88   | -      | -      | -      | -      |
| V(C3,C5)| -     | -      | -       | -      | -    | -      | 1.60   | 1.85   | 1.90   | 2.10   | -      |
| V(O1,C4)| -     | -      | -       | -      | -    | -      | -      | 0.82   | 1.34   | -      | -      |
| IRC     | -10.973 | -1.291 | -0.968  | -0.323 | 0.000 | 1.292  | 1.615  | 1.937  | 3.228  | 3.552  | 9.988  |

CDFT Analysis of the processes
The analysis of the reactivity indices defined in the framework of Conceptual DFT (CDFT) constitute a powerful tool to understand the reactivity of the different reagents engaged in the process of polar cycloaddition reactions, such as Diels-Alder and 32CA reactions.$^{1,2}$ These indices are reported in Table S10 for the reactants of the studied process.

Table S10: ωB97X-D/6-311G(d) electronic chemical potential, μ; chemical hardness, η; electrophilicity, ω; and nucleophilicity, N in eV, for the reagents involved in the studied reaction.

| Species     | μ    | η    | ω    | N    |
|-------------|------|------|------|------|
| 1           | -3.07| 11.85| 0.40 | 2.40 |
| Ethylene    | -3.71| 11.99| 0.57 | 1.69 |
| 2a          | -4.16| 10.92| 0.79 | 1.78 |
| 2b          | -4.24| 10.52| 0.86 | 1.89 |
| 2c          | -4.20| 10.34| 0.85 | 2.02 |

From the results listed in table S10, it can be seen that the electronic chemical potential (μ) of dipole 1, μ = -3.07 eV is higher than those of dipolarophiles, 2a-c (μ = -4.16-4.24 eV) suggesting that along the polar reaction cycloaddition, the global electron density transfer (GEDT)$^3$ will take place from the dipole 1 to dipolarophiles, 2a-c.
Ethylene presents a nucleophilicity (N) index of 1.69 eV and an electrophilicity ω index of 0.57 eV, whereas the compound 2a resulting from the substitution of the two hydrogen atoms within the ethylene molecule, possesses as nucleophilicity and electrophilicity indices 1.78 and 0.79 eV.
respectively. The substitution of a hydrogen atom in compound 2a by a halogen atom, either Cl or Br, also increases the \( N \) and \( \omega \) indices of 2b and 2c to 1.89 and 2.02 \( eV \) and 0.86 and 0.85 \( eV \), respectively. Then the different dipolarophiles 2a, 2b, and 2c are considered strong nucleophiles participating in a polar reaction.

In order to determine the most electrophilic and nucleophilic centers among the species, the analysis of the nucleophilic \( P_k^- \) and electrophilic \( P_k^+ \) Parr functions, coming from the changes of spin electron density for the nucleophile/electrophile interaction, is a powerful tool that makes possible to study the local reactivity in polar processes.\(^4\) The analysis of the nucleophilic Parr functions at dipole indicates that the O1 oxygen atom is the most nucleophilic center with a maximum value of \( P_k^- = 0.70 \), holding 1.68 \( eV \) of local nucleophilicity \( N_k \) index, compared with the C3 carbon which has \( P_k^- = 0.39 \) (see figure 1).

![Figure S1: Three-dimensional representations of the atomic spin density of radical cation 1\(^+\) and radical anions 2a-c\(^-\), together with the nucleophilic \( P_k^- \) Parr functions of 1 and the electrophilic \( P_k^+ \) of 2a-c.](image)

On the other hand, analysis of the electrophilic Parr functions of 2a shows that the C5 carbon of these species is the most electrophilic center, \( P_k^+ = 0.40 \), with local electrophilicity \( \omega_k \) value 0.316 \( eV \), while the adjacent alkene C4 carbon is poorly electrophilically activated, \( P_k^+ = 0.25 \). The substitution of the C5 hydrogen atom by chlorine and bromine atoms in order to form diporaphiles 2b-c, increase the electrophilic \( P_k^+ \) Parr functions of these two species. Theirs C5 atoms present the values of 0.44 and 0.45, respectively, with local electrophilicity \( \omega_k \) values of 0.34 \( eV \) each. However, this atomic substitution also increases the value of \( P_k^+ \) at the C4 atom position, that becomes 0.34 compared to 0.25 for 2a. Therefore, the most favorable electrophile-nucleophile interaction along the nucleophilic attack of nitrile oxide 1 to compounds 2a, 2b and 2c will take place between the most nucleophilic center of nitrile oxide 1, the O1 oxygen, and the C5 carbon atom of dipolarophiles 2a, 2b and 2c, which is the most electrophilic center in the three cases as we can see in figure S1. Therefore, the activation barriers along the para channels (in which the O1-C5 bonds are formed) should be lower than the corresponding barriers along the meta channels, in which the O1-C4 bonds are formed instead, as we have found.
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**BET Analysis for the syn attack along the meta channel**

*The mechanism of the reaction between 1 and 2a.*

As in the case of the para-syn reactive channel, a BET analysis associated with the formation of C3-C5 and O1-C4 bonds was also performed along the meta-syn attack of 1 over the C-C double bond of 2a. The formation of two new sigma bonds takes place along six structural stability domains (SSDs) in accordance with Figure S2, which shows the evolution of the ELF basins engaged in the process.
Figure S2: Population (in electrons) evolution of selected basins along the TS-MSa pathway for the 1,3-dipolar rearrangement between 1 and 2a. The relative energy (in kcal/mol) along the reaction coordinate is represented by black lines with dots.

In SSD-I, the three main basins associated with the topology of reactants are: one disynaptic basin V(N2,C3) associated with the N-C triple bond, one V(O1) monosynaptic basin of oxygen atom for 1, and one V(C4,C5) for the double C-C bond of 2a. At the first point of the second SSD-II domain, the initial V(N2,C3) disynaptic basin has undergone a drop in population with a loss of 1.52 $|e|$; This drop corresponds to the formation of the V(N2) monosynaptic basin with a population of 1.59 $|e|$, which illustrates the lone pair around the N2 atom of acetonitrile oxide (see Figure S3).
The SSD-III and SSD-IV domains correspond to the formation of the pseudo radical centers around the C3 and C5 atoms, which are involved in the formation of the C3-C5 bond. The V(C3) basin starts with a population of 0.31 |e| in the SSD-III domain but quickly reaches a value of 0.73 |e| at the end of the SSD-IV domain, while that of V(C5) is equal to 0.60 |e| (see Figure S2). The last two turning points are identical to those observed during the para-syn attack, namely a simultaneous appearance of V(C3,C5) and V(C4) basins in the SSD-V domain (concomitantly with the reduction of the initial V(C4,C5) basin, which loses a population of 0.22 |e|) and finally the appearance of the V(O1,C4) basin.

The electronic flows, obtained from the analysis of the evolution of the populations of the different basins along the process, are depicted by using curly arrows in Scheme S1 for the path along TS-MSa.
Scheme S1: Curly arrows describing the electronic flows observed along the meta-syn path of the reaction between 1 and 2a. The turning points between SSDs are indicated.

In this case, Sy is calculated to be 0.92 and Sy^{abs}=0.87, both values being slightly lower than those obtained for the para-syn case. This value implies that the topological changes also take place in a very synchronous way, at 87% of the maximum absolute synchronicity. The Cossío synchronicity is also slightly lower than in the para-syn case: 0.82. The TS can also be found slightly displaced to the products along the IRC (at approximately 67%), and therefore it has a product-like character in terms of its position along the IRC pathway.

The mechanism of the reaction between 1 and 2b-c.

In this case, the substitution of halogen atoms on 2a does not affect the number of SSDs recorded, of which there are also six along the meta reactive path. However, the catastrophes taking place in the turning points between the SSDs are different. The first two SSD domains are identical, but the SSD-III and IV domains present notable changes: the two monosynaptic basins V(C3) and V(C5) appear in the SSD-III domain (see Figures S4 to S7) while the V(C4) monosynaptic basin appears at the SSD-IV domain.

The calculated synchronicities (Sy=0.90 for TS-MSb and Sy=0.89 for TS-MSc) are slightly lower than that of TS-MSa, with the absolute synchronicity values around 83% in both cases. In these cases, the Cossío et al synchronicities are slightly greater than that of TS-MSa: 0.87 and 0.88 for TS-MSb and TS-MSc, respectively. All and all, the differences between the synchronicity values obtained with the two approaches are
always very small, as can be seen. Although they are calculated from different parameters (topological changes vs bond order evolution), both are intimately related with the modifications of the bonding scheme and therefore is not surprising that the values obtained are so similar.

Figure S4: Population (in electrons) evolution of selected basins along the TS-MSb pathway of the reaction between 1 and 2b.
Figure S5: ELF basin isosurfaces ($\eta=0.7$) for selected points that are representative of each of the SSDs found along the IRC associated with the TS-MSb regioisomeric channel.
Figure S6: Population (in electrons) evolution of selected basins along the TS-MSc pathway of the reaction between 1 and 2c.
Figure S7: ELF basin isosurfaces (η=0.7) for selected points that are representative of each of the SSDs found along the IRC associated with the TS-MSc regioisomeric channel.

The electronic flows, obtained from the analysis of the evolution of the populations of the different basins along the process, are depicted by using curly arrows in Scheme S2 for the path along TS-MSb and TS-MSc.
Scheme S2: Curly arrows describing the electronic flows observed along the meta-syn path of the reaction between 1 and 2b (R=Cl) or 2c (R=Br). The turning points between SSDs are indicated.

It is worth noting that in the case of the syn attack along the meta channel for these halogenated compounds, the O-C bond is formed from some electron-density of the nitrile oxygen lone pairs and the V(C4) monosynaptic basin, i.e., there is no formation of a second monosynaptic basin on the O1 atom. The halogen atoms are in these cases far from the place where the O-C bond forms, and therefore they have no noticeable influence in the intimate mechanism by which the bond is formed.

**Cartesian coordinates of the stationary points found in vacuo**

**Reactants**

### 1

| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| N     | -0.732655 | -0.000042 | -0.000146 |
| O     | -1.935879 | 0.000145  | 0.000399 |
| C     | 0.422484  | -0.000436 | -0.001249 |
| C     | 1.881025  | 0.000145  | 0.000427 |
| H     | 2.263663  | 0.832110  | 0.595173 |
| H     | 2.264472  | -0.930338 | 0.424062 |
| H     | 2.266432  | 0.099101  | -1.016475 |

### 2a

| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| C     | 0.128267 | 0.527681 | 0.282499 |
| C     | 1.264693 | 0.384660 | 1.328408 |
| C     | 2.355729 | -0.310869 | 0.466125 |
| C     | 1.877513 | -1.722796 | 0.173100 |
| C     | 0.920172 | -1.589645 | -0.738145 |
| C     | 0.829872 | -0.097872 | -0.997288 |
| O     | 2.155935 | 0.342603 | -0.783702 |
| O     | -1.018056 | -0.170378 | 0.770750 |
| C     | -0.219266 | 1.932451 | 0.038361 |
| H     | 0.924552 | -0.197173 | 2.183933 |
H  1.61380400  1.35840400  1.66987800
H  3.37791400 -0.17976400  0.81169100
H  0.43864500  0.24963200 -1.94551700
C -2.03405300 -0.41142100 -0.09325900
N -0.47483800  3.03871400 -0.13930300
C -3.16974200 -1.08922700  0.61546400
O -1.99746200 -0.11412000 -1.25283200
H -2.81087100 -1.97351200  1.14493300
H -3.93483300 -1.36546900 -0.10636400
H -3.59240100 -0.40938800  1.35849200
H  0.26295100 -2.33928900 -1.15548100
H  2.20166500 -2.61706100  0.68824000

2b
C  0.71154000 -0.65852800  0.31538800
C -0.44793900 -1.07516900  1.25822000
C -1.59924700 -1.24077800  0.23163300
C -1.93638700  0.14805700 -0.28862900
C -0.95939300  0.49611000 -1.11492800
C -0.02676000 -0.70028100 -1.09055500
O -0.90286900 -1.79284300 -0.87432200
O  1.18177000  0.62240600  0.73102100
C  1.81733800 -1.62290800  0.34138100
H -0.62439000 -0.30851000  2.01174400
H -0.24137400 -2.02515400  1.74878000
H -2.42932600 -1.87184800  0.53735800
H  0.62058300 -0.86837200 -1.94222800
C  1.99661800  1.30684200 -0.11086300
N  2.67011500 -2.39245700  0.37292700
C  2.44484800  2.58819600  0.52580800
O  2.28981700  0.91349800 -1.20332800
H  1.57907800  3.17529600  0.83804000
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 3.04827900 | 3.15385600 | -0.18021500|
| H    | 3.03088300 | 2.36724000 | 1.42035400 |
| H    | -0.78346800| 1.43722200 | -1.61360200|
| Cl   | -3.26144300| 1.07610200 | 0.29044600 |

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 1.30961200 | -0.61441700| 0.32583000 |
| C    | 0.20026700 | -1.19943400| 1.23859000 |
| C    | -0.86527600| -1.57920800| 0.17666600 |
| C    | -1.41006900| -0.27766700| -0.39486300|
| C    | -0.47049100| 0.20817600 | -1.19579400|
| C    | 0.64745300 | -0.81399300| -1.10345200|
| O    | -0.04191800| -2.03195500| -0.88751700|
| O    | 1.53922700 | 0.73808700 | 0.71666400 |
| C    | 2.55982400 | -1.37709700| 0.42123600 |
| H    | -0.13281600| -0.45736900| 1.96298500 |
| H    | 0.54449000 | -2.08975100| 1.76262200 |
| H    | -1.58839000| -2.33475600| 0.47085000 |
| H    | 1.34868400 | -0.88962000| -1.92528100|
| C    | 2.27044200 | 1.52423000 | -0.11304100|
| N    | 3.52689600 | -1.99155000| 0.50866200 |
| C    | 2.45602200 | 2.88501200 | 0.48895000 |
| O    | 2.68281300 | 1.15139600 | -1.17376200|
| H    | 1.48336300 | 3.34995000 | 0.66297100 |
| H    | 3.04918900 | 3.50163000 | -0.18230600|
| H    | 2.95548700 | 2.79758400 | 1.45556400 |
| H    | -0.43022800| 1.15374300 | -1.71546800|
| Br   | -3.01559200| 0.50044600 | 0.16113200 |

**Transition States**

**TS-PSa**
C  -1.22017900  -0.80894500  0.07980500
C  -0.67662300  -2.01306000  -0.80894500
C   0.85259000  -1.81051400  -0.58000100
C   1.24192600  -0.73470100  -2.01306000
C   0.81699300  -0.55870400  0.85259000
C   0.13192000  -2.73470100  -1.81051400
C   0.81699300  -0.55870400  0.85259000
O   0.90001700  -1.35016000  0.79192600
O  -1.98961000  -0.01651700  -0.79780200
C  -2.06099200  -1.23634600  1.20450900
H  -1.02398300  -1.96210300  -1.76609100
H  -0.98881800  -2.96021100  -0.29586100
H   1.46655200  -2.69761400  -0.68282300
H   0.03164800  -0.37562200  1.53371600
C  -2.31374700  1.26341800  -0.38329000
N  -2.71087700  -1.58670900  2.08530500
C  -3.18206000  1.94039600  -1.40274000
O  -1.94255700  1.73310400  0.65513300
H  -2.72060000  1.88379000  -2.39028000
H  -3.33960000  2.97791700  -1.11697500
H  -4.14386200  1.42596400  -1.45994700
H   0.57839600  1.46773200  -0.94852400
H   3.46114900  2.68302700  1.63919500
H   1.79104000  2.93673800  1.09740300
C   2.67690200  1.14512300  0.41978800
C   2.50863900  2.18900000  1.43859500
N   3.42409300  0.37293200  -0.09975000
O   3.48520200  -0.54645700  -0.89969400
H   2.13368600  1.75707700  2.36940800
H   1.48525400  -0.57163400  -2.39094600

TS-PSb
C  1.41131400  -0.55633800  -0.62052400
|   |   |   |   |   |
|---|---|---|---|---|
| C | 0.70057700 | -1.93128700 | -0.72929700 |
| C | -0.76534400 | -1.47911000 | -0.94568000 |
| C | -1.24419400 | -0.84556000 | 0.34615400 |
| C | -0.65661700 | 0.38642500 | 0.41480200 |
| C | 0.18995800 | 0.42434500 | -0.84872600 |
| O | -0.57990700 | -0.33105800 | -1.76322100 |
| O | 2.03433800 | -0.47609600 | 0.66236000 |
| C | 2.42350700 | -0.36868400 | -1.66666800 |
| H | 0.85997900 | -2.51582600 | 0.17631100 |
| H | 1.05448000 | -2.49568000 | -1.59100700 |
| H | -1.43169100 | -2.19546700 | -1.41622300 |
| H | 0.46060800 | 1.38649600 | -1.26775200 |
| C | 2.45627100 | 0.73543800 | 1.09597000 |
| N | 3.20631400 | -0.23276600 | -2.49696700 |
| C | 3.16100100 | 0.60029000 | 2.41280300 |
| O | 2.27393800 | 1.75338500 | 0.48935100 |
| H | 2.57393900 | -0.01238500 | 3.09839700 |
| H | 3.33577200 | 1.58692100 | 2.83599500 |
| H | 4.11823700 | 0.09695300 | 2.25791600 |
| H | -0.41389100 | 0.90769400 | 1.33042600 |
| H | -2.52174900 | 3.79799600 | -0.75097200 |
| H | -2.01953600 | 3.58551300 | 0.93980700 |
| C | -2.24495100 | 1.78791000 | -0.15968500 |
| C | -1.89350900 | 3.21108700 | -0.07859000 |
| N | -3.07643800 | 0.97537300 | -0.42987500 |
| O | -3.30996300 | -0.21723300 | -0.47173700 |
| H | -0.85010200 | 3.35473700 | -0.36538600 |
| Cl | -1.80297000 | -1.78319300 | 1.68135300 |

**TS-PSc**

|   |   |   |   |   |
|---|---|---|---|---|
| C | -1.65163300 | -0.24485200 | 0.82034300 |
| C | -0.72718400 | -1.14854000 | 1.67860100 |
C   0.57398200 -0.30813700  1.67866700
C   1.13550100 -0.32976000  0.26886900
C   0.34820800  0.50844700 -0.47093600
C  -0.68815700  0.97866700  0.54008700
O   0.04681700  1.01098900  1.74732200
O  -2.05658900 -0.98591300 -0.33161900
C  -2.83963300  0.19549200  1.56127400
H  -0.62393100 -2.13268500  1.22277000
H  -1.10856000 -1.25812200  2.69302300
H   1.27343100 -0.49496400  2.48757000
H  -1.19673000  1.91978300  0.36680800
C  -2.62181400 -0.31071900 -1.36032900
N  -3.75965400  0.53851900  2.15837200
C  -3.04351100 -1.26345900 -2.43881600
O  -2.74327000  0.88190300 -1.37841000
H  -2.19273600 -1.86953000 -2.75646700
H  -3.44433800 -0.70569100 -3.28198900
H  -3.80319900 -1.94506100 -2.05076300
H   0.16652300  0.41477700 -1.53272400
H   1.40756100  4.34961600 -1.31609800
H   1.06794800  3.14476200 -2.57545900
C   1.52735500  2.34240300 -0.67021000
C   0.93732900  3.38567200 -1.51817500
N   2.44159000  2.01984800  0.02649400
O   2.88890100  1.11991000  0.70996000
H  -0.13253800  3.47285100 -1.31957100
Br  2.14352800 -1.76716300 -0.39272600

TS-MSa
C  -1.22073300  0.78480300  0.14198800
C  -0.36701400  1.58891200  1.15817900
C   1.06100800  1.25207500  0.66034900
C  -0.38326000  -0.54994000  0.64737600
C  0.38567500  0.74729300  0.70957800
O  -0.52587400  1.69378900  0.16828500
O  2.13424300  -0.56176400  -0.59860300
C  2.41160600  1.78004000  -0.35216200
H  0.60626300  -0.00727800  -2.36501900
H  0.75722000  1.76049700  -0.59860300
H  -1.62250100  1.49548800  -1.58231400
H  0.77340500  1.07137600  1.66686400
C  2.83010400  -1.01738100  0.47520100
N  3.15047200  2.65773200  -0.28734900
C  3.54577300  -2.28915800  0.13013300
O  2.84337300  -0.45542800  1.53182800
H  2.84500300  -3.01625400  -0.28421100
H  4.02245800  -2.69026500  1.02149400
H  4.30037100  -2.08758500  -0.63320600
H  -0.05403900  -1.48187500  1.07731800
H  -4.08622800  1.56596800  -0.62942000
H  -4.35755000  -1.42083000  -1.02772000
C  -3.11911700  0.18408800  0.64365900
C  -4.24725600  0.57080600  -0.20873900
N  -2.71007100  0.03471400  1.75430400
O  -1.71325900  -0.26180500  2.39335100
H  -5.17172900  0.58219000  0.37137700
Cl  -1.81300100  -1.67954800  -1.43065300

TS-MSc
C  -1.71756700  -0.45649400  -0.69368000
C  -0.71556100  -0.21101800  -1.85190400
C  0.57626500  -0.79941500  -1.24256700
C  1.04716900  0.11043800  -0.10536400
C  0.13447600  -0.07532200  0.89812300
O  -0.05992800  -2.36239300  0.87894700
O  -0.95176200  0.70926700 -0.73225500
C  -2.20489100 -1.28623600 -0.73053200
H   0.80056700 -0.60027900 -1.71846800
H  -0.10664500 -2.12198700 -1.80842300
H   1.63751400 -2.84023700 -0.21847400
H  -1.40214600 -1.05403600  1.78373400
C  -1.72560500  1.53199000  0.02503500
N  -3.19524800 -1.78590100 -1.03054800
C  -1.68145100  2.93233500 -0.50348300
O  -2.34220600  1.14861600  0.97711700
H  -2.45588100  3.52414900 -0.02028300
H  -1.81583100  2.93967600 -1.58594000
H  -0.70067200  3.35287600 -0.27563000
H   3.27831500 -0.53289200 -1.93444600
H   3.97234300  1.09487500 -1.82566300
C   2.51865200  0.65801600 -0.35004000
C   3.61513100  0.24357600 -1.24407000
N   1.90518300  1.60801300  0.04405200
O   1.02661900  1.92952900  0.82793300
H   4.44841700 -0.15723100 -0.66251000
H   0.74083500  0.25516000  2.49471200
H   2.72926900 -1.01912900  1.27233100

TS-MAb
C    1.20718500 -0.76215900  0.41990400
C    0.06758300 -1.11062800  1.41654200
C   -1.01465300 -1.63240000  0.44625200
C   -1.59736500 -0.49609600 -0.40854900
C   -0.62086800 -0.21642000 -1.32430900
C    0.52227800 -1.15395000 -0.94312100
O   -0.18999100 -2.31277300 -0.50746000
| Element | TS-PAb | TS-PAb |
|---------|--------|--------|
| H       | -0.17439000 -0.26555900 -1.82022500 | H       | -0.17439000 -0.26555900 -1.82022500 |
| C       | 2.02488300 1.94772600 0.49576800 | C       | 2.02488300 1.94772600 0.49576800 |
| O       | 0.78188400 -2.27472900 0.67705900 | O       | 0.78188400 -2.27472900 0.67705900 |
| H       | 1.79233200 -2.80411100 -0.72848400 | H       | 1.79233200 -2.80411100 -0.72848400 |

**TS-PAb**

| Element | TS-PAb | TS-PAb |
|---------|--------|--------|
| C       | -0.99191100 -0.94213800 0.19919900 | C       | -0.99191100 -0.94213800 0.19919900 |
| C       | 1.14575200 -1.65749800 -0.56822900 | C       | 1.14575200 -1.65749800 -0.56822900 |
| C       | 0.16978800 -1.11682300 1.23611700 | C       | 0.16978800 -1.11682300 1.23611700 |
| O       | 0.78188400 -2.27472900 0.67705900 | O       | 0.78188400 -2.27472900 0.67705900 |
| C       | -2.02488300 -1.94772600 0.49576800 | C       | -2.02488300 -1.94772600 0.49576800 |
| H       | -0.19862200 -0.39227700 -1.78496800 | H       | -0.19862200 -0.39227700 -1.78496800 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| H | 1.37298700 | -2.30816800 | -1.06396900 |   |   |
| H | -0.68229200 | -1.28782300 | 2.28163600 |   |   |
| C | -2.90039300 | 0.68596000 | -0.70155900 |   |   |
| N | -3.23111400 | -2.77492700 | 0.69123100 |   |   |
| C | -3.38320500 | 2.09079000 | -0.49055300 |   |   |
| O | -3.20563900 | -0.04511200 | -1.59564400 |   |   |
| H | -3.76407200 | 2.21765000 | 0.52432500 |   |   |
| H | -4.16434800 | 2.31608900 | -1.21273500 |   |   |
| H | -2.55034400 | 2.78502000 | -0.62845700 |   |   |
| C | -0.53501600 | 2.72969200 | 1.83623400 |   |   |
| C | 0.08455600 | 2.01701100 | 0.71397200 |   |   |
| O | 0.84262000 | 1.38541000 | -1.35389900 |   |   |
| N | 0.36858800 | 2.05254000 | -0.44579800 |   |   |
| H | -1.43836000 | 2.20204500 | 2.14767600 |   |   |
| H | -0.79852500 | 3.74722500 | 1.54150000 |   |   |
| H | 0.15068900 | 2.78195200 | 2.68410500 |   |   |
| H | 1.22503700 | 0.41398300 | 2.05951300 |   |   |
| Br | 3.29885000 | -0.06045400 | -0.25493500 |   |   |

**Products**

3a

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C | -1.11183600 | -0.81048800 | -0.00899400 |   |   |
| C | -0.47545400 | -1.92808500 | -0.88171800 |   |   |
| C | 1.00426300 | -1.81264600 | -0.48087900 |   |   |
| C | 1.60557200 | -0.56130600 | -1.13261200 |   |   |
| C | 1.00074800 | 0.55355400 | -0.26003100 |   |   |
| C | 0.15476700 | -0.26920400 | 0.73469800 |   |   |
| O | 0.91286200 | -1.44763800 | 0.89582800 |   |   |
| O | -1.76891900 | 0.11509100 | -0.87672100 |   |   |
| C | -2.07956000 | -1.35637400 | 0.95198400 |   |   |
| H | -0.67520400 | -1.73785700 | -1.93648200 |   |   |
H  -0.87164600  -2.90774000  -0.62016800
H   1.60131400  -2.71415100  -0.58891100
H  -0.04871500   0.19322200   1.69404200
C  -2.22693500   1.27293100  -0.33035100
N  -2.83073700  -1.81466200   1.69075100
C  -3.00908900   2.05682500  -1.34087500
O  -2.01700500   1.58532300   0.80591700
H  -2.47968600   2.10076700  -2.29360500
H  -3.19245300   3.05848000  -0.95877300
H  -3.96454200   1.55686300  -1.51725500
H   0.43750700   1.32128600  -0.78985900
H   1.80912900   3.12265900   0.90948800
H   1.72300900   1.97325200   2.24127600
C   2.25492400   1.10680800   0.35993300
C   2.27935400   2.23131300   1.33528100
N   3.31678300   0.52398300  -0.02501900
O   3.01875300  -0.47909800  -0.93584800
H   3.30634900   2.46820400   1.61123700
H   1.40657000  -0.48962800  -2.20312700

3b
C   1.29591000  -0.77251500  -0.29953700
C   0.48334600  -2.02749100   0.12451300
C  -0.89636300  -1.71013200  -0.46598400
C  -1.61905000  -0.59689900   0.31691700
C  -0.78011100   0.64294100  -0.03193400
C   0.19694000   0.03838500 -1.06239400
O  -0.56075100  -1.00072100  -1.65504800
O   1.82009500  -0.16020500   0.87706000
C   2.39749900  -1.11654000  -1.20878300
H   0.50417700  -2.14397000   1.20593500
H   0.88306300  -2.92912700  -0.33633800
H       -1.531501000  -2.560686000  -0.697092000
H        0.575856000   0.715926000  -1.818976000
C       2.377155000   1.073992000   0.751700000
N       3.249389000  -1.416525000  -1.918803000
C       2.970282000   1.514158000   2.055306000
O       2.359534000   1.694058000  -0.272642000
H       2.205907000   1.510018000   2.835083000
H       3.389035000   2.511606000   1.945087000
H       3.750386000   0.813775000   2.359712000
H    -0.294678000   1.115882000   0.819129000
H    -1.296899000   3.539118000  -0.254390000
H    -0.830237000   2.953463000  -1.848192000
C    -1.839630000   1.512257000  -0.639959000
C    -1.618448000   2.912527000  -1.091235000
N     -2.972599000   0.942767000  -0.727902000
O     -2.885153000  -0.364029000  -0.232575000
H     -2.534863000   3.324923000  -1.511560000
Cl   -1.790163000  -0.924209000   2.082501000

3c
C    -1.521718000  -0.367508000   0.771980000
C    -0.512855000  -1.307558000   1.487758000
C     0.668650000  -0.359190000   1.728231000
C    -1.428490000  -0.025723000   0.429145000
C     0.407742000   0.838458000  -0.330939000
C    -0.700751000   0.963416000   0.737272000
O     0.013809000   0.885985000   1.956913000
O    -1.842917000  -0.938989000  -0.494957000
C    -2.752108000  -0.185958000   1.553972000
H    -0.289205000  -2.168231000   0.861344000
H    -0.906401000  -1.655743000   2.441202000
H     1.322610000  -0.603799000   2.560421000
|   |   |   |   |
|---|---|---|---|
| H | -1.30014200 | 1.86594200 | 0.70158500 |
| C | -2.52715500 | -0.16883500 | -1.38195200 |
| N | -3.70310500 | -0.06239700 | 2.18658100 |
| C | -2.89196900 | -0.96911500 | -2.59504200 |
| O | -2.77609100 | 0.98591400 | -1.18453500 |
| H | -2.01611500 | -1.48949000 | -2.98620300 |
| H | -3.31276500 | -0.31055800 | -3.35132100 |
| H | -3.62800000 | -1.72719600 | -2.31827200 |
| H | 0.06711600 | 0.42609700 | -1.27783000 |
| H | 0.56299700 | 3.01149900 | -2.32236000 |
| H | -0.17945900 | 3.67290400 | 0.86893700 |
| C | 1.21070200 | 2.09279000 | -0.50846500 |
| C | 0.75510400 | 3.28060800 | -1.27985400 |
| N | 2.34678000 | 2.05149100 | 0.06030900 |
| O | 2.50650700 | 0.82080800 | 0.70821000 |
| H | 1.51156100 | 4.06376100 | -1.24942100 |
| Br | 2.08762400 | -1.59391200 | -0.55646100 |

4a

|   |   |   |   |
|---|---|---|---|
| C | -0.52446200 | -1.00331400 | -0.25215000 |
| C | 0.58552500 | -1.49749100 | -1.21881300 |
| C | 1.77867800 | -1.59538400 | -0.26450600 |
| C | 2.35799300 | -0.19223900 | 0.02195600 |
| C | 1.31870300 | 0.37450000 | 1.00305000 |
| C | 0.29387300 | -0.79420900 | 1.06560100 |
| O | 1.16635500 | -1.91048200 | 0.99079100 |
| O | -1.15217500 | 0.13316400 | -0.83328700 |
| C | -1.52730800 | -2.05753900 | -0.02651500 |
| H | 0.73131500 | -0.77372300 | -2.01821600 |
| H | 0.34061900 | -2.46718700 | -1.64821100 |
| H | 2.51147000 | -2.35869200 | -0.51163600 |
| H | -0.30736100 | -0.83922400 | 1.96697500 |
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| C    | -2.07939100 | 0.79272000 | -0.09968600 |
| N    | -2.29039600 | -2.90448600 | 0.11586900 |
| C    | -2.67814200 | 1.90610600 | -0.90362700 |
| O    | -2.34240500 | 0.50351600 | 1.03384200 |
| H    | -1.88683700 | 2.50700300 | -1.35511300 |
| H    | -3.30950100 | 2.51988200 | -0.26518600 |
| H    | -3.27628100 | 1.48670300 | -1.71573500 |
| C    | 0.23821200  | 2.79963500 | 0.95305600 |
| C    | 1.01812300  | 1.68664900 | 0.33845300 |
| O    | 2.35648100  | 0.70345600 | -1.09165400 |
| N    | 1.58338900  | 1.82345800 | -0.79516500 |
| H    | -0.71195900 | 2.45362000 | 1.36326300 |
| H    | 0.05921700  | 3.58829900 | 0.22223500 |
| H    | 0.80486700  | 3.22813200 | 1.78600200 |
| H    | 1.70273600  | 0.51499000 | 2.01526700 |
| H    | 3.37388400  | -0.24644300 | 0.41698500 |

**4b**
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| C    | 0.97869700 | -1.07254000 | 0.23910700 |
| C    | -0.07008400 | -1.60130000 | 1.25527700 |
| C    | -1.34360600 | -1.55838700 | 0.40651400 |
| C    | -1.81333000 | -0.09270100 | 0.23302800 |
| C    | -0.87934800 | 0.41908300 | -0.86859500 |
| C    | 0.07719100  | -0.79995200 | -1.01398900 |
| O    | -0.85478100 | -1.86246800 | -0.89951000 |
| O    | 1.63844600  | 0.04165000 | 0.82513400 |
| C    | 1.96349600  | -2.11275100 | -0.09633500 |
| H    | -0.99945800 | -0.96303700 | 2.13495900 |
| H    | 0.14601500  | -2.62595800 | 1.55249000 |
| H    | -2.12485300 | -2.25727200 | 0.68779900 |
| H    | 0.60595000  | -0.85441300 | -1.95879000 |
| C    | 2.47147700  | 0.76872300 | 0.04268400 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| N       | 2.7143  | -2.9498 | -0.3315 |
| C       | 3.0820  | 1.8840  | 0.8328  |
| O       | 2.6436  | 0.5305  | -1.1200 |
| H       | 2.2927  | 2.4694  | 1.3089  |
| H       | 3.6819  | 2.5114  | 0.1776  |
| H       | 3.7094  | 1.4730  | 1.6265  |
| C       | 0.1962  | 2.8416  | -1.0138 |
| C       | -0.4833 | 1.7371  | -0.2789 |
| O       | -1.5804 | 0.7381  | 1.3318  |
| N       | -0.8837 | 1.8890  | 0.9216  |
| H       | 1.1006  | 2.4926  | -1.5149 |
| H       | 0.4434  | 3.6556  | -0.3325 |
| H       | -0.4739 | 3.2313  | -1.7860 |
| H       | -1.3791 | 0.5343  | -1.8304 |
| Cl      | -3.5628 | -0.0178 | -0.2188 |

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 1.4264  | -1.0740 | 0.2352  |
| C       | 0.4031  | -1.6088 | 1.2737  |
| C       | -0.8909 | -1.5641 | 0.4558  |
| C       | -1.3635 | -0.0958 | 0.2984  |
| C       | -0.4605 | 0.4153  | -0.8301 |
| C       | 0.4953  | -0.8021 | -0.9966 |
| O       | -0.4324 | -1.8657 | -0.8611 |
| O       | 2.0949  | 0.0411  | 0.8093  |
| C       | 2.4072  | -2.1095 | -0.1255 |
| H       | 0.3952  | -0.9757 | 2.1574  |
| H       | 0.6267  | 2.6352  | 1.5595  |
| H       | -1.6619 | -2.2670 | 0.7541  |
| H       | 1.0018  | -0.8561 | -1.9536 |
| C       | 2.9071  | 0.7743  | 0.0109  |
| N       | 3.1555  | -2.9430 | -0.3806 |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 3.52859700 | 1.89110100 | 0.79057400 |
| O    | 3.05553300 | 0.53998400 | -1.15584700 |
| H    | 2.74633000 | 2.47106500 | 1.28485100 |
| H    | 4.11122500 | 2.52319900 | 0.12445000 |
| H    | 4.17485400 | 1.48174200 | 1.56981300 |
| C    | 0.60711000 | 2.83939500 | -1.00735700 |
| C    | -0.04929100 | 1.73430600 | -0.25257400 |
| O    | -1.09494100 | 0.73300900 | 1.38966800 |
| N    | -0.41222700 | 1.88527700 | 0.95995100 |
| H    | 1.49884900 | 2.49187700 | -1.53155900 |
| H    | 0.86996900 | 3.65540500 | -0.33441000 |
| H    | -0.08481400 | 3.22538400 | -1.76208800 |
| H    | -0.97772600 | 0.53002700 | -1.78231700 |
| Br   | -3.28433800 | -0.00649400 | -0.13463000 |

| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | -1.11613900 | 0.76203100 | 0.19483400 |
| C    | -0.20426200 | 1.49647900 | 1.21819800 |
| C    | 1.17495300 | 1.30655700 | 0.56895400 |
| C    | 1.64449100 | -0.15252400 | 0.76153500 |
| C    | 0.73465400 | -0.89088600 | -0.23838400 |
| C    | -0.05559600 | 0.27714800 | -0.84840700 |
| O    | 0.86923000 | 1.34921800 | -0.81902800 |
| O    | -1.82039000 | -0.26977400 | 0.88741300 |
| C    | -2.06955400 | 1.69127000 | -0.42627000 |
| H    | -0.30604400 | 1.04100600 | 2.20321900 |
| H    | -0.45903500 | 2.55276600 | 1.28902900 |
| H    | 1.90894000 | 2.07303500 | 0.80879600 |
| H    | -0.42934600 | 0.11177000 | -1.85211500 |
| C    | -2.57673600 | -1.12038900 | 0.13885800 |
| N    | -2.79705500 | 2.45488000 | -0.88192700 |
| C    | -3.32053700 | -2.07462700 | 1.02427800 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | 2.610600  | -1.078166 | -1.055409 |
| H       | 2.621574  | -2.633854 | 1.649585  |
| H       | 3.900474  | -2.759379 | 0.410143  |
| H       | 3.983693  | -1.517814 | 1.689202  |
| H       | 0.119399  | -1.688152 | 0.174278  |
| H       | 4.317442  | 1.136894  | 0.709731  |
| H       | 4.430939  | -0.304806 | 1.720166  |
| C       | 2.987350  | -0.442826 | 0.147864  |
| C       | 4.285451  | 0.043059  | 0.692870  |
| N       | 2.927563  | -1.144460 | -0.910393 |
| O       | 1.614025  | -1.470398 | -1.205443 |
| H       | 5.110121  | -0.316931 | 0.078568  |
| H       | 1.577194  | -0.486362 | 1.799400  |

**5b**

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 1.341415  | 0.709006  | -0.391958 |
| C       | 0.364153  | 1.022714  | -1.557862 |
| C       | -0.956697 | 1.197572  | -0.798989 |
| C       | -1.510191 | -0.155079 | -0.284631 |
| C       | -0.506936 | -0.497757 | 0.831044  |
| C       | 0.367814  | 0.763464  | 0.830661  |
| O       | -0.535264 | 1.784093  | 0.423718  |
| O       | 1.942284  | -0.558635 | -0.647140 |
| C       | 2.378503  | 1.742520  | -0.268370 |
| H       | 0.372365  | 0.215269  | -2.287001 |
| H       | 0.628932  | 1.953526  | -2.056587 |
| H       | -1.694987 | 1.829334  | -1.287466 |
| H       | 0.824210  | 1.005082  | 1.783172  |
| C       | 2.712089  | -1.097360 | 0.339586  |
| N       | 3.169845  | 2.573212  | -0.209338 |
| C       | 3.343840  | -2.372493 | -0.129182 |
| O       | 2.833851  | -0.588370 | 1.414935  |
H  2.59035300  -3.03923500  -0.55191800
H  3.84909500  -2.85310500  0.70529700
H  4.06648900  -2.14998100  -0.91739900
H  0.02629100  -1.43585400  0.70109800
H  -4.04736400  1.37221600  -0.47402000
H  -4.41838600  -0.32511200  -0.79135800
C  -2.76880800  -0.01440000  0.53079000
C  -4.09441200  0.37780700  -0.02016000
N  -2.59296000  -0.25275300  1.76759000
O  -1.27821200  -0.58339900  2.02742200
H  -4.83532200  0.39583700  0.77784100
Cl  -1.71328000  -1.39391900  -1.57332200

5c
C  -1.60237100  -0.48466700  -0.64965900
C  -0.54977600  -0.34693800  -1.78384800
C  0.66779500  -1.02505300  -1.14370300
C  1.30520200  -0.15527700  -0.03087000
C  0.22683300  -0.21381600  1.06613500
C  -0.75888000  -1.21577800  0.44547600
O  0.07286100  -2.04629900  -0.35535500
O  -2.05908500  0.82905000  -0.30975200
C  -2.73605900  -1.32052500  -1.06790500
H  -0.40771400  0.70046600  -2.04163800
H  -0.85315100  -0.89362600  -2.67514400
H  1.38302700  -1.45290300  -1.84241800
H  -1.32363200  -1.80494900  1.15807300
C  -2.87027100  0.94106700  0.77842400
N  -3.60211500  -1.97870300  -1.43739600
C  -3.34483300  2.35459600  0.92539300
O  -3.14002700  0.01695600  1.48749700
H  -2.51288300  3.05351700  0.82732800
H  -3.83144200  2.47456900  1.89054000
H  -4.05849600  2.57770000  0.12870700
Br  1.84307000  1.62986700 -0.62037300
H  -0.20782700  0.74060700  1.89054000
H  3.62897600 -1.89684600 -0.74357400
H  4.23321900 -0.28682900 -0.33717800
C  2.43760000 -0.84471800  0.68347600
C  3.75330000 -1.17843800  0.07250300
N  2.15756600 -1.15318800  1.88558100
O  0.87336000 -0.76506000  2.21074300
H  4.40618600 -1.62138400  0.82340000

6a
C  -0.88536700 -0.69794700 -0.39045000
C  0.27916500 -1.32672500 -1.20700400
C  1.21279500 -1.79918900 -0.08423800
C  1.95107200 -0.62116000  0.60460300
C  0.81911800 -0.01843600  1.45452700
C  -0.37661700 -0.93112500  1.07050000
O  0.28390000 -2.18010000  0.93180100
O  -1.05109600  0.64386900 -0.81585400
C  -2.13724300 -1.44571400 -0.59376000
H  0.69940900 -0.57867100 -1.87832500
H  -0.06193000 -2.17697300 -1.79566000
H  1.84169100 -2.64890000 -0.33912300
H  -1.16535900 -0.99856400  1.81007300
C  -1.78979500  1.46488600 -0.01960900
N  -3.09252200 -2.05612100 -0.78066300
C  -1.72808000  2.86885200 -0.51334200
O  -2.37475700  1.07234600  0.94771400
H  -0.70483500  3.23190000 -0.41074800
H  -2.41334200  3.49393300  0.03650600
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | -3.495622 | 1.433405 | 1.605639 |
| H       | -2.252917 | 0.711510 | 2.623473 |
| C       | -1.627444 | 1.141247 | 0.622107 |
| C       | -2.428121 | 1.452759 | 1.838024 |
| N       | -0.822886 | 1.987122 | 0.109447 |
| O       | -0.227302 | 1.474397 | -1.031487 |
| H       | -2.165531 | 2.439556 | 2.217023 |
| H       | -0.978602 | -0.002930 | -2.226652 |
| Cl      | -3.325252 | -0.474208 | -0.771866 |

| 6c      |         |         |         |
|---------|---------|---------|---------|
| C       | 1.606413 | -0.806893 | 0.425156 |
| C       | 0.554858 | -1.024767 | 1.548367 |
| C       | -0.711816 | -1.314254 | 0.726962 |
| C       | -1.260226 | -0.023263 | 0.064012 |
| C       | -0.273731 | 0.157562 | -1.101209 |
| C       | 0.717994 | -1.012229 | -0.844053 |
| O       | -0.182576 | -2.011934 | -0.396076 |
| O       | 2.188030 | 0.472773 | 0.603914 |
| C       | 2.647875 | -1.845818 | 0.466621 |
| H       | 0.510424 | -0.145029 | 2.188401 |
| H       | 0.798519 | -1.892576 | 2.159342 |
| H       | -1.459129 | -1.921958 | 1.228519 |
| H       | 1.258299 | -1.349794 | -1.720216 |
| C       | 2.899859 | 0.986379 | -0.439520 |
| N       | 3.440500 | -2.674537 | 0.535737 |
| C       | 3.310950 | 2.392148 | -0.138986 |
| O       | 3.120383 | 0.363474 | -1.436678 |
| H       | 2.413154 | 3.014587 | -0.120129 |
| H       | 3.991579 | 2.745393 | -0.910146 |
| H       | 3.782543 | 2.453370 | 0.842855 |
| H       | -2.833732 | 1.783112 | 1.877304 |
|   | X          | Y            | Z            |
|---|------------|--------------|--------------|
| H | -1.61325300| 0.92221200   | 2.81041300   |
| C | -1.08134500| 1.28703700   | 0.76895100   |
| C | -1.75760000| 1.68119000   | 2.03595500   |
| N | -0.26833800| 2.06783800   | 0.17239400   |
| O | 0.20113800  | 1.49168500   | -0.99698500  |
| H | -1.36084100| 2.63132000   | 2.39154100   |
| H | 0.71321100  | 0.53012200   | -2.08862800  |
| Br| -3.12899100 | -0.16589800  | -0.48237500  |

**Cartesian coordinates of the stationary points found in benzene**

**Reactants**

### 1

|   | X          | Y            | Z            |
|---|------------|--------------|--------------|
| N | -0.72996200| 0.00033400   | 0.00000000   |
| O | 0.13944900 | 0.00000000   | 0.00000000   |
| C | 0.42368600 | -0.00086500  | 0.00015400   |
| C | 1.88213700 | 0.00000000   | 0.00000000   |
| H | 2.26396100 | -1.02071800  | -0.05593200  |
| H | 2.26301000 | 0.55981500   | -0.85621400  |
| H | 2.26341500 | 0.46299500   | 0.91195800   |

### 2a

|   | X          | Y            | Z            |
|---|------------|--------------|--------------|
| C | 0.12607000 | 0.51556100   | 0.28867200   |
| C | 1.26579900 | 0.37142000   | 1.33083400   |
| C | 2.36152700 | -0.30368200  | 0.45913100   |
| C | 1.89607500 | -1.71622800  | 0.15335300   |
| C | 0.93337000 | -1.58487700  | -0.75303600  |
| C | 0.82808800 | -0.09226600  | -0.99949900  |
| O | 2.15056200 | 0.36101600   | -0.78644500  |
| O | -1.01471800| -0.19465900  | 0.76783800   |
| C | -0.22649000| 1.92207600   | 0.05685600   |
2b

C   0.02962200  -0.69223300  1.08915800
C   0.24777900  -2.01019600  1.75780200
H   0.24777900  -2.01019600  1.75780200
H   2.42985500  -1.87071400  -0.54074700
H   -0.61854400  -0.85779100  1.94088600
C   -2.02249700  1.99525700  0.10331200
N   -2.65386500  -2.39516000  -0.37616900
C   -2.43955300  2.59858400  -0.50520300
O   -2.36057000  0.86115700  1.16863600
|   |   |   |   |
|---|---|---|---|
| H | -1.55873400 | 3.19471600 | -0.75086700 |
| H | -3.07663600 | 3.13972700 | 0.19014800 |
| H | -2.97988300 | 2.41262500 | -1.43557000 |
| H | 0.79330000 | 1.44256300 | 1.61474200 |
| Cl | 3.27481400 | 1.07336000 | -0.27985000 |

2c

|   |   |   |   |
|---|---|---|---|
| C | -1.30364100 | -0.60824300 | -0.32695800 |
| C | -0.19377300 | -1.18901500 | -1.24178500 |
| C | 0.87176300 | -1.57248400 | -0.18174400 |
| C | 1.41655200 | -0.27290300 | 0.39331900 |
| C | 0.47710600 | 0.21432000 | 1.19389800 |
| C | -0.64078100 | -0.80756400 | 1.10201200 |
| O | 0.04732900 | -2.02659800 | 0.88430100 |
| O | -1.54020700 | 0.74316800 | -0.71171200 |
| C | -2.54909900 | -1.38075600 | -0.42029800 |
| H | 0.13996300 | -0.44380100 | -1.96227600 |
| H | -0.53469200 | -2.07676700 | -1.77182000 |
| H | 1.59275400 | -2.32822900 | -0.47901200 |
| H | -1.34017200 | -0.88327300 | 1.92551400 |
| C | -2.30100600 | 1.51362200 | 0.10655900 |
| N | -3.50943800 | -2.00637400 | -0.50380200 |
| C | -2.46973400 | 2.88436200 | -0.47302100 |
| O | -2.75056400 | 1.11340900 | 1.14354300 |
| H | -1.49256400 | 3.34823200 | -0.62126400 |
| H | -3.07341700 | 3.49223900 | 0.19660800 |
| H | -2.95255000 | 2.81476200 | -1.44950500 |
| H | 0.43802200 | 1.15927100 | 1.71485100 |
| Br | 3.02548400 | 0.50383700 | -0.15621200 |

**Transition States**
### TS-PSa

| Element | x   | y   | z   | x   | y   | z   |
|---------|-----|-----|-----|-----|-----|-----|
| C       | -1.22130000 | -0.80799100 | 0.06855300 |
| C       | -0.67810800 | -2.01180000 | -0.74630500 |
| C       | 0.85041100 | -1.81755700 | -0.55880100 |
| C       | 1.24921600 | -0.58078400 | -1.33166900 |
| C       | 0.82321700 | 0.47308700  | -0.57265100 |
| C       | 0.13026200 | -0.18673500 | 0.61085700  |
| O       | 0.89119200 | -1.36160900 | 0.79545800  |
| O       | -1.97762600 | 0.02623700  | -0.80955300 |
| C       | -2.06917300 | -1.23841600 | 1.18773600  |
| H       | -1.01604200 | -1.95511600 | -1.78021500 |
| H       | -0.99709400 | -2.96035400 | -0.31583500 |
| H       | 1.45787200  | -2.70880200 | -0.68288700 |
| H       | 0.02774500  | 0.36737600  | 1.53675000  |
| C       | -2.31919600 | 1.26340700  | -0.37883700 |
| N       | -2.72022200 | -1.59393000 | 2.06575200  |
| C       | -3.13345500 | 1.97331300  | -1.41766100 |
| O       | -1.99564200 | 1.69777900  | 0.69192300  |
| H       | -2.61877400 | 1.95326300  | -2.37961400 |
| H       | -3.30995200 | 2.99989900  | -1.10526300 |
| H       | -4.08886100 | 1.45974900  | -1.54496100 |
| H       | 0.58655100  | 1.46207600  | -0.94225100 |
| H       | 3.45230800  | 2.68834500  | 1.64520200  |
| H       | 1.80450100  | 2.96497700  | 1.04918800  |
| C       | 2.67734900  | 1.14694900  | 0.42859200  |
| C       | 2.49655700  | 2.20996500  | 1.42466500  |
| N       | 3.43086000  | 0.37622300  | -0.08314100 |
| O       | 3.49593700  | -0.55131500 | -0.87939400 |
| H       | 2.08653000  | 1.79921900  | 2.34979100  |
| H       | 1.49517700  | -0.57604400 | -2.38252700 |

### TS-PSb
|   | C         |          |          |
|---|-----------|----------|----------|
|   | 0.72131900| -1.14294900| -1.68138400|
|   | -0.57634200| -0.29829400| -1.68010000|
|   | -1.13939000| -0.32167600| -0.27113900|
|   | -0.35140000| 0.51201200| 0.47360300|
|   | 0.68889300| 0.98139500| -0.53347600|
| O | -0.04371800| 1.02088800| -1.74301700|
| O | 2.04181700| -0.99221200| 0.33473100|
| C | 2.83702200| 0.19152100| -1.55533700|
| H | 0.61402700| -2.12922600| -1.23168500|
| H | 1.10193800| -1.24992200| -2.69613700|
| H | -1.27303100| -0.48161100| -2.49187600|
| H | 1.20082600| 1.91947000| -0.35378300|
| C | 2.63812900| -0.32509400| 1.35240300|
| N | 3.75510900| 0.53487100| -2.15534800|
| C | 3.01542600| -1.27195700| 2.44985700|
| O | 2.81445700| 0.86178800| 1.33986800|
| H | 2.13693400| -1.82896600| 2.78092400|
| H | 3.44341600| -0.71688800| 3.28118500|
| H | 3.74162900| -1.99658100| 2.07605200|
| H | -0.17227800| 0.41334600| 1.53537600|
| H | -1.54406100| 4.27757700| 1.52159100|
| H | -0.80111100| 3.02945800| 2.54342400|
| C | -1.52954000| 2.34335800| 0.68262100|
| C | -0.91815700| 3.38382000| 1.51777400|
| N | -2.45028500| 2.02396400| -0.00620800|
| O | -2.89945100| 1.12080900| -0.69166900|
| H | 0.06782400| 3.64955000| 1.13198900|
| Br | -2.14712800| -1.76332300| 0.38518800|

**TS-MSa**

|   | C         |          |          |
|---|-----------|----------|----------|
|   | -1.22126900| 0.77564100| 0.15704400|
|   | -0.36165200| 1.57330800| 1.17319600|
C  1.06286500  1.25040100  0.65713600
C  1.36935100 -0.21281800  0.96209700
C  0.58695500 -0.90864100  0.08274300
C -0.08975800  0.14832400 -0.75038800
O  0.84444900  1.21255400  0.87700800
C  0.58695500 -0.90864100  0.08274300
O -2.01752600 -0.16444600  1.11090400
C -2.08402900  1.66411000 -0.63264900
H -0.55618200  2.30729000  2.18861300
H -0.56189300  2.64234000  1.11090400
H  1.81788000  1.99254000  0.90531900
H -0.39611800  0.14832400 -1.76521300
C -2.70268500 -1.09143000  0.16194700
N -2.73909000  2.38835500 -0.23881600
C -3.48692200 -1.98502900  1.07453900
O -2.65472400 -1.15917900 -1.03389000
H -2.80377300 -2.54821900  1.71417900
H -4.08638500 -2.67231600  0.48231100
H -4.12973000 -1.38772400  1.72300000
H  0.26032900 -1.93402600  0.15634000
H  4.27760900  1.33959300  0.84797500
H  4.56339000 -0.12637300  1.79947400
C  3.38378400 -0.41104300  0.06864700
C  4.47109900  0.26693700  0.78542500
N  3.08476000 -1.06435800 -0.88532600
O  2.14317900 -1.59676400 -1.45322600
H  5.41771300  0.11626600  0.26386700
H  1.68799200 -0.57152900  1.93320800

TS-MSb
C  1.44227000  0.66944600 -0.47381700
C  0.51499800  0.83600600 -1.70604000
C -0.85983200  0.97036800 -1.01429800
C  -1.23644200  -0.38100600  -0.40542800
C  -0.38647300  -0.57465000  -0.59477100
C   0.38596500   0.74745300   0.70568300
O  -0.52319900   1.69366000   0.16103800
O   2.12705600  -0.54775100  -0.65382700
C   2.40804000   1.77100100  -0.36774800
H   0.59623200  -0.02715700  -2.36567100
H   0.75104500   1.73937400  -2.26658400
H  -1.62511100   1.48743200  -1.58772100
H   0.77769200   1.07697100   1.65967900
C   2.84673700  -1.00827200   0.47234700
N   3.14186400   2.65338900  -0.30815600
C   3.52952200  -2.30251300   0.15321400
O   2.89984400  -0.40572900   1.50699800
H   2.80615700  -3.02787400  -0.22295800
H   4.01837100  -2.68608800   1.04552100
H   4.27142800  -2.13904000  -0.63141000
H  -0.05704200  -1.47913600   1.08499400
H  -4.07217600   1.55487700  -0.65803800
H  -4.36454700   -0.15818300  -1.01790100
C  -3.12089300   0.19179000   0.64543600
C  -4.24454500   0.57153800  -0.21573300
N  -2.71435000   0.04934000  -1.75774700
O  -1.71318800  -0.24466200   2.39815100
H  -5.16691100   0.60623200   0.36669600
Cl  -1.81930300  -1.68963700  -1.41233700

TS-MSc
C  -1.71429100  -0.45190300  -0.69141800
C  -0.71124400  -0.21468300  -1.85038400
C   0.57878500  -0.80464200  -1.23907400
C   1.05116700   0.10758400  -0.10433100
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -0.54147000 | -1.04747900 | 1.10751100 |
| O    | -0.04392900 | -2.36305700 | 0.86819200 |
| O    | -0.96098400 | 0.70846100 | -0.73134200 |
| C    | -2.19428400 | -1.29872000 | -0.72253800 |
| H    | 0.80510700 | -0.58409800 | -1.72178100 |
| H    | -0.09216900 | -2.10898700 | -1.82057100 |
| H    | 1.65632400 | -2.82591300 | -0.23878200 |
| H    | -1.38547700 | -1.06264100 | 1.78612500 |
| C    | -1.74556300 | 1.52376500 | 0.01917400 |
| N    | -3.18317800 | -1.80833200 | -1.01105400 |
| C    | -1.69983800 | 2.92674100 | -0.49931300 |
| O    | -2.37606300 | 1.12973000 | 0.96013000 |
| H    | -2.46558900 | 3.52121800 | -0.00593400 |
| H    | -1.84608000 | 2.94089500 | -1.58017600 |
| H    | -0.71389000 | 3.34014500 | -0.28140500 |
| H    | 3.29783400 | -0.52437100 | -1.91381100 |
| H    | 3.96134500 | 1.11761800 | -1.82772000 |
| C    | 2.51766600 | 0.67516700 | -0.35194600 |
| C    | 3.62098500 | 0.26734100 | -1.23503900 |
| N    | 1.89428400 | 1.61684100 | 0.05036200 |
| O    | 1.01009000 | 1.92327300 | 0.83919100 |
| H    | 4.45960700 | -0.10915900 | -0.64578700 |
| H    | 0.75414500 | 0.23992800 | 2.50252600 |
| H    | 2.74383200 | -1.01210100 | 1.25816300 |

**TS-MAb**

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 1.20140600 | -0.75745500 | 0.42128900 |
| C    | 0.06302800 | -1.09713500 | 1.42205800 |
| C    | -1.02092600 | -1.62377600 | 0.45743900 |
| C    | -1.60331500 | -0.49382800 | -0.40485100 |
| C    | -0.62917800 | -0.22008500 | -1.32528800 |
| C    | 0.51444600 | -1.15399300 | -0.94006900 |
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| O | -0.19564800 | -2.31152600 | -0.49382700 |
| O | 1.58822000  | 0.59279900  | 0.61026900  |
| C | 2.36744200  | -1.63270000 | 0.63227500  |
| H | -0.20228500 | -0.21500800 | 1.99963600  |
| H | 0.35923200  | -1.88992100 | 2.10693900  |
| H | -1.75078300 | -2.29837200 | 0.89622900  |
| H | 1.20738600  | -1.40012700 | -1.73526100 |
| C | 2.40887600  | 1.14554400  | -0.32244400 |
| N | 3.26299600  | -2.32609800 | 0.82604000  |
| C | 2.73467700  | 2.56414900  | 0.02404800  |
| O | 2.79367600  | 0.53953400  | -1.28237100 |
| H | 3.62514800  | 2.87378300  | -0.51904900 |
| H | 2.88039800  | 2.68255800  | 1.09754100  |
| H | 1.89308800  | 3.18936600  | -0.28019900 |
| H | -2.36052400 | 0.56575200  | 2.61657900  |
| H | -2.50123400 | 2.32751600  | 2.46856000  |
| C | -1.69156600 | 1.37147300  | 0.77794800  |
| C | -2.59936300 | 1.82097000  | 1.93309700  |
| N | -0.98660000 | 2.03734200  | 0.07839000  |
| O | -0.27802300 | 1.97744600  | -0.91762300 |
| H | -3.63251600 | 1.26369400  | 1.60405700  |
| H | -0.75879000 | 0.16405800  | -2.32306000 |
| Cl| -3.31958200 | -0.50198700 | -0.80280200 |

**TS-MAc**

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | 1.60358700 | -0.78214800 | 0.42524200 |
| C | 0.52671900 | -1.01252300 | 1.52004900 |
| C | -0.65910100 | -1.50213700 | 0.66107900 |
| C | -1.24063600 | -0.36411600 | -0.19367500 |
| C | -0.32223400 | -0.18010900 | -1.19218400 |
| C | 0.78914300  | -1.17389400 | -0.86439200 |
| O | 0.04701400  | -2.26922500 | -0.32515200 |
O  2.09104700  0.54352200  0.53710100
C  2.72240800 -1.72829800  0.57856500
H  0.36140400 -0.09382400  2.07693600
H  0.82516100 -1.79646700  2.21406200
H -1.38674500 -2.11842900  1.18116300
H  1.40008600 -1.48727800 -1.70211900
C  2.86605500  1.01596100 -0.47511000
C  3.29840700  2.42263000 -0.20484100
O  3.13730700  0.35920900 -1.44042900
H  4.18133400  2.65138600 -0.79825100
H  3.49809700  2.57617800  0.85526700
H  2.48502000  3.08752400 -0.50182000
H -1.64424000  0.87642900  2.87132900
H -1.77330400  2.62689300  2.61741000
C -1.12943000  1.54501000  0.93064700
C -1.93081500  1.65033200  2.15728100
N -0.43241600  2.13747700  0.16081500
O  0.19327800  2.00013400 -0.88247000
H -2.99025800  1.53032700  1.92815600
H -0.49787200  0.18595700 -2.18961700
Br -3.12590800 -0.28829900 -0.51267500

TS-PAa
C  -1.06245900  -0.19720300  0.18723800
C  -0.85782400  -0.83935200 -1.21398200
C  -0.30762700  -2.22775900 -0.80592900
C  1.13724800  -2.11128600 -0.34576100
C  1.07244000  -1.46776400  0.86070300
C  -0.43206800  -1.30213700  1.10502400
O  -0.98140300  -2.44049600  0.45054300
O  -0.43226600  1.05678300  0.40902600
|    | X       | Y       | Z       |
|----|---------|---------|---------|
| C  | -2.48985300  | -0.08382900  | 0.53334300  |
| H  | -0.15795400  | -0.27027900  | -1.81966900  |
| H  | -1.80241700  | -0.92706200  | -1.74648100  |
| H  | -0.53092300  | -3.03562600  | -1.49666200  |
| H  | -0.75202700  | -1.25230900  | 2.14272700   |
| C  | -0.76236500  | 2.08477300   | -0.41516400  |
| N  | -3.59342700  | -0.01155700  | 0.84558700   |
| C  | 0.07647900   | 3.29022200   | -0.11478300  |
| O  | -1.59728400  | 1.99251300   | -1.26800900  |
| H  | 0.17252100   | 3.44497000   | 0.96001000   |
| H  | -0.36414600  | 4.16619600   | -0.58530700  |
| H  | 1.07724900   | 3.13226500   | -0.52619200  |
| C  | 2.45431300   | 1.19890900   | 1.66417300   |
| C  | 2.20808600   | 0.37518800   | 0.47495000   |
| O  | 2.16131000   | -0.50531500  | -1.64038100  |
| N  | 2.40467900   | 0.25100700   | -0.69845200  |
| H  | 3.09303900   | 0.66615400   | 2.37147900   |
| H  | 1.50652600   | 1.42744600   | 2.15224800   |
| H  | 2.94552100   | 2.13225300   | 1.38365900   |
| H  | 1.75935700   | -1.61117900  | 1.68455000   |
| H  | 1.95340400   | -2.69543600  | -0.73861000  |

**TS-PAb**

|    | X       | Y       | Z       |
|----|---------|---------|---------|
| C  | -0.99142800  | -0.93374000  | 0.19843900  |
| C  | -0.23572400  | -1.24494700  | -1.12517400  |
| C  | 1.14622700  | -1.65213500  | -0.56799500  |
| C  | 1.90379000  | -0.42845300  | -0.05941000  |
| C  | 1.26124200  | -0.03769000  | 1.08170400   |
| C  | 0.16819400  | -1.10410600  | 1.23676000   |
| O  | 0.77939400  | -2.26644600  | 0.67994100   |
| O  | -1.56429600  | 0.35910700   | 0.31464800   |
| C  | -2.01864000  | -1.94744600  | 0.49280200   |
H  -0.19473100  -0.38134100  -1.78155200
H  -0.69825400  -2.07617500  -1.65301800
H   1.72146500  -2.33610200  -1.18473600
H  -0.16614900  -1.28640200   2.25461600
C  -2.48719600   0.72924400  -0.61289100
N  -2.80269500  -2.74151200   0.76669100
C  -2.89494700   2.15561600  -0.40218400
O  -2.87412000  -0.00757900  -1.47282800
H  -3.09007500   2.35171600   0.65269400
H  -3.77897100   2.37453100  -0.99645400
H  -2.07746600   2.80758900  -0.72169600
C   0.05884800   2.74096900   1.79352200
C   0.59382700   2.00771000   0.64246700
O   1.26070900   1.33433100  -1.44463800
N   0.83598200   2.02844200  -0.52646200
H   0.82041500   2.85043700   2.56766200
H  -0.79010200   2.19673800   2.21000300
H  -0.27176100   3.73439200   1.48528000
H   1.75280000   0.37951600   1.95031700
Cl  3.57065700  -0.15816700  -0.42058400

TS-PAc
C  -1.41907900  -0.94587400   0.18929900
C  -0.59984600  -1.23637700  -1.10067000
C   0.76430400  -1.62024500  -0.48433800
C   1.47830900  -0.38176000   0.05475800
C   0.77626000  -0.00476200   1.16625200
C  -0.30178900  -1.09328500  -1.27644300
O   0.35521600  -2.24197900   0.74662300
O  -2.02769300   0.33239000   0.28310500
C  -2.43472400  -1.98348200   0.43752300
H  -0.54552600  -0.36838000  -1.75053300
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| H       | -1.02316900 | -2.07274900 | -1.65269700 |
| H       | 1.37379100  | -2.29636000 | -1.07607600 |
| H       | -0.67605800 | -1.28239100 | 2.27912700  |
| C       | -2.91763000 | 0.68377780  | -0.68298700 |
| N       | -3.21232400 | -2.79519400 | 0.67577900  |
| C       | -3.36929900 | 2.09898300  | -0.48670200 |
| O       | -3.24785800 | -0.05832900 | -1.56179100 |
| H       | -3.60319700 | 2.29099300  | 0.56093400  |
| H       | -4.23847200 | 2.29498900  | -1.11015200 |
| H       | -2.55907200 | 2.77173300  | -0.78093100 |
| C       | -0.55582900 | 2.72068600  | 1.82294900  |
| C       | 0.06744000  | 2.01313200  | 0.69986200  |
| O       | 0.86018700  | 1.38299100  | -1.35679300 |
| N       | 0.36599000  | 2.05219900  | -0.45588300 |
| H       | 0.16657500  | 2.88218900  | 2.62491000  |
| H       | -1.38568200 | 2.12717800  | 2.20933300  |
| H       | -0.93561900 | 3.68890300  | 1.49215200  |
| H       | 1.21615800  | 0.42626300  | 2.05576100  |
| Br      | 3.30534600  | -0.05962200 | -0.24670300 |

Products

3a
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.10722800 | -0.80998700 | -0.01782500 |
| C       | -0.46702000 | -1.92415600 | -0.89209200 |
| C       | 1.01032700  | -1.81216800 | -0.48367000 |
| C       | 1.61612700  | -0.56137600 | -1.13022900 |
| C       | 1.00351300  | 0.55469800  | -0.26509200 |
| C       | 0.15628200  | -0.26688000 | 0.72962800  |
| O       | 0.91417300  | -1.44588800 | 0.89478500  |
| O       | -1.76587300 | 0.11606200  | -0.88032800 |
| C       | -2.07000000 | -1.36357000 | 0.94528100  |
H  -0.65930200  -1.72841400  -1.94689200
H  -0.86406700  -2.90575300  -0.64029800
H   1.60326500  -2.71619200  -0.58991700
H  -0.04824000   0.19768900   1.68773300
C  -2.24220400   1.26386200  -0.32811000
N  -2.81234900  -1.82956000   1.68821600
C  -2.99409800   2.06586700  -1.34463000
O  -2.06568800   1.55042200   0.82214700
H  -2.43716500   2.12673000  -2.28033900
H  -3.18862100   3.06062900  -0.95069700
H  -3.94393600   1.56933000  -1.55684800
H   0.44104000  -0.00168300  -0.80168300
H   1.79381900   3.13457400   0.88559800
H   1.68690000   1.99750600   2.22668600
C   2.24946400   1.11648900   0.36289400
C   2.25855800   2.24912900   1.32866000
N   3.31673200   0.53376700  -0.00800000
O   3.02925900  -0.47766500  -0.91691500
H   3.27970700   2.49164100   1.62089400
H   1.42863300  -0.49005900  -2.20207600

3b
C    1.29085400  -0.77507300  -0.28529200
C    0.47121800  -2.02474900   0.14090300
C   -0.90285100  -1.70634200  -0.46221100
C   -1.62928700  -0.59040700   0.30976400
C   -0.78164200   0.64583100  -0.02968200
C    0.19897500   0.03835200  -1.05549700
O   -0.55789000  -1.00059400  -1.65145300
O    1.81453600  -0.15900500   0.88709500
C    2.38987300  -1.13133400  -1.19468100
H    0.48378300  -2.13351700   1.22314400
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | 1.315696  | -0.642451| 2.553802 |
| H    | -1.31405  | 1.843775 | 0.722113 |
| C    | -2.55005  | -0.165963| -1.379993|
| N    | -3.69553  | -0.126565| 2.191423 |
| C    | -2.84261  | -0.916282| -2.641200|
| O    | -2.86173  | 0.963037 | -1.124481|
| H    | -1.90607  | -1.191591| -3.131143|
| H    | -3.43986  | -0.295181| -3.304215|
| H    | -3.37530  | -1.840217| -2.410304|
| H    | 0.067627  | 0.438160 | -1.273529|
| H    | 0.53499   | 3.031803 | -2.285516|
| H    | -0.212106 | 3.674854 | -0.825306|
| C    | 1.192115  | 2.106388 | -0.481070|
| C    | 0.725382  | 3.296203 | -1.241818|
| N    | 2.326325  | 2.070679 | 0.092476 |
| O    | 2.49559   | 0.832236 | 0.729497 |
| H    | 1.47285   | 4.087613 | -1.206767|
| Br   | 2.114487  | -1.567241| -0.573446|

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | -0.516208 | -0.980508| -0.258074|
| C    | 0.599291  | -1.455982| -1.227736|
| C    | 1.786022  | -1.583279| -0.267810|
| C    | 2.379061  | -0.193066| 0.046869 |
| C    | 1.325608  | 0.378760 | 1.010136 |
| C    | 0.297450  | -0.786592| 1.063809 |
| O    | 1.161698  | -1.909163| 0.981103 |
| O    | -1.152689 | 0.160286 | -0.818995|
| C    | -1.508623 | -2.049286| -0.047991|
| H    | 0.753816  | -0.713758| -2.008271|
| H    | 0.354884  | -2.412005| -1.686450|
| H    | 2.510622  | -2.351019| -0.523170|
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -0.30507800 | -0.83365800 | 1.96428400 |
| C       | -2.12041100 | 0.77114300  | -0.09348000 |
| N       | -2.25802500 | -2.91019400 | 0.08347500  |
| C       | -2.73243800 | 1.89033700  | -0.87625500 |
| O       | -2.40914800 | 0.43040400  | 1.02050900  |
| H       | -1.95485100 | 2.49479500  | -1.34495900 |
| H       | -3.35110100 | 2.50009400  | -0.22184400 |
| H       | -3.35171800 | 1.47263200  | -1.67360400 |
| C       | 0.21545500  | 2.78712800  | 0.92405900  |
| C       | 1.02808400  | 1.68530900  | 0.33367400  |
| O       | 0.0        | 2.41734400  | -1.05834500 |
| N       | 1.62282000  | 1.82669800  | -0.78424400 |
| H       | -0.73124600 | 2.42305000  | 1.32658100  |
| H       | 0.02512600  | 3.56436300  | 0.18422100  |
| H       | 0.76047900  | 3.23487600  | 1.76089700  |
| H       | 1.69428500  | 0.52967300  | 2.02607800  |
| H       | 3.38383400  | -0.26751700 | 0.46424900  |

**4b**

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 0.96597700 | -1.04985500 | 0.25079400 |
| C       | -0.08638400 | -1.54437400 | 1.28034700 |
| C       | -1.35951300 | -1.53008700 | 0.42825200 |
| C       | -1.84014500 | -0.07274100 | 0.22837500 |
| C       | -0.88596500 | 0.43735600  | -0.85760100 |
| C       | 0.06329000  | -0.78702100 | -1.00107500 |
| O       | -0.86829600 | -1.84909800 | -0.87454400 |
| O       | 1.64895600  | 0.06498400  | 0.80580000  |
| C       | 1.92724600  | -2.11767300 | -0.07106800 |
| H       | -0.11917400 | -0.87592100 | 2.13714800  |
| H       | 0.12726500  | -2.55636400 | 1.61857100  |
| H       | -2.13235200 | -2.23231000 | 0.72295700  |
| H       | 0.58570400  | -0.84763600 | -1.94890800 |
C          2.53309200      0.72485300      0.01690200
N          2.65404500       -2.97862700     -0.29522600
C          3.18151500      1.83805000      0.77660900
O          2.72187900      0.42690100     -1.13017200
H          2.42158200      2.44429200      1.27257800
H          3.77556000      2.44727400      0.09955900
H          3.82635100     -1.42000300     -1.9522600
C          0.24390100      2.83410400     -0.97014200
O          -0.48279700      1.74754900     -0.25519400
H          -1.64970200      0.77120200      1.32382200
N          -0.91974400      1.91067200      0.93097400
H          1.14883700      2.46018300     -1.45187200
H          0.49918700      3.64068600     -0.28357200
H          -0.39612300      3.23957700     -1.75910800
H          -1.36968000      0.56936800     -1.82536200
Cl         -3.58183900     -0.02507900     -0.26714400

4c
C          1.41544700     -1.05167300      0.24830300
C          0.39236500     -1.54841900      1.30574400
C         -0.90489300     -1.53160500      0.48991400
C         -1.38834400     -0.07122900      0.30711600
C         -0.46703400      0.43665000     -0.80939700
C          0.47796300     -0.78845400     -0.97806700
O         -0.45042000     -1.84987600     -0.82563000
O          2.11208300      0.06320400      0.78578500
C          2.36842200     -2.11807500     -0.10162000
C          0.38496000     -0.88340200      2.16574200
H          0.61422200     -2.56208500      1.63371900
H         -1.66634100     -2.23679800      0.80580400
H          0.97365500     -0.84992400     -1.94011800
C          2.97382600      0.72538900     -0.02544100
N  3.08924000  -2.97816600  -0.34742500
C  3.63779000   1.84064400   0.71773900
O  3.13395200   0.42813900  -1.17704800
H  4.21534000   2.44990900   0.02656800
H  4.30059200   1.42506100   1.47996600
C  2.88806300   2.44629500   1.22979100
H  0.65988800  -2.83330600  -0.95767100
C  -0.04308100   1.74646800  -0.21982200
O  -1.15812200   0.77067700   1.39564800
N  -0.43958500   1.90938600   0.98052400
H  1.54929400   2.46051000  -1.46815800
H  0.93607500   3.64024900  -0.27966000
H  -0.00564400   3.23799200  -1.72566400
H  -0.97126800   0.57035900  -1.76596900
Br  -3.30287300  -0.01005300  -0.16813000

5a
C  1.11256400   0.75644300   0.20279800
C  -0.19757100   1.48552500   1.22726700
C   1.17984600   1.29903900   0.57417800
C   1.65025500  -0.15986700   0.76006800
C   0.73576400  -0.89701800  -0.23540300
C  -0.05521200   0.27166500  -0.84336900
O   0.86954700   1.34404100  -0.81592500
O  -1.82134000  -0.27497100   0.88764000
C  -2.05897800   1.69343400  -0.41964700
H  -0.29511500   1.02475700   2.20982100
H  -0.45017700   2.54145100   1.30669000
H   1.91299200   2.06522900   0.81480100
H  -0.43124700   0.10703100  -1.84652200
C  -2.59457800  -1.10844700   0.13797400
N  -2.77634400   2.46390800  -0.87996600
| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| C     | -3.31555700 | -2.08557400 | 1.01414100 |
| O     | -2.65568700 | -1.03164100 | -1.05533500 |
| H     | -2.60055100 | -2.65814700 | 1.60805000 |
| H     | -3.90869000 | -2.75654900 | 0.39767900 |
| H     | -3.96410100 | -1.54720300 | 1.70790200 |
| H     | 0.12311100  | -1.69421200 | 0.18055400 |
| H     | 4.30801000  | 1.14061600 | 0.70969000 |
| H     | 4.43165400  | -0.30634300 | 1.71033300 |
| C     | 2.99117000  | -0.44380300 | 0.14018900 |
| C     | 4.28688600  | 0.04700500  | 0.68527600 |
| N     | 2.92999400  | -1.14462900 | -0.91874700 |
| O     | 1.61185300  | -1.47534400 | -1.20837300 |
| H     | 5.11561900  | -0.30214600 | 0.07028300 |
| H     | 1.59120600  | -0.49653500 | 1.79683700 |

5b

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| C     | 1.34089900 | 0.70203500 | -0.39812200 |
| C     | 0.36150300 | 1.01490900 | -1.56234800 |
| C     | -0.95709300 | 1.19471600 | -0.80170100 |
| C     | -1.51092300 | -0.15552000 | -0.28069100 |
| C     | -0.50545200 | -0.49709500 | 0.83337100 |
| C     | 0.37147200  | 0.76269800  | 0.82742900 |
| O     | 0.53092800  | 1.78369700  | 0.42081900 |
| O     | 1.93734600  | -0.56717500 | -0.64630800 |
| C     | 2.37756700  | 1.73774500  | -0.27895000 |
| H     | 0.36690500  | 0.20597700  | -2.28961100 |
| H     | 0.62462000  | 1.94306800  | -2.06621400 |
| H     | 1.69414500  | 1.82642700  | -1.29080300 |
| H     | 0.83091400  | 1.00598500  | 1.77823100 |
| C     | 2.72906200  | -1.09132800 | 0.33083400 |
| N     | 3.16301100  | 2.57416400  | -0.22179900 |
| C     | 3.30012500  | -2.40381800 | -0.10602000 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -2.377129 | 2.989532  | 1.152244  |
| H    | -3.972397 | 2.476696  | 1.763447  |
| H    | -3.713466 | 2.785858  | 0.022898  |
| Br   | 1.849696  | 1.612967  | -0.640025 |
| H    | -0.208606 | 0.763466  | 1.338832  |
| H    | 3.617152  | -1.908128 | -0.725555 |
| H    | 4.231548  | -0.301906 | -0.323288 |
| C    | 2.432503  | -0.844483 | 0.696462  |
| C    | 3.746735  | -1.189442 | 0.088961  |
| N    | 2.150356  | -1.135855 | 1.902405  |
| O    | 0.864680  | -0.736480 | 2.221905  |
| H    | 4.397838  | -1.633648 | 0.840506  |

**6a**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -0.876673 | -0.699470 | -0.390861 |
| C    | 0.289295  | -1.319606 | -1.211493 |
| C    | 1.227119  | -1.790794 | -0.092171 |
| C    | 1.957582  | -0.612265 | 0.602522  |
| C    | 0.824417  | -0.020492 | 1.457167  |
| C    | -0.366779 | -0.936182 | 1.069856  |
| O    | 0.297312  | -2.181906 | 0.923256  |
| O    | -1.054808 | 0.642389  | -0.812652 |
| C    | -2.126164 | -1.453384 | -0.592391 |
| H    | 0.705221  | -0.568628 | -1.881849 |
| H    | -0.045872 | -2.169548 | -1.803608 |
| H    | 1.860873  | -2.634572 | -0.351750 |
| H    | -1.153961 | -1.010370 | 1.810591  |
| C    | -1.805953 | 1.454378  | -0.022556 |
| N    | -3.081143 | -2.066320 | -0.773103 |
| C    | -1.753059 | 2.860430  | -0.527105 |
| O    | -2.399813 | 1.051642  | 0.937434  |
| H    | -0.734107 | 3.232479  | -0.399090 |
|  | X   | Y   | Z   |
|---|-----|-----|-----|
| H | 3.21331900 | 2.56709000 | 1.06713400 |
| H | -3.50511200 | 1.45992600 | 1.58651600 |
| H | -2.28380700 | 0.70791400 | 2.60785700 |
| C | -1.63395100 | 1.14611200 | 0.61753200 |
| C | -2.43982500 | 1.45976100 | 1.82918200 |
| N | -0.82660200 | 1.98938200 | 0.10456800 |
| O | -0.22670700 | 1.47163400 | -1.03463600 |
| H | -2.16622500 | 2.43854300 | 2.22059100 |
| H | -0.97864600 | -0.00769400 | -2.22777800 |
| Cl | -3.32675500 | -0.47658800 | -0.77566100 |

| 6c  | X   | Y   | Z   |
|-----|-----|-----|-----|
| C   | 1.60247100 | -0.80253000 | 0.42840700 |
| C   | 0.55252300 | -1.01596900 | 1.55349800 |
| C   | -0.71459000 | -1.30855800 | 0.73497800 |
| C   | -1.26254200 | -0.02184700 | 0.06368500 |
| C   | -0.27695800 | 0.15325400 | -1.10283400 |
| C   | 0.71450300 | -1.01446800 | -0.84056400 |
| O   | -0.18452000 | -2.01280800 | -0.38638300 |
| O   | 2.18771800 | 0.47640900 | 0.60132900 |
| C   | 2.64456300 | -1.84202500 | 0.46997100 |
| H   | 0.50833200 | -0.13519900 | 2.19171500 |
| H   | 0.79389300 | -1.88091200 | 2.16888000 |
| H   | -1.45989500 | -1.91320600 | 1.24212200 |
| H   | 1.25318100 | -1.35534600 | -1.71643700 |
| C   | 2.91147500 | 0.98075900 | -0.43603600 |
| N   | 3.43833400 | -2.47014700 | 0.53376200 |
| C   | 3.32278900 | 2.38729200 | -0.1412300 |
| O   | 3.14448100 | 0.34599700 | -1.42494900 |
| H   | 2.42633600 | 3.01158400 | -0.13010800 |
| H   | 4.00596400 | 2.73657900 | -0.91464100 |
| H   | 3.79234900 | 2.45310200 | 0.83830300 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -2.83837400| 1.80312400 | 1.86247100 |
| H    | -1.63124200| 0.92935400 | 2.80039700 |
| C    | -1.08547400| 1.29226600 | 0.76337500 |
| C    | -1.76428800| 1.69103700 | 2.02730700 |
| N    | -0.27137200| 2.06984800 | 0.16377800 |
| O    | 0.20018700 | 1.48721200 | -1.00416300|
| H    | -1.36200900| 2.63699000 | 2.38739500 |
| H    | -0.71483600| 0.02127800 | -2.09013000|
| Br   | -3.13120500| -0.27071400| -0.48329700|