

# Origins of Stereoselectivity in Intramolecular Aldol Reactions Catalyzed by Cinchona Amines

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## Supporting Information

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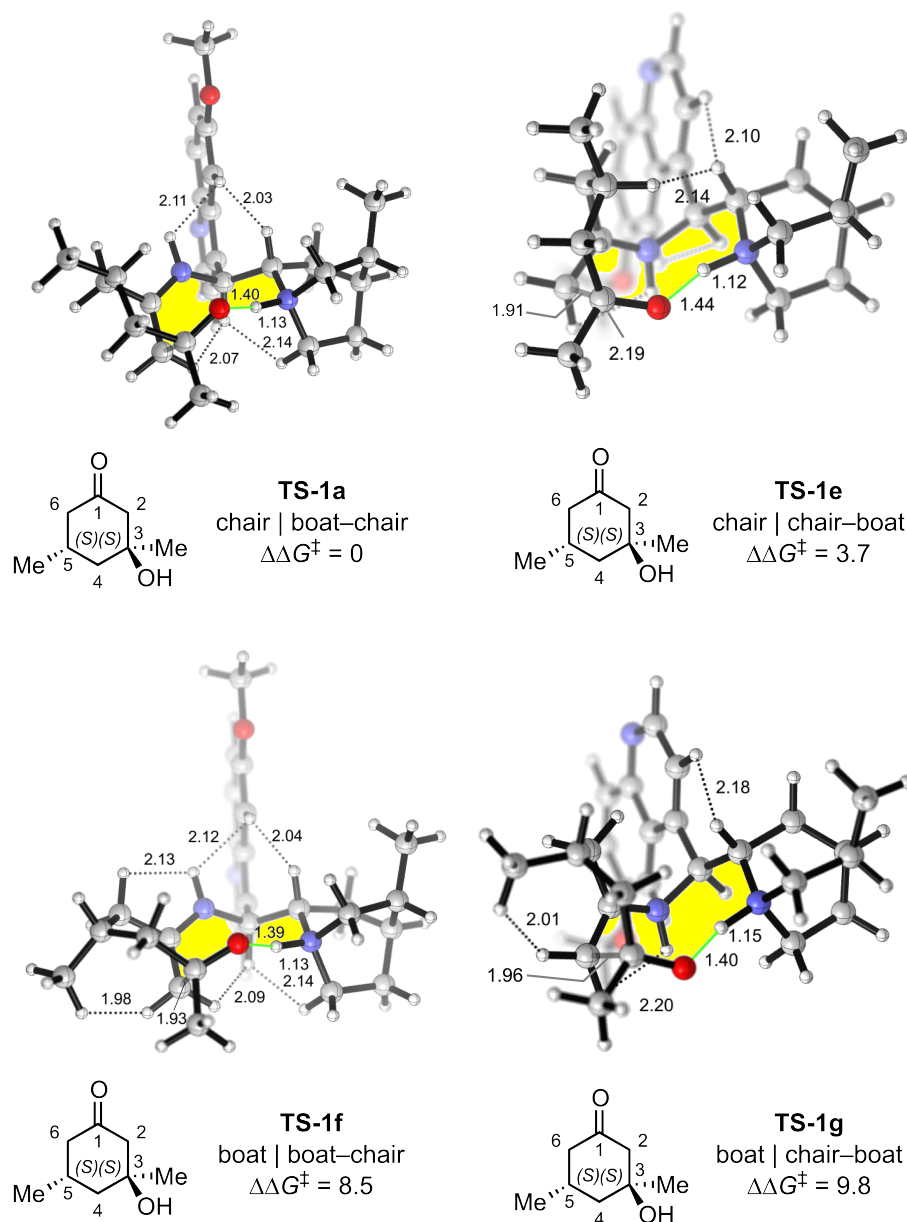
## A. Complete set of TS-1a–1p (B3LYP-D3(BJ)/def2-TZVPP-IEF-PCM (toluene)//B3LYP/6-31G(d)-IEF-PCM (toluene))

For each of the four stereoisomers of aldol adduct **4**, four transition state conformers that combine different conformations of the forming six-membered ring and the hydrogen-bonded nine-membered ring were located, resulting in a total of 16 transition structures (**TS-1a–1p**). Their conformational properties and relative energies, as well as the resulting configurations of the aldol adduct and cyclohexenone, are listed in Table S1. The lowest-energy transition structures that lead to the four stereoisomeric aldols are collected in entries 1 to 4 as **TS-1a–1d** and illustrated in Figure 4 of the Main Text. **TS-1a–1p** are illustrated in Figures S1–S4, organized by the stereochemistry of the resulting aldol adduct. For **TS-1a–1d**, transition structures differing only in the orientation of the quinoline ring, that is, the *syn* versus *anti* conformation, have also been checked. These are denoted **TS-1a'–1d'** and shown alongside **TS-1a–1d** in Table S1. The  $\Delta\Delta G^\ddagger$  values in Table S1 show that among the four transition structures that lead to a given stereoisomer of **4**, only one transition structure needs to be considered as the other three conformers are significantly higher in energy. The ring conformations found for the truncated system (diketone **10** and model catalyst **III**) are mostly retained in **TS-1a–1p**, although in the high-energy transition structure **TS-1o** ( $\Delta\Delta G^\ddagger = 8.0$ , Figure S4) the crown is distorted in order to alleviate steric hindrance from the axial methyl group. The medium rings in the lowest-energy transition structures are either boat–chairs or crowns, and the (*S*)-configured quinoline ring of the catalyst is equatorial.

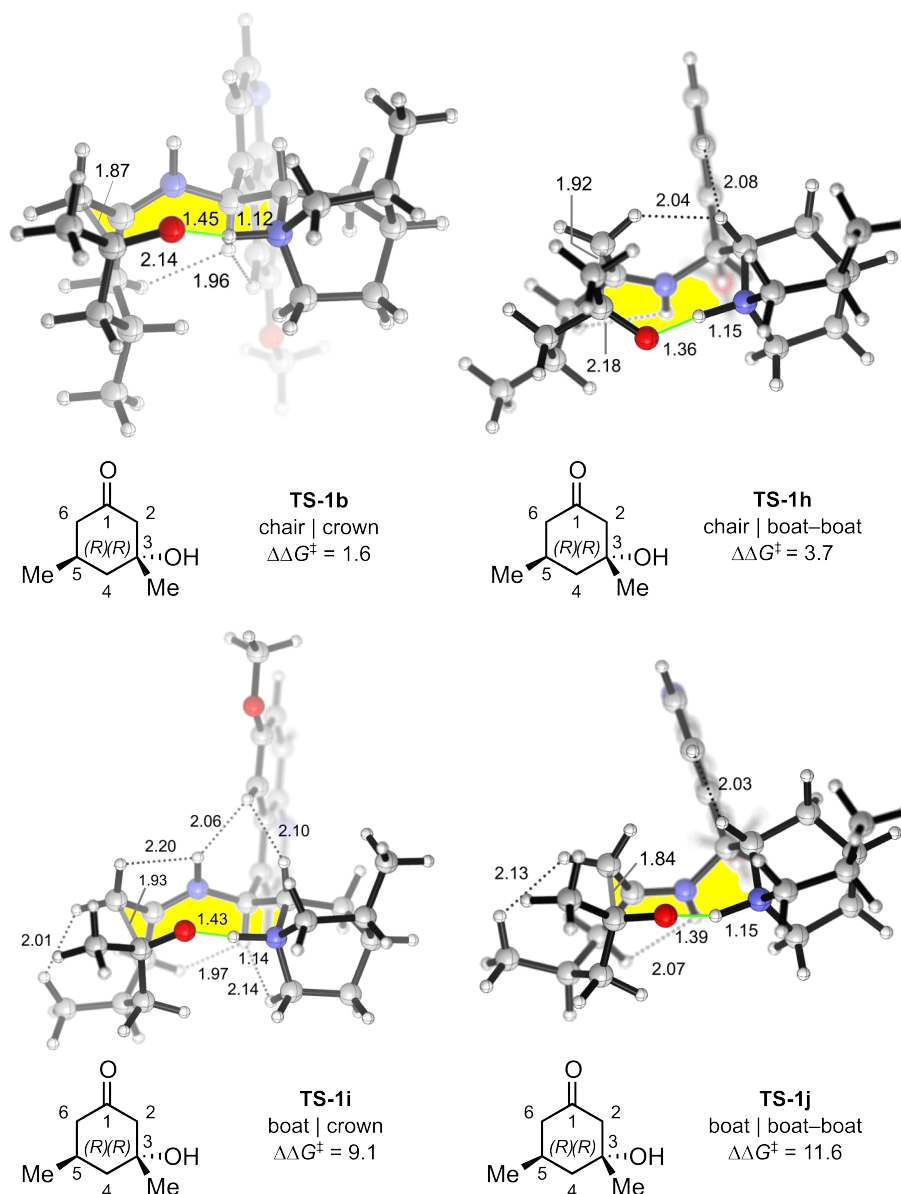
**Table S1.** Intramolecular Aldol Addition Transition Structures of **1** Catalyzed by **III**. <sup>a</sup>

| Entry                                                                | TS                                        | Ring Conformation  | Methyl Group Disposition | Configuration of Aldol (4) | Configuration of Cyclohexenone (7) | $\Delta\Delta G^\ddagger$ |
|----------------------------------------------------------------------|-------------------------------------------|--------------------|--------------------------|----------------------------|------------------------------------|---------------------------|
| Lowest-Energy Transition Structure for Each Stereoisomer of <b>4</b> |                                           |                    |                          |                            |                                    |                           |
| 1                                                                    | <b>TS-1a</b> / <b>TS-1a'</b> <sup>b</sup> | chair   boat–chair | equatorial               | (3 <i>S</i> ,5 <i>S</i> )  | <i>S</i>                           | 0 / 0.1                   |
| 2                                                                    | <b>TS-1b</b> / <b>TS-1b'</b> <sup>b</sup> | chair   crown      | equatorial               | (3 <i>R</i> ,5 <i>R</i> )  | <i>R</i>                           | 1.6 / 2.0                 |
| 3                                                                    | <b>TS-1c</b> / <b>TS-1c'</b> <sup>b</sup> | chair   boat–chair | axial                    | (3 <i>S</i> ,5 <i>R</i> )  | <i>R</i>                           | 2.7 / 3.4                 |
| 4                                                                    | <b>TS-1d</b> / <b>TS-1d'</b> <sup>b</sup> | boat   crown       | equatorial               | (3 <i>R</i> ,5 <i>S</i> )  | <i>S</i>                           | 4.9 / 5.0                 |
| Other Higher-Energy Transition Structures                            |                                           |                    |                          |                            |                                    |                           |
| 5                                                                    | <b>TS-1e</b>                              | chair   chair–boat | equatorial               | (3 <i>S</i> ,5 <i>S</i> )  | <i>S</i>                           | 3.7                       |
| 6                                                                    | <b>TS-1f</b>                              | boat   boat–chair  | axial                    | (3 <i>S</i> ,5 <i>S</i> )  | <i>S</i>                           | 8.5                       |
| 7                                                                    | <b>TS-1g</b>                              | boat   chair–boat  | axial                    | (3 <i>S</i> ,5 <i>S</i> )  | <i>S</i>                           | 9.8                       |
| 8                                                                    | <b>TS-1h</b>                              | chair   boat–boat  | equatorial               | (3 <i>R</i> ,5 <i>R</i> )  | <i>R</i>                           | 3.7                       |
| 9                                                                    | <b>TS-1i</b>                              | boat   crown       | axial                    | (3 <i>R</i> ,5 <i>R</i> )  | <i>R</i>                           | 9.1                       |
| 10                                                                   | <b>TS-1j</b>                              | boat   boat–boat   | axial                    | (3 <i>R</i> ,5 <i>R</i> )  | <i>R</i>                           | 11.6                      |
| 11                                                                   | <b>TS-1k</b>                              | chair   chair–boat | axial                    | (3 <i>S</i> ,5 <i>R</i> )  | <i>R</i>                           | 10.7                      |
| 12                                                                   | <b>TS-1l</b>                              | boat   chair–boat  | equatorial               | (3 <i>S</i> ,5 <i>R</i> )  | <i>R</i>                           | 6.1                       |
| 13                                                                   | <b>TS-1m</b>                              | boat   boat–chair  | equatorial               | (3 <i>S</i> ,5 <i>R</i> )  | <i>R</i>                           | 4.4                       |
| 14                                                                   | <b>TS-1n</b>                              | chair   boat–boat  | axial                    | (3 <i>R</i> ,5 <i>S</i> )  | <i>S</i>                           | 6.2                       |
| 15                                                                   | <b>TS-1o</b>                              | chair   crown      | axial                    | (3 <i>R</i> ,5 <i>S</i> )  | <i>S</i>                           | 8.0                       |
| 16                                                                   | <b>TS-1p</b>                              | boat   boat–boat   | equatorial               | (3 <i>R</i> ,5 <i>S</i> )  | <i>S</i>                           | 7.0                       |

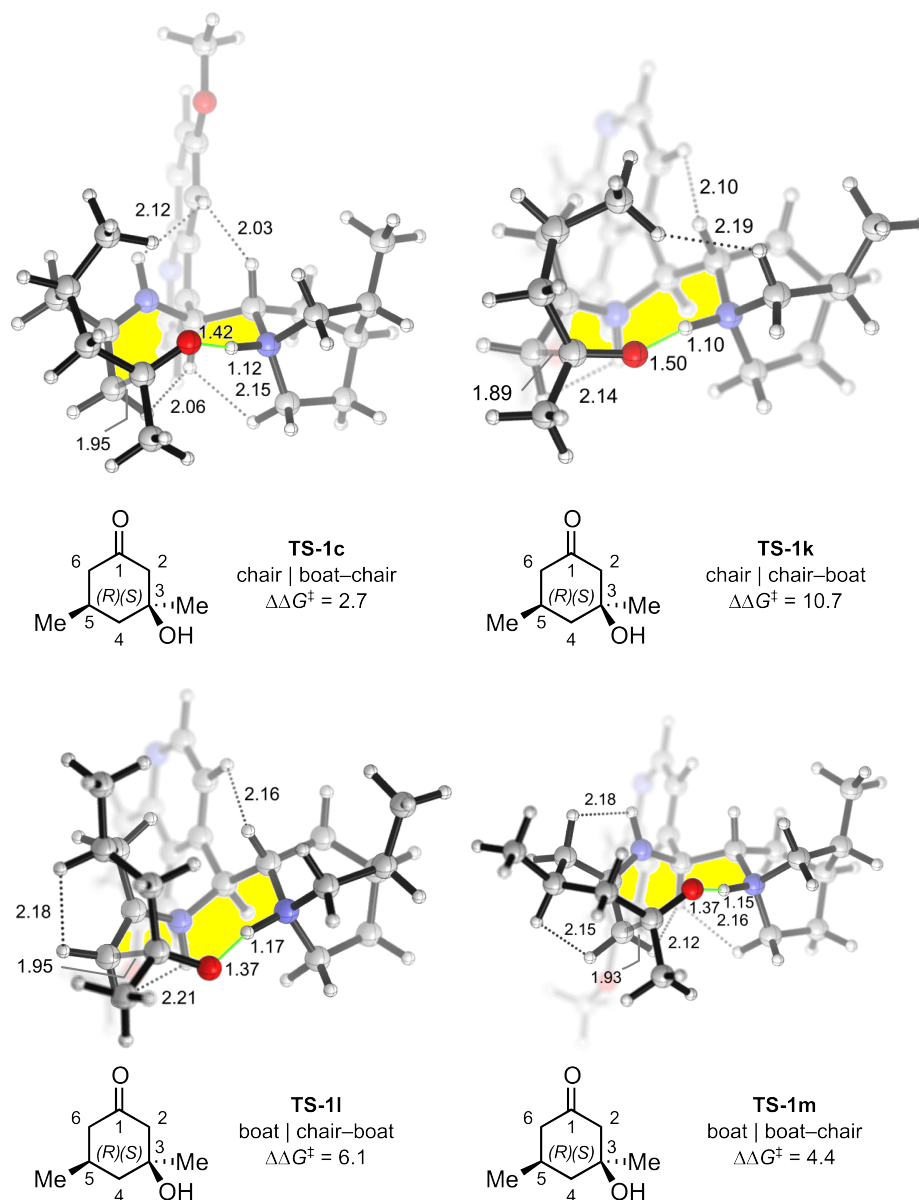
<sup>a</sup> B3LYP-D3(BJ)/def2-TZVPP–IEF-PCM (toluene)//B3LYP/6-31G(d)–IEF-PCM (toluene). The relative free energies of activation ( $\Delta\Delta G^\ddagger$ ) are reported in kcal/mol relative to the lowest-energy transition structure, **TS-1a**. <sup>b</sup> **TS-1a'**–**1d'** are the same as **TS-1a**–**1d** except that the orientation of the quinoline ring (*syn* vs. *anti*) is opposite.



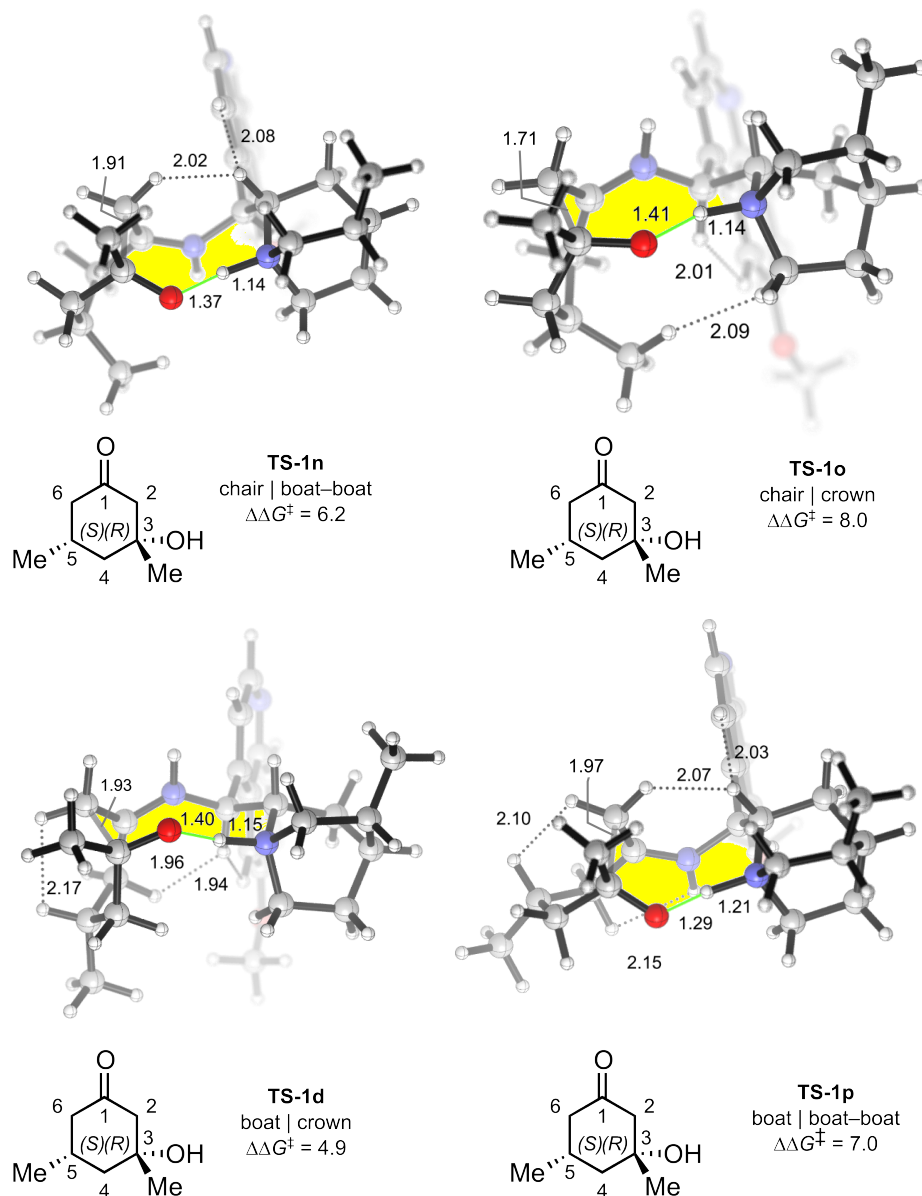
**Figure S1.** Aldol addition transition structures of **1** involving model catalyst **III** (B3LYP-D3(BJ)/def2-TZVPP-IEF-PCM (toluene)//B3LYP/6-31G(d)-IEF-PCM (toluene)), leading to (3*S*,5*S*)-**4**. The two conformational designators for each transition structure refer to the forming six-membered ring and the medium ring, respectively. The relative free energies of activation ( $\Delta\Delta G^\ddagger$ ) are reported in kcal/mol compared with **TS-1a**. In the illustrations, the close H–H contacts ( $< 2.20$  Å) are annotated, and the hydrogen-bonded nine-membered ring is color-filled.



**Figure S2.** Aldol addition transition structures of **1** involving model catalyst **III** (B3LYP-D3(BJ)/def2-TZVPP-IEF-PCM (toluene)//B3LYP/6-31G(d)-IEF-PCM (toluene)), leading to (3*R*,5*R*)-**4**. The two conformational designators for each transition structure refer to the forming six-membered ring and the medium ring, respectively. The relative free energies of activation ( $\Delta\Delta G^\ddagger$ ) are reported in kcal/mol compared with **TS-1a** (Figure S1). In the illustrations, the close H-H contacts ( $< 2.20$  Å) are annotated, and the hydrogen-bonded nine-membered ring is color-filled.



**Figure S3.** Aldol addition transition structures of **1** involving model catalyst **III** (B3LYP-D3(BJ)/def2-TZVPP-IEF-PCM (toluene)//B3LYP/6-31G(d)-IEF-PCM (toluene)), leading to (3*S*,5*R*)-**4**. The two conformational designators for each transition structure refer to the forming six-membered ring and the medium ring, respectively. The relative free energies of activation ( $\Delta\Delta G^\ddagger$ ) are reported in kcal/mol compared with **TS-1a** (Figure S1). In the illustrations, the close H–H contacts ( $< 2.20$  Å) are annotated, and the hydrogen-bonded nine-membered ring is color-filled.



**Figure S4.** Aldol addition transition structures of **1** involving model catalyst **III** (B3LYP-D3(BJ)/def2-TZVPP-IEF-PCM (toluene)//B3LYP/6-31G(d)-IEF-PCM (toluene)), leading to (3*R*,5*S*)-**4**. The two conformational designators for each transition structure refer to the forming six-membered ring and the medium ring, respectively. The relative free energies of activation ( $\Delta\Delta G^\ddagger$ ) are reported in kcal/mol compared with **TS-1a** (Figure S1). In the illustrations, the close H–H contacts ( $< 2.20$  Å) are annotated, and the hydrogen-bonded nine-membered ring is color-filled.

## B. Computational results by other density functionals

To study the extent to which the stereoselectivities depend on dispersion interactions, single-point energies of the aldol transition structures **TS-1a–1d**, **TS-2a–2c**, **TS-3a–3c**, and **TS-10a–10d** were computed using M06-2X/def2-TZVPP and M06-2X-D3(zero damping)/def2-TZVPP, in addition to the B3LYP-D3(BJ)/def2-TZVPP results discussed in the Main Text. The results are listed in Table S2. Results using the plain B3LYP functional, in conjunction with the 6-31G(d) and the larger def2-TZVPP basis sets are also listed. B3LYP/6-31G(d)–IEF-PCM (toluene) geometries and thermal corrections were used.

**Table S2.** Selectivity Data ( $\Delta\Delta G^\ddagger$ ) Predicted for Intramolecular Aldol Additions of **1–3** and **10**. <sup>a</sup>

|               | B3LYP/<br>6-31G(d) | B3LYP/<br>def2-TZVPP | B3LYP-D3(BJ)/<br>def2-TZVPP | M06-2X/<br>def2-TZVPP | M06-2X-D3/<br>def2-TZVPP |
|---------------|--------------------|----------------------|-----------------------------|-----------------------|--------------------------|
| <b>TS-10a</b> | <b>0</b>           | <b>0</b>             | <b>0</b>                    | <b>0</b>              | <b>0</b>                 |
| <b>TS-10b</b> | 3.6                | 3.7                  | 3.3                         | 2.5                   | 2.5                      |
| <b>TS-10c</b> | <b>3.5</b>         | <b>3.3</b>           | <b>2.6</b>                  | <b>1.4</b>            | <b>1.4</b>               |
| <b>TS-10d</b> | 4.2                | 4.2                  | 2.9                         | 2.3                   | 2.2                      |
|               |                    |                      |                             |                       |                          |
| <b>TS-1a</b>  | <b>0</b>           | <b>0</b>             | <b>0</b>                    | <b>0</b>              | <b>0</b>                 |
| <b>TS-1b</b>  | <b>2.6</b>         | <b>2.5</b>           | <b>1.6</b>                  | <b>0.8</b>            | <b>0.6</b>               |
| <b>TS-1c</b>  | 3.3                | 4.2                  | 2.7                         | 3.2                   | 2.9                      |
| <b>TS-1d</b>  | 5.7                | 5.5                  | 4.9                         | 4.4                   | 4.0                      |
|               |                    |                      |                             |                       |                          |
| <b>TS-2a</b>  | <b>0</b>           | <b>0</b>             | <b>0</b>                    | <b>0</b>              | <b>0</b>                 |
| <b>TS-2b</b>  | <b>2.7</b>         | <b>2.6</b>           | <b>0.9</b>                  | <b>0.2</b>            | <b>0.3</b>               |
| <b>TS-2c</b>  | 3.2                | 4.1                  | 2.4                         | 2.8                   | 2.6                      |
|               |                    |                      |                             |                       |                          |
| <b>TS-3a</b>  | <b>0</b>           | <b>0</b>             | <b>0</b>                    | <b>0</b>              | <b>0</b>                 |
| <b>TS-3b</b>  | <b>3.3</b>         | <b>3.1</b>           | <b>1.5</b>                  | <b>0.9</b>            | <b>0.5</b>               |
| <b>TS-3c</b>  | 5.7                | 7.2                  | 3.7                         | 5.0                   | 4.0                      |

<sup>a</sup> Single-point energies calculated by the specified method within the IEF-PCM (toluene) model, using B3LYP/6-31G(d)–IEF-PCM (toluene) geometries and thermal corrections. All of the free energies are reported in kcal/mol. Values for the stereoselectivity-determining transition structures are in boldface.

All of the methods in Table S2 agree on the identity of the lowest-energy stereoselectivity-determining transition structures: **TS-10a/10c**, **TS-1a/1b**, **TS-2a/2b**, and **TS-3a/3b**. However, using a

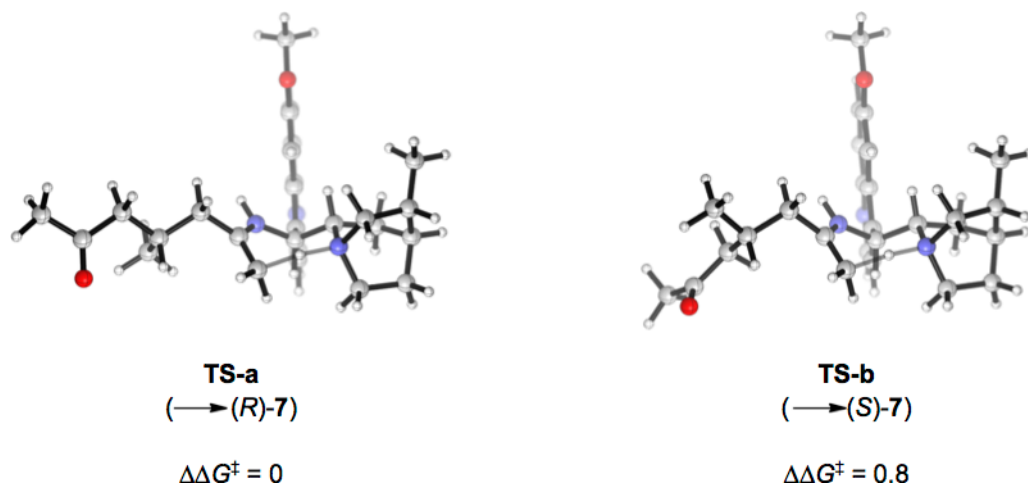
dispersion-inclusive method significantly decreases the energy differences within these pairs. For example, using the def2-TZVPP basis set, the energy difference between **TS-10a** and **TS-10c** is 3.3 kcal/mol by plain B3LYP but 2.6 kcal/mol by B3LYP-D3(BJ). Importantly, inclusion of dispersion effects results in changes in the predicted levels of stereoselectivities that are experimentally observable. Thus, **TS-1b** is predicted to be 2.5–2.6 kcal/mol higher in energy than **TS-1a** by plain B3LYP, but only 1.6 kcal/mol higher by B3LYP-D3(BJ). Also, the size by which the energy gap is reduced by the D3(BJ) correction increases with system size. Thus, the stabilities of **TS-2b**, relative to **TS-2a**, computed with and without D3(BJ) differ by as much as 1.7 kcal/mol ( $\Delta\Delta G^\ddagger = 0.9$  kcal/mol with dispersion and 2.6 kcal/mol without dispersion). Similarly, a 1.6 kcal/mol reduction in energy gap is found between **TS-3b** and **TS-3a** ( $\Delta\Delta G^\ddagger = 1.5$  kcal/mol with dispersion and 3.1 kcal/mol without dispersion). Thus, although B3LYP successfully reproduces the senses of enantioselectivity for the reactions of **1–3** with or without dispersion corrections, the plain functional erroneously predicts a completely enantioselective aldol condensation, irrespective of the ketone substituent. Use of the D3(BJ) dispersion correction scheme reproduces the level of enantioselectivities in remarkably close agreement to experiment. The performance of M06-2X, with or without D3 correction, in single-point calculations is also reasonable, although the stereoselectivities are underestimated.

### C. Calculations on enamine formation and stereoselectivity

We have explored ways to establish that the aldol C–C bond formation step is indeed the rate and stereoselectivity-determining step. Because of issues with properly accounting for energetics of the various steps involving protonations and ion pairs by DFT, we did not attempt to prove that the transition states we computed are the rate determining steps by energetics. Instead, we explored whether the rates of formation of the enamines from attack of the primary amine of **III** on one or the other carbonyl of 4-methylheptane-2,6-dione (**1**) could explain the stereoselectivity. We make the assumption that the attack of amine and dehydration are reversible and that the rds and stereoselectivity-determining step is therefore the intramolecular deprotonation of the iminium intermediate. This assumption follows from our previous work on the mechanism of the Hajos-Parrish reaction (ref. 9 in main text), in which this step has the highest activation barrier among all of the elementary steps of enamine formation.

Figure S5 shows these two transition states. **TS-a** forms the enamine that will, upon aldol cyclization, form the cyclohexenone enantiomer (*R*)-**7**, the minor enantiomer experimentally found, while **TS-b** corresponds to the enamine that will form the major cyclohexenone product, (*S*)-**7**. **TS-b** is *higher* in energy than **TS-a** by 0.8 kcal/mol. The disfavored transition state places the partially positive hydrogens  $\alpha$  to the carbonyl group near the iminium, and this could lead to the small difference in energy between **TS-a** and **TS-b**.

As the predicted stereocontrol is in the wrong direction than that experimentally observed, the proposal that stereocontrol occurs at the enamine formation step can be ruled out.



**Figure S5.** Intramolecular deprotonation transition structures for enamine formation between **1** and **III** (B3LYP-D3(BJ)/def2-TZVPP-IEF-PCM (toluene)//B3LYP/6-31G(d)-IEF-PCM (toluene)). The relative free energies of activation ( $\Delta\Delta G^\ddagger$ ) are reported in kcal/mol compared with **TS-a**.

## D. Cartesian coordinates and energies

TS-10a            C16H29N2O1(1+)  
C,2.3237417784,-1.2174002874,-0.5889869001  
C,2.4089483131,-0.0393095014,-1.3522221269  
C,3.6300729762,0.8952462378,0.8542901903  
C,3.6669018264,-0.536442209,1.389630651  
C,3.5167237919,-1.5834781811,0.2472608556  
H,1.5799316509,0.2401746528,-1.9966612961  
H,3.711679417,1.5970053323,1.6951672186  
H,2.8528167837,-0.6680072219,2.1093000989  
H,3.4247029087,-2.5927236896,0.6630736973  
H,-3.0403768774,-2.2218963148,-0.0651294665  
N,1.1802779006,-1.8521505936,-0.3236845668  
C,-0.1191359537,-1.7094474166,-0.9776089999  
C,-1.211776807,-1.0467347801,-0.1169341264  
H,0.0156534243,-1.1992289879,-1.9331377324  
H,-1.088049261,-1.412836832,0.9065101668  
C,-2.6400549967,-1.3724622387,-0.6257646841  
N,-1.0836914247,0.4532382869,0.0010205498  
C,-3.5284733496,-0.1196969187,-0.4835288026  
H,-2.6133202218,-1.6758238401,-1.6800616499  
H,4.4116671278,-1.5649524498,-0.3831027673  
C,-1.9392977067,0.9145571105,1.1518505458  
C,-1.5160715708,1.1629472064,-1.2506153082  
C,-3.4187267204,0.4816339526,0.9392896601  
H,-4.5706080453,-0.3765963752,-0.6966221976  
C,-3.0271319749,0.9282354276,-1.4954124902  
H,-1.5018550468,0.4872529116,2.0578103266  
H,-1.8220229548,1.9990344772,1.2087407415  
H,-0.9020105729,0.7953189622,-2.075284515  
H,-1.2711455301,2.2179038249,-1.1081725839  
H,-4.0380018342,1.3862546572,0.9544232633  
H,-3.5837828217,1.8637257075,-1.3808561764  
H,1.226129894,-2.5797591042,0.3817637105  
H,-0.0151873318,0.7360272906,0.2749624361  
H,3.38061177,0.1689609014,-1.7888407183  
H,4.4835835813,1.0874285826,0.1927372142  
C,2.3190838505,2.5440832657,-0.6309787289  
H,3.1794520418,2.6425949061,-1.29943036  
H,2.3606415932,3.3574275882,0.1049889496  
H,1.4001360838,2.6707793121,-1.2118910745  
C,2.3073477097,1.2199050086,0.1362104943  
O,1.2420308246,0.9590496324,0.8375174547  
H,-3.1905395716,0.5794207162,-2.5200699474  
C,-3.9288678845,-0.4448465386,2.0502421499  
H,-3.3468153141,-1.3711206538,2.123379074  
H,-3.874756015,0.0545783816,3.0237277062  
H,-4.9745213833,-0.7202152782,1.8748505993  
H,4.6083762225,-0.731081033,1.9132657622  
H,-0.4744902997,-2.7193138873,-1.2101662971  
Electronic energy = -811.7009362  
Zero-point electronic energy = -811.259658  
Thermal energy = -811.242102  
Enthalpy = -811.241157  
Free energy = -811.303683  
Free energy with quasiharmonic approximation = -811.301915  
Frequencies = -365.0159, 32.8093, 53.4981, 86.0536, 100.0739

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1140469  
SCF (M06-2X/def2-TZVPP) = -811.6466099  
SCF (M06-2X-D3/def2-TZVPP) = -811.6502422  
SCF (B3LYP/def2-TZVPP) = -812.011304

TS-10b C16H29N2O1(1+)

C,-2.2799297196,-1.0749997106,-0.6918901161  
C,-2.2134676065,0.1167688136,-1.4436801242  
C,-3.6401132359,1.1236618632,0.5616234877  
C,-3.8402591784,-0.29366116,1.1006402619  
C,-3.5734253849,-1.3736950514,0.01026447  
H,-1.3116797258,0.3247110196,-2.0119748054  
H,-4.3807535558,1.3633390618,-0.2108583128  
H,-4.8599379498,-0.4299941816,1.4743120642  
H,-4.3808160067,-1.3473690298,-0.7294471288  
H,2.8922457352,-0.3950578878,-2.0474619132  
N,-1.2042456758,-1.7734408742,-0.3331859291  
C,0.1325287264,-1.8053145224,-0.9480290789  
C,1.0527456969,-0.5619438176,-0.8705425386  
H,0.6367248695,-2.6580866829,-0.4891692168  
H,0.7063559395,0.177346955,-1.5950964581  
C,2.5265283489,-0.9594144706,-1.1850658549  
N,1.0164843078,0.1555615726,0.4471439639  
C,3.3972978044,-0.6877704141,0.0598441623  
H,2.5868752379,-2.0188989273,-1.4589111729  
H,-3.5664288148,-2.3738490629,0.4566870395  
C,1.9623131555,1.3229792263,0.3924070149  
C,1.4046843839,-0.7410976825,1.5832055544  
C,3.4330304052,0.8297157489,0.367461331  
H,4.4119839517,-1.060074308,-0.1118888567  
C,2.7662173194,-1.40905005,1.2693547637  
H,1.7092181423,1.8932791661,-0.5069459657  
H,1.7411188922,1.9518989133,1.2580473973  
H,0.5955890048,-1.4571239481,1.7385471936  
H,1.4483100089,-0.1076776616,2.4719443016  
H,3.853325143,0.9462904436,1.3743294563  
H,3.4233446343,-1.3416632023,2.1417804232  
H,-1.3655174278,-2.5064146807,0.3484943854  
H,-0.0573285408,0.5830772713,0.6142414601  
H,-3.1209348435,0.382644708,-1.9773310429  
H,-3.7830954849,1.8424330034,1.3790368206  
C,-1.9882539854,2.6580549139,-0.6977466476  
H,-2.734374665,2.8424501279,-1.476603357  
H,-0.9894564645,2.6990659354,-1.1443497478  
H,-2.0543258143,3.4647817394,0.0429758837  
C,-2.2082625064,1.3308393659,0.0320889778  
O,-1.293417445,0.9906081231,0.9068509685  
H,2.6368869248,-2.4748252083,1.0496456127  
C,4.2982123907,1.6529820448,-0.5922684545  
H,4.2750947561,2.7149611107,-0.3229742301  
H,5.3415377543,1.3227376833,-0.5527500618  
H,3.9562608287,1.5682818656,-1.6304432417  
H,-3.1534706072,-0.4526369167,1.9366802621  
H,0.0278402767,-2.0393012251,-2.0138830008

Electronic energy = -811.6953092

Zero-point electronic energy = -811.254056

Thermal energy = -811.236637

Enthalpy = -811.235692

Free energy = -811.297475

Free energy with quasiharmonic approximation = -811.296149

Frequencies = -499.3210, 37.9565, 68.1234, 93.6826, 116.6151

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1089374  
SCF (M06-2X/def2-TZVPP) = -811.6428025  
SCF (M06-2X-D3/def2-TZVPP) = -811.6464418  
SCF (B3LYP/def2-TZVPP) = -812.0055407

TS-10c            C16H29N2O1(1+)  
C,-2.2712314311,-0.9935938307,-1.0178604825  
C,-3.118334055,0.1172125221,-1.2612956521  
C,-3.0832830981,0.3202084071,1.365608067  
C,-2.4659398413,-1.0772518182,1.4550312226  
C,-2.632883179,-1.8849967199,0.1296367529  
H,-2.8879476943,0.7340763301,-2.1292486131  
H,-4.1764844284,0.2433592333,1.3185878768  
H,-2.9259297616,-1.6519997825,2.2651088997  
H,-3.6845862599,-2.1663558489,0.0174117237  
H,3.2007486482,-1.2087358372,-1.6780033123  
N,-1.0601476865,-0.9859958331,-1.5662695255  
C,0.1691138245,-1.6653971804,-1.1574655173  
C,1.2715192212,-0.6354180721,-0.8670001806  
H,-0.0314488502,-2.3078904659,-0.2990853381  
H,1.2706316648,0.0780044121,-1.697717016  
C,2.686310145,-1.2401880833,-0.7137391032  
N,0.9725096584,0.210357874,0.3497907989  
C,3.4479314123,-0.446012565,0.3698778423  
H,2.628503207,-2.2955950891,-0.4202326189  
H,-2.0508102657,-2.8096454735,0.155876984  
C,1.8184834849,1.456700701,0.2718347691  
C,1.2841209645,-0.5195295902,1.6280331706  
C,3.3231858822,1.0809553729,0.1363036546  
H,4.5029803193,-0.7355869219,0.3706551995  
C,2.8076484816,-0.7718867502,1.7321570558  
H,1.4459033688,2.0311490431,-0.5796702061  
H,1.6051486148,2.0307565433,1.175950154  
H,0.7190137878,-1.4531741419,1.6249195424  
H,0.8973788097,0.0975455837,2.4420045304  
H,3.8639447283,1.5731420661,0.9531338438  
H,3.2480219175,-0.1478031,2.516335574  
H,-0.9230946938,-0.2835403433,-2.2872366446  
H,-0.1020313441,0.5691552524,0.3207088627  
H,-4.1828948968,-0.0568085609,-1.1284676762  
H,-2.8433777627,0.8793896939,2.2792281057  
C,-3.3816616403,2.436321164,-0.0532733323  
H,-3.2172365067,3.1001747833,0.8044455147  
H,-4.456362526,2.2496393258,-0.1437706755  
H,-3.0264810427,2.9543652337,-0.948635362  
C,-2.5666116575,1.1545622216,0.1674895384  
O,-1.2703087326,1.3535417469,0.0889363573  
H,2.9930967536,-1.8149639087,2.0070707506  
C,3.9397230547,1.5673338972,-1.1814074548  
H,3.4445115204,1.1387175779,-2.0605395407  
H,3.8650654677,2.6573197363,-1.2619687661  
H,5.0010108799,1.3017279504,-1.2336817204  
H,-1.4026478896,-0.9926167321,1.6963087515  
H,0.5177294265,-2.3093200229,-1.9730268046  
Electronic energy = -811.6961777  
Zero-point electronic energy = -811.254162  
Thermal energy = -811.236760  
Enthalpy = -811.235816  
Free energy = -811.297667  
Free energy with quasiharmonic approximation = -811.296324  
Frequencies = -243.3663, 33.8552, 70.3246, 100.7655, 102.1850

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1108138  
SCF (M06-2X/def2-TZVPP) = -811.6451867  
SCF (M06-2X-D3/def2-TZVPP) = -811.6488931  
SCF (B3LYP/def2-TZVPP) = -812.0068209

TS-10d C16H29N2O1(1+)

C,-2.1985806711,1.3950989061,0.1462608723  
C,-3.2418554329,0.7739694462,-0.5780686426  
C,-2.8358915143,-1.2068769972,1.1117930263  
C,-1.9887660426,-0.2744770833,1.9792416281  
C,-2.204171549,1.2361111477,1.6353238033  
H,-3.2629552305,0.9358936814,-1.6549668708  
H,-2.5568015962,-2.2466261124,1.3272492043  
H,-0.9320893118,-0.5313335023,1.8581919881  
H,-1.4544639009,1.8563202116,2.1347544591  
H,2.9145241168,1.321761098,1.5768677746  
N,-1.1104618039,1.7781061415,-0.522396426  
C,0.2218971705,2.1312527276,-0.0317122285  
C,1.0883450056,0.9412855561,0.4395965249  
H,0.7155741652,2.6665496714,-0.8459929752  
H,0.722759233,0.6194643377,1.4164995501  
C,2.5962307163,1.3038069145,0.5312585244  
N,0.9253765687,-0.2731669957,-0.4397081457  
C,3.4154632655,0.2824475515,-0.2848293691  
H,2.7707680803,2.3108339553,0.1339505019  
H,-3.1860611886,1.5444533512,2.007868705  
C,1.6541129846,-1.4343696023,0.1831314476  
C,1.4563383669,-0.0421540663,-1.8270692529  
C,3.1825469472,-1.1578229515,0.2342945864  
H,4.479125359,0.531151464,-0.2179468035  
C,2.9529731258,0.3489356393,-1.7542511233  
H,1.2297951354,-1.5730956275,1.1815453636  
H,1.3985681004,-2.3152484835,-0.4094227468  
H,0.8415204816,0.7267109287,-2.2981599812  
H,1.2841971609,-0.9692819669,-2.3768701962  
H,3.6747399667,-1.8350649719,-0.4740250275  
H,3.5482403662,-0.3317782126,-2.3702753869  
H,-1.2020189427,1.7505242382,-1.5319676537  
H,-0.160533641,-0.5666496547,-0.5206221454  
H,-4.2250988972,0.7989284683,-0.1169911772  
H,-3.8959645174,-1.1025663618,1.3730954191  
C,-3.6974797409,-1.7409575082,-1.2443252937  
H,-3.5722703296,-1.5011427387,-2.3039487894  
H,-4.7253502569,-1.5205892431,-0.9398573753  
H,-3.525199247,-2.8175894953,-1.1224870812  
C,-2.6505695409,-0.991234761,-0.4108939402  
O,-1.4383051632,-1.0903481664,-0.8961007635  
H,3.105273652,1.3573580645,-2.1525607539  
C,3.7714449256,-1.4365792933,1.6221138676  
H,3.3205022288,-0.8096584834,2.4005455726  
H,3.6081267462,-2.4817791869,1.9076220706  
H,4.8514624902,-1.2558480136,1.6272703656  
H,-2.2229959416,-0.4147695108,3.0391737092  
H,0.1424481009,2.8369854899,0.8003811851

Electronic energy = -811.6953818

Zero-point electronic energy = -811.253103

Thermal energy = -811.235699

Enthalpy = -811.234755

Free energy = -811.296343

Free energy with quasiharmonic approximation = -811.295280

Frequencies = -270.0206, 51.8134, 61.8159, 102.9147, 111.6048

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.110447  
SCF (M06-2X/def2-TZVPP) = -811.64407  
SCF (M06-2X-D3/def2-TZVPP) = -811.647803  
SCF (B3LYP/def2-TZVPP) = -812.0057781

TS-10e C16H29N2O1(1+)  
C,2.2409508508,-1.2809438223,-0.5049981818  
C,2.4565492075,-0.0820290691,-1.2192671391  
C,3.017844924,0.5436184524,1.3764344324  
C,4.0494688995,-0.5436252717,1.0522581027  
C,3.3679969939,-1.7607255304,0.3730531871  
H,1.7097934296,0.257106705,-1.9311740119  
H,2.2121861015,0.1211372777,1.9910279877  
H,4.5535131548,-0.8858087243,1.9615783064  
H,2.9872605605,-2.4570395365,1.129748292  
H,-3.1422622976,-2.1650492849,-0.2775299688  
N,1.0616839297,-1.8855843296,-0.3618742949  
C,-0.190109697,-1.6539645237,-1.0815000596  
C,-1.2900654443,-1.0314024852,-0.2020709796  
H,0.0128713299,-1.0609613491,-1.9744092001  
H,-1.1981254343,-1.4760726732,0.7939458694  
C,-2.7200459816,-1.2726329097,-0.7485100867  
N,-1.1162811959,0.4476140032,0.0199799869  
C,-3.5788796582,-0.0171958623,-0.483496441  
H,-2.6923862085,-1.4702931452,-1.8278094791  
H,4.0906539945,-2.3167330845,-0.2370136998  
C,-1.9464788933,0.8539410741,1.2070010312  
C,-1.5391032284,1.252015314,-1.1814045663  
C,-3.4367836097,0.4589722937,0.984237171  
H,-4.6292569074,-0.2320894103,-0.7020370284  
C,-3.0621189496,1.1071063629,-1.4022166802  
H,-1.512309827,0.3624196111,2.0821477972  
H,-1.8083169001,1.9303575572,1.3286945101  
H,-0.9591785687,0.8958677245,-2.0347161835  
H,-1.2196056744,2.2762546417,-0.98567228  
H,-4.0415817908,1.3677572936,1.084236178  
H,-3.5747844546,2.0475258719,-1.1749565717  
H,1.0288652724,-2.6507563685,0.3039803339  
H,-0.043169149,0.7654502517,0.2241288898  
H,3.4719691197,0.0205730298,-1.5934901635  
H,3.4832923461,1.3371258273,1.9742550634  
C,3.2189288905,2.3234445274,-0.4759749654  
H,3.1874639104,3.1831537417,0.2036579288  
H,2.8064727729,2.6402975076,-1.4380217308  
H,4.2643521946,2.0284703834,-0.6121302669  
C,2.355249215,1.212783313,0.1418234345  
O,1.1031491416,1.56024618,0.2852209538  
H,-3.268168401,0.8730923347,-2.4513553031  
C,-3.9448503718,-0.5464166962,2.0256373187  
H,-3.3795229233,-1.4860000747,2.0158901325  
H,-4.9981144481,-0.78880926,1.8477504312  
H,-3.8662008511,-0.1269388064,3.0346894546  
H,4.8314539933,-0.1399232693,0.3996614681  
H,-0.5554893671,-2.6281457925,-1.4226989796

Electronic energy = -811.6926602

Zero-point electronic energy = -811.252038

Thermal energy = -811.234320

Enthalpy = -811.233376

Free energy = -811.296229

Free energy with quasiharmonic approximation = -811.294567

Frequencies = -360.8016, 43.9860, 47.4380, 80.8544, 101.3917

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1052145  
SCF (M06-2X/def2-TZVPP) = -811.6381548  
SCF (M06-2X-D3/def2-TZVPP) = -811.6417262  
SCF (B3LYP/def2-TZVPP) = -812.0035626

TS-10f C16H29N2O1(1+)

C,-2.2772667963,-1.075752412,-0.7624498307  
C,-2.2021641635,0.0809872651,-1.5516629425  
C,-3.7028944256,1.1416626584,0.4993450743  
C,-4.4640911245,-0.1138310307,0.024161766  
C,-3.570966055,-1.3640220557,-0.0429670846  
H,-1.2885874252,0.2906705858,-2.0986237533  
H,-4.9046929857,0.0666078644,-0.9625869527  
H,-4.098968922,-2.1752893994,-0.5617033676  
H,2.9134262845,-0.4258723674,-2.0293238875  
N,-1.2071033116,-1.7742156366,-0.3863758069  
C,0.1289635421,-1.8189982867,-0.9957828942  
C,1.0504887539,-0.5776463382,-0.8862112105  
H,0.6223707943,-2.6822382789,-0.5444985173  
H,0.7275970014,0.1602544705,-1.6231312241  
C,2.5338443147,-0.9706627986,-1.1603334031  
N,0.965694614,0.1369206879,0.4297843472  
C,3.3754989301,-0.6634512545,0.0952357301  
H,2.6092188021,-2.0366597396,-1.4041921625  
H,-3.3415003477,-1.7301999728,0.9657833556  
C,1.8923740304,1.3185535104,0.4004898374  
C,1.3481393142,-0.7541231912,1.5711987037  
C,3.3750595166,0.8569928499,0.3872099558  
H,4.4008939824,-1.0160816861,-0.0537649343  
C,2.7371040519,-1.3859159868,1.2994798795  
H,1.6423892043,1.8974968379,-0.4943034106  
H,1.651414255,1.934248784,1.270711999  
H,0.5580627755,-1.4964381031,1.7016132524  
H,1.3470778205,-0.1256540931,2.4649868872  
H,3.7884532035,0.9924923432,1.3945530694  
H,3.3714211675,-1.2886830319,2.1859492471  
H,-1.3582553349,-2.4522841758,0.3518373197  
H,-0.1639911979,0.5608567091,0.5935244988  
H,-3.100431246,0.3740830736,-2.0832964934  
C,-1.9458747651,2.6081832903,-0.7201480109  
H,-2.6581137475,2.8186125546,-1.5231471676  
H,-0.9316432826,2.631773345,-1.1293426681  
H,-2.0226482425,3.4110001536,0.0248607236  
C,-2.2415181252,1.2891558465,-0.0036804353  
O,-1.3637561013,0.8936911039,0.8868312875  
H,2.6444147213,-2.4576011102,1.0895685861  
C,4.2283536376,1.689704326,-0.5753186905  
H,4.184119705,2.7528282331,-0.3130981444  
H,5.2778806378,1.3800860746,-0.5299014104  
H,3.8922588878,1.5921359262,-1.6143089833  
H,-5.3055759642,-0.3144819037,0.6946648492  
H,0.0296311568,-2.0380173963,-2.0648896265  
H,-3.6257599938,1.1334068028,1.5912474353  
H,-4.2824578369,2.0284567727,0.2203868483

Electronic energy = -811.6870175

Zero-point electronic energy = -811.247145

Thermal energy = -811.229308

Enthalpy = -811.228364

Free energy = -811.291196

Free energy with quasiharmonic approximation = -811.289698

Frequencies = -819.2905, 38.6401, 57.3786, 91.2725, 99.4619

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1010654  
SCF (M06-2X/def2-TZVPP) = -811.6347796  
SCF (M06-2X-D3/def2-TZVPP) = -811.6383831  
SCF (B3LYP/def2-TZVPP) = -811.9977408

TS-10g C16H29N2O1(1+)

C,-2.2479756925,-1.0763038632,-0.875364796  
C,-3.0942564887,-0.0278560879,-1.2756865449  
C,-2.6557462984,0.5290623118,1.3939470037  
C,-3.3401047216,-0.8464862781,1.3493955064  
C,-2.615241863,-1.8155612831,0.3825158065  
H,-2.8749788433,0.4758207268,-2.2144452339  
H,-3.2453675432,1.1974622183,2.0324993312  
H,-4.3858866396,-0.7361716254,1.0445066607  
H,-3.2734715736,-2.6547603263,0.1234646497  
H,2.5443599812,-2.391100691,-0.0513616718  
N,-1.0457576254,-1.1697571716,-1.4500911014  
C,0.1904753153,-1.7918919165,-0.9823626953  
C,1.3120661945,-0.754551828,-0.8242621236  
H,0.0068811578,-2.3323595062,-0.0546071265  
H,1.3894215845,-0.2078938176,-1.7700988928  
C,2.681182664,-1.3875711298,-0.4733778305  
N,0.9871230139,0.3078821048,0.1998762957  
C,3.3943980765,-0.4927210333,0.5622669288  
H,3.2747209759,-1.5074608974,-1.3836668133  
H,-1.7378758956,-2.2525977168,0.8671159349  
C,1.9336988505,1.4633137788,0.001270376  
C,1.1299809738,-0.2078145275,1.6030137198  
C,3.4117629152,0.9858049478,0.1024747204  
H,4.4191243935,-0.8457069307,0.713215794  
C,2.6078096993,-0.576356655,1.8845308283  
H,1.6995587984,1.8979437438,-0.9741015127  
H,1.6782105392,2.2052857553,0.760971526  
H,0.4640344624,-1.0659986005,1.7145212482  
H,0.760238186,0.5802891809,2.2627969411  
H,3.8964538694,1.5624220581,0.89906229  
H,3.0379335738,0.107408348,2.6233034061  
H,-0.9327931605,-0.5960696319,-2.2803612059  
H,-0.074962655,0.7450353027,0.0289134395  
H,-4.1537245926,-0.1363329363,-1.0685389172  
H,-1.6763741779,0.431263542,1.8765482493  
C,-3.3918556226,2.3878294042,-0.2502619394  
H,-3.2679646566,2.7669331549,-1.2678959266  
H,-3.1420466565,3.1994855697,0.4447853329  
H,-4.4377369679,2.1087512562,-0.0894109491  
C,-2.4228201679,1.230989972,0.0168556818  
O,-1.1864913992,1.5003370823,-0.3105875048  
H,2.6685750125,-1.5850779526,2.3047040935  
C,4.2021310013,1.2303493703,-1.1891426677  
H,5.2399499617,0.8983453421,-1.0769193814  
H,3.77303559,0.7027080043,-2.0491008488  
H,4.219123065,2.297955173,-1.4341793785  
H,-3.3609422221,-1.2914388018,2.3496967382  
H,0.5262156084,-2.5299271398,-1.7199274409

Electronic energy = -811.6910332

Zero-point electronic energy = -811.249921

Thermal energy = -811.232513

Enthalpy = -811.231569

Free energy = -811.293000

Free energy with quasiharmonic approximation = -811.292099

Frequencies = -386.4724, 55.1019, 72.6535, 94.9738, 112.1256

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1053966  
SCF (M06-2X/def2-TZVPP) = -811.6383102  
SCF (M06-2X-D3/def2-TZVPP) = -811.6419815  
SCF (B3LYP/def2-TZVPP) = -812.0016798

TS-10h C16H29N2O1(1+)

C,-2.2563475268,1.3442489009,0.0518297147  
C,-3.2138221359,0.662839241,-0.7169414431  
C,-2.2715851397,-1.2452280508,1.0549298221  
C,-2.9158335808,-0.150365245,1.9194075306  
C,-2.3784407527,1.2581095896,1.5480218499  
H,-3.176983628,0.7705647906,-1.7981457704  
H,-1.2001630601,-1.3041407813,1.2817778241  
H,-2.7222501164,-0.3387853191,2.9803132859  
H,-1.423159023,1.45238645,2.0425427555  
H,2.6805781632,1.1794458566,1.8435187459  
N,-1.1413643463,1.7709616601,-0.548227335  
C,0.1601525071,2.1014421699,0.0328909345  
C,1.0031122564,0.8845304103,0.4729094952  
H,0.6943556826,2.6891685693,-0.7175770526  
H,0.539896293,0.4513972805,1.3633334538  
C,2.4774318843,1.2737537575,0.7733917969  
N,0.9790329727,-0.2322195812,-0.5378168564  
C,3.4187150148,0.3765947675,-0.0564468581  
H,2.65277019,2.3240619341,0.5121594537  
H,-3.0754934103,2.0299979773,1.8973380706  
C,1.6871009375,-1.4256077813,0.0421342782  
C,1.6457441673,0.1573936119,-1.8254652556  
C,3.1921829369,-1.1183286036,0.2742508956  
H,4.4587625937,0.6481200398,0.1499055774  
C,3.1069682957,0.5964357387,-1.5502240845  
H,1.1751326454,-1.6711916628,0.9775201399  
H,1.5239761037,-2.2543245615,-0.6505450878  
H,1.0517148924,0.9463873258,-2.2916729437  
H,1.5833319888,-0.7160047799,-2.478105711  
H,3.7762571861,-1.698875657,-0.4501131539  
H,3.7959072382,0.0158744611,-2.1716563678  
H,-1.1632011424,1.7287683265,-1.5610288261  
H,-0.1184458375,-0.5731145472,-0.7604853426  
H,-4.2177632838,0.5954126353,-0.3102311091  
H,-2.6942762662,-2.2174394851,1.3349638726  
C,-3.5288396053,-1.9319423388,-1.0984537334  
H,-3.2096300591,-2.9805056821,-1.0462469194  
H,-3.6804730317,-1.6786361756,-2.1507411359  
H,-4.4759665872,-1.8342443848,-0.5592736928  
C,-2.4139714837,-1.0745494868,-0.491131505  
O,-1.3114776195,-1.076652244,-1.1938643899  
H,3.2468058457,1.6498331716,-1.8147050606  
C,3.652722334,-1.5307916725,1.6769750759  
H,4.7213103829,-1.3313879277,1.8096543257  
H,3.1085082254,-0.9945605494,2.4633276206  
H,3.4917544577,-2.6025848439,1.8380067227  
H,-4.0037638764,-0.1716953067,1.7975325736  
H,0.0324163173,2.7540480019,0.900873819

Electronic energy = -811.6909971

Zero-point electronic energy = -811.250195

Thermal energy = -811.232664

Enthalpy = -811.231720

Free energy = -811.293964

Free energy with quasiharmonic approximation = -811.292355

Frequencies = -444.7116, 33.2738, 65.0817, 82.5577, 102.9666

SCF (B3LYP-D3(BJ)/def2-TZVPP) = -812.1058676  
SCF (M06-2X/def2-TZVPP) = -811.6392526  
SCF (M06-2X-D3/def2-TZVPP) = -811.6429652  
SCF (B3LYP/def2-TZVPP) = -812.0011924

syn-open-12a C27H38N3O2(1+)  
C,1.4994686076,-1.7030807832,-1.2215611909  
C,2.0989243162,-1.3793076699,-2.3806764806  
C,4.0564801939,-2.5086398399,0.4902902898  
C,2.6087323149,-2.9496413927,0.7698219589  
C,1.7657688164,-3.0237954322,-0.5301995355  
H,1.9289308548,-0.4533393216,-2.9194126305  
H,4.6907189708,-2.7727976934,1.3525576017  
H,2.1574098636,-2.2105215209,1.4426342457  
H,0.8006544182,-3.4916707147,-0.2851450654  
H,-1.4999010742,2.9621413555,-0.0728710237  
N,0.6288075832,-0.8794958482,-0.4788189494  
C,-0.0081891918,0.3187094516,-1.0314692863  
C,0.0607523281,1.4622163625,0.011431075  
H,0.5893021329,0.6295083386,-1.8892406525  
C,-1.4251334787,0.0998044926,-1.5592869816  
H,-0.4564827972,1.142265612,0.9171306669  
C,-0.4802266523,2.8342638343,-0.4447404352  
N,1.4989578979,1.660792642,0.4679016965  
C,-2.5160710231,-0.3743903817,-0.7524222004  
C,-1.6735367031,0.3548277306,-2.8917222481  
C,0.462249487,3.9459288817,0.0660066282  
H,-0.5401304549,2.8813176471,-1.5381538801  
H,2.2605165422,-3.6993381683,-1.2364260599  
C,1.5013287043,2.4237024216,1.7723337526  
C,2.3392630573,2.4002576263,-0.5511714658  
C,-2.4365135548,-0.6938287651,0.625715052  
C,-3.7839550459,-0.5404755498,-1.4112833011  
C,-2.9658831249,0.1579163877,-3.4355546267  
H,-0.8781937853,0.7044518266,-3.5439608283  
C,0.7672984591,3.782409906,1.5767396674  
H,0.0091830432,4.9258522607,-0.110376894  
C,1.7904217463,3.8363797149,-0.7074846894  
H,1.0113556046,1.7848298257,2.5113227886  
H,2.5476980745,2.5384386156,2.0623684036  
H,2.3032744776,1.8256744001,-1.4773303345  
H,3.3631017384,2.3593600436,-0.1789758948  
C,-3.5416477327,-1.1493669951,1.331033286  
H,-1.5175606713,-0.591813567,1.1914372971  
C,-4.8933110883,-1.0085067321,-0.6626283378  
N,-3.9908721241,-0.2716280467,-2.7329442885  
H,-3.1429005243,0.3651633322,-4.4896040225  
H,1.4700426417,4.5785899438,1.8482093978  
H,2.5128954428,4.5633494221,-0.3234090695  
C,-4.7892340859,-1.3097163939,0.675259296  
O,-3.3369577795,-1.4153628324,2.6474227352  
H,-5.8356776763,-1.1224465147,-1.1884529727  
H,-5.6573553965,-1.6661150134,1.2165538672  
C,-4.4287025316,-1.8914131026,3.4353277387  
H,-4.0267855019,-2.0290877347,4.4396971325  
H,-5.2459481287,-1.1616624897,3.46770824  
H,-4.8044449684,-2.8500804087,3.0596859993  
H,0.0011037477,-1.4269213213,0.0991033829  
H,1.9335689388,0.7318418813,0.617470926  
H,2.780159536,-2.0825889482,-2.8450200701  
H,4.478467273,-3.0642905061,-0.3568766369

C,5.5213417721,-0.6414871248,-0.5128660485  
 H,6.3926703258,-1.2310706259,-0.2060449836  
 H,5.7346202959,0.424094322,-0.4072011255  
 H,5.3361607577,-0.872373278,-1.5695734611  
 C,4.2997430416,-1.0233778594,0.2898304096  
 O,3.5852574641,-0.1669905846,0.8016885291  
 C,2.5962401034,-4.3173091803,1.4700994333  
 H,3.0618058559,-5.0878500105,0.8430269062  
 H,1.5718386002,-4.6401054736,1.6870660922  
 H,3.1445556806,-4.2815107605,2.4180546035  
 H,1.6371269454,4.0625365522,-1.7669286032  
 C,-0.4622402662,3.9216040811,2.4831833675  
 H,-0.9431372338,4.8936886137,2.3310246974  
 H,-1.2117772131,3.1441478135,2.2964278503  
 H,-0.1741278471,3.8552732468,3.5380492601  
 Electronic energy = -1366.2859522  
 Zero-point electronic energy = -1365.665926  
 Thermal energy = -1365.635255  
 Enthalpy = -1365.634310  
 Free energy = -1365.727017  
 Free energy with quasiharmonic approximation = -1365.721224  
 Frequencies = 25.9916, 28.9874, 38.7084, 45.5496, 50.6446  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.8932758

anti-open-12a C27H38N3O2(1+)  
 C,-1.3543861526,-1.9554914615,0.1496092345  
 C,-1.0139194907,-2.1251493549,1.4394468873  
 C,-4.517189634,-2.1106419696,0.4087732988  
 C,-3.7070833665,-2.3741857223,-0.8728043701  
 C,-2.2869555903,-2.9144777081,-0.5600102773  
 H,-0.3434249654,-1.4699896336,1.9852469831  
 H,-5.5911064358,-2.0800872444,0.1617895018  
 H,-3.6140131313,-1.4217291105,-1.4084117903  
 H,-1.8207115552,-3.2204914224,-1.508418272  
 H,1.2599253141,2.9091208738,-1.1926164362  
 N,-0.9695697589,-0.875018875,-0.6692707809  
 C,0.1539861689,0.0157304297,-0.3694772773  
 C,-0.2804638418,1.4697791951,-0.671559415  
 H,0.3597242005,-0.0626575482,0.6957285277  
 C,1.4234044206,-0.3244790493,-1.1520764898  
 H,-0.534815821,1.5292374517,-1.7342153122  
 C,0.7308550723,2.5774207726,-0.2960825278  
 N,-1.5918276247,1.7790212039,0.0349712118  
 C,2.6623298467,-0.6513380742,-0.5085265229  
 C,1.3918946429,-0.3249330223,-2.5322708731  
 C,-0.0180056602,3.7422417372,0.3862427851  
 H,1.4922993839,2.1848568316,0.3874186684  
 H,-2.3791824626,-3.825521397,0.0409781575  
 C,-2.2155204572,3.0080144932,-0.5831043058  
 C,-1.4151764003,1.9940704604,1.5216655635  
 C,2.855142302,-0.697037207,0.8918710853  
 C,3.7809728126,-0.9492595116,-1.3637090892  
 C,2.5531882252,-0.6423101731,-3.2757425809  
 H,0.4817192095,-0.0835748518,-3.0770361996  
 C,-1.230388263,4.2074233728,-0.459409113  
 H,0.6662002277,4.5826185093,0.535842369  
 C,-0.5420472409,3.2476873603,1.7484126844  
 H,-2.4382754717,2.758177671,-1.6234202602  
 H,-3.1608253518,3.1714139704,-0.0620875695  
 H,-0.9725442666,1.0844279846,1.9280811494  
 H,-2.4220904393,2.0786128065,1.9310301498

C,4.088603281,-1.0137365914,1.4393368835  
 H,2.0465910747,-0.5023035426,1.5863644224  
 C,5.0289685523,-1.2699323354,-0.7721076621  
 N,3.710687418,-0.9406899659,-2.7252926451  
 H,2.5117050885,-0.6408234027,-4.3637033758  
 H,-1.7351812744,4.9948536575,0.1120388796  
 H,-1.1269004205,4.0339787523,2.2356492789  
 C,5.1918022164,-1.3024289537,0.5931635945  
 O,4.1523130789,-1.0249198606,2.7968119625  
 H,5.8565087903,-1.4903682633,-1.4385499767  
 H,6.1593883056,-1.550225869,1.0131800168  
 C,5.3858266463,-1.3648078013,3.4287278108  
 H,6.1771536018,-0.6506455578,3.1723604626  
 H,5.1893963615,-1.3167562531,4.500427028  
 H,5.7052470595,-2.3793741013,3.1632240499  
 H,-1.0229449549,-1.1060358617,-1.6558565632  
 H,-2.231372576,0.9727377286,-0.0887689486  
 H,-1.3945974306,-2.9800581273,1.9855260039  
 H,-4.4111262177,-2.940513407,1.1192298039  
 C,-4.6339398008,-0.7507105943,2.593712408  
 H,-4.6503507361,0.2803012971,2.9529411138  
 H,-3.8906831608,-1.3215645195,3.1649931978  
 H,-5.6052026181,-1.2259650063,2.7708070202  
 C,-4.2623770377,-0.7991680664,1.1297462625  
 O,-3.8330227233,0.1955922697,0.5532557387  
 C,-4.448961527,-3.3715838457,-1.7760294411  
 H,-4.5884749171,-4.3355683183,-1.2711533412  
 H,-3.89012238,-3.5590267114,-2.6996504882  
 H,-5.4391181943,-2.9929682872,-2.0531384546  
 H,0.2921961071,3.005233591,2.4133413505  
 C,-0.8563488888,4.7910071611,-1.8270994582  
 H,-0.1617339165,5.629726964,-1.7122574827  
 H,-0.3833341864,4.0488246439,-2.4801519266  
 H,-1.7471230661,5.1644273906,-2.3439563188  
 Electronic energy = -1366.2861265  
 Zero-point electronic energy = -1365.666381  
 Thermal energy = -1365.635626  
 Enthalpy = -1365.634682  
 Free energy = -1365.728226  
 Free energy with quasiharmonic approximation = -1365.721713  
 Frequencies = 18.5321, 27.6219, 34.3250, 40.8920, 51.6149  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.892802

syn-open-12b C27H38N3O2(1+)  
 C,1.1991166449,-2.1956079146,0.5179588138  
 C,0.8949327418,-3.0796995083,1.4831997643  
 C,4.2186858066,-1.769793642,0.9731386197  
 C,3.5757950453,-1.6814975189,-0.4216213485  
 C,2.2587359651,-2.4960728292,-0.5183956633  
 H,0.1293249917,-2.8806810286,2.22929461  
 H,4.1563550919,-2.7875458026,1.3768597568  
 H,3.3578360596,-0.6236016465,-0.6063249354  
 H,2.5070820707,-3.5595176087,-0.4318220153  
 H,-1.4483666852,2.3675669286,-1.4664426072  
 N,0.6103300893,-0.9062287949,0.5160210565  
 C,0.1449767456,-0.2507115096,-0.713445513  
 C,0.109345395,1.271986917,-0.441290389  
 H,0.9082105523,-0.4275970408,-1.4756911564  
 C,-1.1615754923,-0.7880068381,-1.3039472642  
 H,-0.4984511891,1.4501494081,0.447755026  
 C,-0.378428277,2.1801963258,-1.5875115682

N,1.493413335,1.7603829296,-0.0270290866  
 C,-2.4198491402,-0.8054910685,-0.6094970977  
 C,-1.1242834812,-1.3195701796,-2.5764903099  
 C,0.444291072,3.4884048474,-1.573622485  
 H,-0.2557394175,1.6815870543,-2.5559890375  
 H,1.8520332302,-2.3734418445,-1.5316500457  
 C,1.338910005,3.0587105462,0.7325792948  
 C,2.4071920876,1.9793278322,-1.2127521376  
 C,-2.6417335759,-0.3025975163,0.6955556288  
 C,-3.5370704659,-1.3852616427,-1.3067441721  
 C,-2.2900279667,-1.8604749819,-3.1702070351  
 H,-0.1952162982,-1.3346148845,-3.1407726305  
 C,0.5513689289,4.0771975442,-0.1441434625  
 H,-0.0142691675,4.2247872534,-2.2397706595  
 C,1.8691116306,3.1554503288,-2.057007811  
 H,0.8240848066,2.8197522088,1.6659749946  
 H,2.3471028387,3.399694216,0.9768915791  
 H,2.436768665,1.0453798336,-1.7740166217  
 H,3.4036772593,2.1547877391,-0.8034984866  
 C,-3.8913813406,-0.3612738587,1.2957836714  
 H,-1.8539085902,0.1546033306,1.2816697618  
 C,-4.800682768,-1.4323380866,-0.6655119575  
 N,-3.4582145393,-1.8991504154,-2.5683899466  
 H,-2.2397073286,-2.2742084945,-4.1760389544  
 H,1.1614066113,4.9847319442,-0.2173963837  
 H,2.5197505018,4.0299038506,-1.9563208725  
 C,-4.9874171096,-0.9374730732,0.6039726773  
 O,-3.9734029064,0.1592987976,2.5481666743  
 H,-5.6225340758,-1.8766976885,-1.2174256264  
 H,-5.9667209155,-0.9904246397,1.06421336  
 C,-5.2250432623,0.1157065009,3.2341418074  
 H,-5.0422342195,0.5732896147,4.2070177428  
 H,-5.9929785985,0.6887312912,2.7016162097  
 H,-5.5667925997,-0.9159852618,3.376121057  
 H,-0.0880328316,-0.8471770367,1.2506906401  
 H,1.9325719158,1.0472532893,0.5912988955  
 H,1.4095675333,-4.0312297802,1.5502715113  
 H,5.2968674065,-1.5561450031,0.8923136501  
 C,3.9403445119,-1.1528083272,3.4623480196  
 H,3.7518333625,-0.2955835261,4.1113107383  
 H,4.9575714584,-1.5293740226,3.6192121522  
 H,3.2543134439,-1.9672533742,3.7272656517  
 C,3.7165920806,-0.7819646749,2.0158166239  
 O,3.204494334,0.2917000099,1.7151656249  
 C,4.5532749503,-2.1608511518,-1.5062469257  
 H,4.8568599377,-3.2003921206,-1.3329634349  
 H,5.4602299725,-1.5461703352,-1.52184267  
 H,4.0962091335,-2.112190904,-2.5013261277  
 H,1.8624114308,2.8744760457,-3.1143604589  
 C,-0.7944530185,4.476239364,0.4747390443  
 H,-1.3092365616,5.2027973393,-0.16276781  
 H,-1.4652625073,3.6210796264,0.614874561  
 H,-0.6441753137,4.9414926585,1.454925489  
 Electronic energy = -1366.2816483  
 Zero-point electronic energy = -1365.662035  
 Thermal energy = -1365.631156  
 Enthalpy = -1365.630212  
 Free energy = -1365.724176  
 Free energy with quasiharmonic approximation = -1365.717499  
 Frequencies = 22.0245, 28.4338, 35.6577, 42.8933, 51.3894  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.8904676

anti-open-12b C27H38N3O2(1+)

C,0.9227763406,-1.9326466676,1.5875612979  
C,1.2375221005,-2.4679979334,2.7793185721  
C,3.0101465359,-3.2622182138,-0.2535728745  
C,1.6126852195,-2.8500063833,-0.7477656714  
C,0.5708289473,-2.800614284,0.4009681119  
H,1.4891142835,-1.8539197143,3.6405125162  
H,2.9487427754,-4.0911261999,0.4619386115  
H,1.7095736589,-1.8510524018,-1.1884772691  
H,0.4230683732,-3.8199901206,0.7738212056  
H,-0.4531629532,3.3088046081,0.0418447608  
N,1.0261071106,-0.5369959076,1.3772020004  
C,0.0579810016,0.2304029413,0.5861134036  
C,0.7775304831,1.5348187391,0.1734689442  
H,-0.155541352,-0.3520531076,-0.3096943815  
C,-1.2617124593,0.5434128998,1.297268379  
H,1.1472546388,1.9990554154,1.0934283909  
C,-0.0149250088,2.5780488888,-0.6415067914  
N,2.0449366981,1.208110817,-0.6096273227  
C,-2.5360354765,0.2835686617,0.6917634208  
C,-1.2492804336,1.0894652384,2.5639983615  
C,0.939520857,3.2440365382,-1.6596114585  
H,-0.848947745,2.1087661399,-1.1749951644  
H,-0.3977282175,-2.5008285844,-0.0219105987  
C,2.9958979757,2.3785970081,-0.5078512904  
C,1.7575757712,0.9165321008,-2.0667808235  
C,-2.7182913713,-0.2664350569,-0.5999236782  
C,-3.7044225657,0.6072928875,1.4661862904  
C,-2.4627993734,1.3774268229,3.232331885  
H,-0.3164399075,1.3019465659,3.080847793  
C,2.2744587379,3.6697976667,-0.9954610605  
H,0.4565155396,4.1193374349,-2.1032404379  
C,1.2632432121,2.2081621937,-2.7532996315  
H,3.3116765784,2.439524358,0.5364652034  
H,3.8694192394,2.1257413073,-1.1120988072  
H,1.0142063937,0.1190689903,-2.0955361559  
H,2.6834486113,0.5226760507,-2.4899524096  
C,-3.9851581492,-0.5008088656,-1.1123585691  
H,-1.8805733092,-0.5297485483,-1.2357484574  
C,-4.9855002078,0.3551940164,0.9129781264  
N,-3.6516652995,1.1493877082,2.7160258824  
H,-2.4356821297,1.8098654725,4.2311128801  
H,2.8949393777,4.1122497279,-1.7831589949  
H,2.0275030549,2.5985260145,-3.4326466402  
C,-5.1356600697,-0.1856417775,-0.3426045073  
O,-4.0319501399,-1.0344138324,-2.3616222893  
H,-5.8496407911,0.6055814929,1.5197598316  
H,-6.1294150834,-0.3675648634,-0.7341640538  
C,-5.3032490639,-1.3145514399,-2.9469269821  
H,-5.0873830852,-1.7342277482,-3.9301662414  
H,-5.8634771798,-2.047482884,-2.3547814317  
H,-5.8996420268,-0.4021854377,-3.0644621988  
H,1.2502459412,-0.0623680902,2.2477663089  
H,2.4883646486,0.3624560205,-0.1947838988  
H,1.2524385437,-3.5423600926,2.920647713  
H,3.5953527915,-3.654180275,-1.1014458468  
C,4.9864815982,-2.5921771983,1.2617907798  
H,5.6711023263,-1.7643872276,1.4556836459  
H,5.5350658193,-3.4470457915,0.8497982103  
H,4.5397804162,-2.9255675531,2.2066860608

C,3.8830774167,-2.1590525449,0.3261660114  
O,3.752384018,-0.9799488279,0.0127255247  
C,1.1174548299,-3.807056365,-1.8432464744  
H,1.0526288153,-4.8358033234,-1.4683758532  
H,1.7943147846,-3.8071893208,-2.7048667046  
H,0.1204398354,-3.5212109774,-2.1975869996  
H,0.3758182767,1.9883599057,-3.3541213752  
C,2.1200296632,4.7207026508,0.111432661  
H,1.6234029082,5.6155519465,-0.2782036045  
H,1.5322961734,4.3569773828,0.961958489  
H,3.1005710767,5.0247409464,0.4936156761  
Electronic energy = -1366.2829153  
Zero-point electronic energy = -1365.663302  
Thermal energy = -1365.632523  
Enthalpy = -1365.631579  
Free energy = -1365.725111  
Free energy with quasiharmonic approximation = -1365.718681  
Frequencies = 19.4292, 25.7948, 38.9531, 46.6434, 52.3817  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.8916151

TS-1a C27H38N3O2(1+)  
C,1.6467964722,-1.7427731693,-1.0095361977  
C,2.7445263263,-1.1409686762,-1.6485306624  
C,4.0972501811,-2.3167122386,0.363815102  
C,2.829157912,-3.0927547463,0.7376744352  
C,1.8415373015,-3.1313363515,-0.4716349456  
H,2.6397423245,-0.1466228568,-2.0742345551  
H,4.7593760885,-2.2740084412,1.2394380414  
H,2.3364929511,-2.5414293663,1.5475115764  
H,0.8908724568,-3.5817080704,-0.164654683  
H,-1.6513307663,2.492162955,0.2932878702  
N,0.5730539748,-1.0748698264,-0.5778966409  
C,0.0732094154,0.2394527119,-1.0213893729  
C,0.169512278,1.3296726438,0.088927477  
H,0.7048997926,0.5439841025,-1.8569355584  
C,-1.3383056773,0.0711654616,-1.587166285  
H,-0.14462092,0.8801758215,1.0318433405  
C,-0.677229735,2.5975146231,-0.1906058342  
N,1.5904520642,1.7769284784,0.3547138747  
C,-2.4563654437,-0.3917036698,-0.8137315815  
C,-1.5409174697,0.3416005744,-2.9238679513  
C,0.0867345999,3.8412373251,0.3092210895  
H,-0.8748799197,2.70524707,-1.2629002048  
H,2.2668814716,-3.7634630248,-1.2592355678  
C,1.6288968857,2.4540619865,1.7027910095  
C,2.0942430768,2.7314657545,-0.6913883179  
C,-2.4188900097,-0.7164976708,0.5643715452  
C,-3.7057032525,-0.5397081257,-1.5112122764  
C,-2.8207789637,0.1689291522,-3.5048099346  
H,-0.7222012264,0.6869592477,-3.5492406408  
C,0.6156205059,3.6331640955,1.7486088751  
H,-0.5706975163,4.7153671596,0.2785534264  
C,1.2950718652,4.0543732516,-0.6231050758  
H,1.4141594153,1.6816106403,2.4456542612  
H,2.661763888,2.7766711597,1.8529409132  
H,1.9999372738,2.2424834379,-1.6634683401  
H,3.1602741825,2.8693878186,-0.4980762357  
C,-3.5484813408,-1.1668259,1.2348031968  
H,-1.5189547944,-0.6126376119,1.1598873171  
C,-4.8408120624,-1.001557296,-0.797484807  
N,-3.8693675209,-0.257063594,-2.8352081304

H,-2.9659341759,0.3899784648,-4.5606612768  
 H,1.1691116306,4.5387516529,2.0238732345  
 H,1.9274009375,4.8657963328,-0.2483738613  
 C,-4.7776837388,-1.3122427333,0.540705073  
 O,-3.3845906707,-1.4403502956,2.5528450948  
 H,-5.7691239786,-1.1017829136,-1.3502508694  
 H,-5.6645051813,-1.6626619512,1.0549663873  
 C,-4.5031940928,-1.9040419774,3.3117824826  
 H,-4.1284405725,-2.0477966882,4.3255675431  
 H,-5.3108137629,-1.1634336405,3.323778388  
 H,-4.8801329679,-2.8572606123,2.9240732593  
 H,-0.0851531956,-1.6095602701,-0.0213191717  
 H,2.299588396,0.8989217117,0.4529570829  
 H,3.3612553218,-1.8024833424,-2.2485506551  
 H,4.6501803578,-2.8406124424,-0.4268684545  
 C,5.0258140358,-0.1417155734,-0.6569116737  
 H,5.7678943743,0.0048323517,0.1385411824  
 H,4.7468246023,0.8473389287,-1.033836266  
 H,5.4964824098,-0.7107542048,-1.4639450741  
 C,3.8194694569,-0.8590081038,-0.0436826759  
 O,3.1155660094,-0.1844395954,0.8177625426  
 C,3.1332752972,-4.51679723,1.2145136616  
 H,3.6408167151,-5.0968632408,0.4340114545  
 H,2.214995304,-5.0499021002,1.4863963756  
 H,3.7834238551,-4.4994891463,2.0957395328  
 H,0.9616698311,4.3409849092,-1.6253308447  
 C,-0.4874778016,3.4303286238,2.7953218189  
 H,-1.1705037046,4.2865691044,2.8062486753  
 H,-1.0838419308,2.5300410518,2.6071401639  
 H,-0.0555888455,3.3358980944,3.797617318  
 Electronic energy = -1366.2634509  
 Zero-point electronic energy = -1365.645101  
 Thermal energy = -1365.616254  
 Enthalpy = -1365.615310  
 Free energy = -1365.703088  
 Free energy with quasiharmonic approximation = -1365.698125  
 Frequencies = -371.5756, 22.6832, 31.6377, 42.8973, 48.6856  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.942465  
 SCF (B3LYP/def2-TZVPP) = -1366.7767593  
 SCF (M06-2X/def2-TZVPP) = -1366.1967429  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.2039362

TS-1a-primed C27H38N3O2(1+)  
 C,-1.1346823429,-1.9685664229,-0.2602756599  
 C,-1.3649787837,-2.025760548,1.1252050682  
 C,-3.8442897247,-2.707595155,0.3200023321  
 C,-3.3186009592,-2.8530570048,-1.11307603  
 C,-1.7677088322,-3.0346886818,-1.1068591776  
 H,-0.9031356951,-1.2887759338,1.7770209192  
 H,-4.9295227439,-2.5400883889,0.2843033872  
 H,-3.5365300558,-1.9137322974,-1.634970229  
 H,-1.3837568178,-3.0127222795,-2.1330282065  
 H,0.5211885827,3.2581105263,-1.1264991604  
 N,-0.6717776084,-0.8887449927,-0.8956762916  
 C,0.1155742679,0.2391844966,-0.3595192797  
 C,-0.665968478,1.5803911329,-0.4085060317  
 H,0.3407713497,0.006557587,0.6792347075  
 C,1.4199086539,0.3046439485,-1.1552743672  
 H,-1.1492798569,1.6452611653,-1.3872353523  
 C,0.2099216316,2.8397831765,-0.1670033199  
 N,-1.8145623734,1.6283757868,0.5754634255

C,2.6506403677,-0.2015726631,-0.6210042403  
 C,1.42237097,0.8000185202,-2.4440235215  
 C,-0.5856450296,3.8648918756,0.6680811132  
 H,1.1307084736,2.5746535699,0.3656583658  
 H,-1.5243503207,-4.0162554508,-0.6846080986  
 C,-2.7540107413,2.7293451783,0.1531113044  
 C,-1.3528745757,1.8840405589,1.9841743396  
 C,2.7997475385,-0.7667903788,0.6663481074  
 C,3.8066617151,-0.1232121371,-1.4748170513  
 C,2.6206709541,0.8186886923,-3.1977239274  
 H,0.5186058107,1.1904861524,-2.9053993579  
 C,-1.9997205561,4.0884190684,0.0787445466  
 H,-0.0431727694,4.8148092301,0.6979651381  
 C,-0.7399050375,3.2992640903,2.0915400606  
 H,-3.1753540822,2.4282637161,-0.80959963  
 H,-3.5678390362,2.7353903005,0.8815768229  
 H,-0.6358736593,1.1039308892,2.2478103696  
 H,-2.228563441,1.7505189374,2.6231408731  
 C,4.0296984852,-1.2300082467,1.1094513274  
 H,1.9637399029,-0.8724364428,1.3483412503  
 C,5.0506108655,-0.5991171707,-0.988709148  
 N,3.7745214271,0.3825678914,-2.7402067718  
 H,2.6107546874,1.2157536003,-4.2112051565  
 H,-2.5162467363,4.79517839,0.7389409597  
 H,-1.3820591403,3.9510305652,2.6924301358  
 C,5.1715707336,-1.1394782117,0.2698578243  
 O,4.051748907,-1.7565712761,2.3603438751  
 H,5.9079440512,-0.5238795182,-1.6495422392  
 H,6.1361124574,-1.4948891279,0.6118823009  
 C,5.2815571837,-2.2670470797,2.8766895765  
 H,5.6634955455,-3.0881998498,2.259124132  
 H,6.0399764598,-1.4794465066,2.954262597  
 H,5.0469730697,-2.6423970159,3.8732778847  
 H,-0.6907488787,-0.9294214677,-1.909733198  
 H,-2.4391105785,0.6817198391,0.5622866205  
 H,-1.3966880122,-3.0209840036,1.5567664879  
 H,-3.684263512,-3.6343769132,0.8862437171  
 C,-3.5499681085,-1.4831737578,2.566789354  
 H,-3.001951097,-0.6806055536,3.0698561771  
 H,-3.3236740589,-2.4327617968,3.0607512159  
 H,-4.6217547522,-1.2793424103,2.68651222  
 C,-3.2420282294,-1.5040869475,1.0666548052  
 O,-3.3494293002,-0.3729320602,0.4316337392  
 C,-3.9824168069,-4.0104087495,-1.8662157229  
 H,-3.7993027936,-4.9679456789,-1.3634944073  
 H,-3.6007393979,-4.0900610818,-2.8905780913  
 H,-5.0662768848,-3.8637374276,-1.9236974043  
 H,0.2308629986,3.2496127819,2.5940978208  
 C,-2.0011935288,4.6889274101,-1.3325265526  
 H,-1.5237866384,4.0299201942,-2.0670354041  
 H,-3.025987127,4.8729103147,-1.6730497908  
 H,-1.4686879876,5.6459510423,-1.3465920825  
 Electronic energy = -1366.2637044  
 Zero-point electronic energy = -1365.645456  
 Thermal energy = -1365.616584  
 Enthalpy = -1365.615640  
 Free energy = -1365.703446  
 Free energy with quasiharmonic approximation = -1365.698633  
 Frequencies = -368.7122, 19.6376, 36.3335, 44.6490, 50.5872  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9420399  
 SCF (B3LYP/def2-TZVPP) = -1366.777451

SCF (M06-2X/def2-TZVPP) = -1366.1967999  
SCF (M06-2X-D3/def2-TZVPP) = -1366.2037517

TS-1b C27H38N3O2(1+)  
C,1.4553748384,-1.7835758179,1.355382101  
C,2.6696180329,-2.0639660337,2.0225206214  
C,3.4755277405,-2.6266429662,-0.4416432378  
C,2.0180952844,-2.6268792007,-0.9217624794  
C,1.0299351309,-2.7409019689,0.2869807813  
H,2.962268084,-1.3971712527,2.8323263418  
H,3.7363165172,-3.6231196576,-0.0614098569  
H,1.8303348785,-1.66573253,-1.4145939284  
H,1.0934788116,-3.7553256297,0.6945357925  
H,-0.7679872706,3.137127658,0.0726972045  
N,0.9644604729,-0.5480489053,1.4462262651  
C,-0.0059653545,0.1553486259,0.5920530032  
C,0.6389464958,1.4858347229,0.1282265336  
H,-0.1894786635,-0.4760086939,-0.2739145791  
H,1.014753668,1.9853076264,1.0271517005  
C,-0.2920690655,2.4563182655,-0.6368903511  
N,1.8732678429,1.2560193419,-0.7197819519  
C,0.5463078793,3.2128084278,-1.6929261054  
H,-1.0999152676,1.9088773037,-1.1358338403  
H,-0.0021476731,-2.5914550811,-0.0422794778  
C,2.7162875284,2.506526003,-0.6649051281  
C,1.5208390406,0.9599871844,-2.1542400008  
C,1.8711635887,3.7426381162,-1.0885759499  
H,-0.0348302161,4.0455181179,-2.1000168178  
C,0.9032639727,2.2153829287,-2.8113332199  
H,3.0984430625,2.5801678393,0.3560775883  
H,3.5692910345,2.330182007,-1.3229996315  
H,0.8266713382,0.1174243207,-2.1574834694  
H,2.4424208161,0.6300961356,-2.6388845169  
H,2.410333138,4.2495948792,-1.8975108221  
H,1.6084360725,2.66918322,-3.5153532626  
H,1.3889400927,0.0248198332,2.1685685621  
H,2.5168286546,0.4362942625,-0.302865689  
H,2.8769849724,-3.1113691808,2.2229404796  
H,4.131657627,-2.4363210997,-1.3017805661  
C,5.1851310838,-1.7873528185,1.2739265816  
H,5.9548557582,-1.6357478008,0.5068439471  
H,5.3027321687,-2.794826266,1.6845775137  
H,5.3522992528,-1.0505834804,2.0644935949  
C,3.8125391164,-1.5578703259,0.6265972223  
O,3.588122399,-0.304450648,0.3248862597  
H,0.0124071591,1.9350576693,-3.3817617488  
C,1.6847140061,4.7600107287,0.0445340682  
H,1.1683746626,4.3356382931,0.9134811277  
H,2.6548654587,5.1343757719,0.3889686405  
H,1.1005072563,5.619304972,-0.3018296992  
C,1.7387768983,-3.7420548669,-1.9360285627  
H,2.3870153332,-3.6394752289,-2.8127780133  
H,1.9250076851,-4.7284618797,-1.4952254948  
H,0.6987436945,-3.7182365163,-2.2815124301  
C,-1.3180688926,0.4049947467,1.3347509214  
C,-2.5813985264,-0.0054795794,0.7976829933  
C,-1.3032784605,1.0358553789,2.561354503  
C,-2.7585805099,-0.6513116382,-0.4488992038  
C,-3.7436814684,0.264677618,1.6019270197  
C,-2.5120050786,1.2574070204,3.2626518999  
H,-0.3748026784,1.3671020058,3.0192486707

C,-4.0177182412,-1.0304471759,-0.889940625  
 H,-1.9244751084,-0.8709300546,-1.1059725407  
 C,-5.0164056046,-0.1354246114,1.1212919691  
 N,-3.6922799628,0.8882530244,2.8124131097  
 H,-2.4876889587,1.7558232871,4.2299907263  
 C,-5.1620503401,-0.768407706,-0.0905195274  
 O,-4.0650245179,-1.6465404543,-2.0985553014  
 H,-5.8766873834,0.0769522423,1.7475668085  
 H,-6.1484529972,-1.0630395116,-0.4277205943  
 C,-5.3289547406,-2.0699322918,-2.6121776529  
 H,-5.1120774339,-2.5395490935,-3.572120757  
 H,-5.8044688051,-2.8012291224,-1.9485823948  
 H,-6.0023253296,-1.2190104898,-2.7673051239  
 Electronic energy = -1366.2605074  
 Zero-point electronic energy = -1365.641466  
 Thermal energy = -1365.612688  
 Enthalpy = -1365.611743  
 Free energy = -1365.699767  
 Free energy with quasiharmonic approximation = -1365.694421  
 Frequencies = -252.8756, 11.5833, 28.4859, 44.4864, 57.8260  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9407191  
 SCF (B3LYP/def2-TZVPP) = -1366.7744359  
 SCF (M06-2X/def2-TZVPP) = -1366.1965763  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.2038842

TS-1b-primed C27H38N3O2(1+)  
 C,1.4740443755,-2.0633365255,0.4837685226  
 C,1.9987304814,-2.3656246751,1.7630309305  
 C,4.2523260236,-1.5591339227,0.6283880221  
 C,3.5890982534,-1.6303173595,-0.7543347248  
 C,2.2819360959,-2.4899904744,-0.7001464107  
 H,1.3892132892,-2.103642344,2.6267743113  
 H,4.6670636906,-2.5428085256,0.8854081791  
 H,3.3036083285,-0.6105347336,-1.0398635618  
 H,2.5601204481,-3.5404539102,-0.5640950895  
 H,-1.4984541453,2.341361396,-1.0854764773  
 N,0.5268351618,-1.1311268135,0.402010099  
 C,0.1216695489,-0.3075368157,-0.7503630233  
 C,0.1632595568,1.1828132662,-0.3187128937  
 H,0.8763235902,-0.4569889991,-1.5234768754  
 H,-0.367548253,1.2682858276,0.6314292995  
 C,-0.4413601106,2.1926134023,-1.3196380747  
 N,1.5747351874,1.6290501112,0.0069227231  
 C,0.3635293245,3.5092494826,-1.2355049899  
 H,-0.4003165821,1.8037099073,-2.3437887739  
 H,1.7331555581,-2.4201129937,-1.643282488  
 C,1.480518857,2.8394583519,0.9036702703  
 C,2.3492235986,1.9929933555,-1.2313923615  
 C,0.5956644666,3.9335986221,0.2369368913  
 H,-0.1657060574,4.3026731963,-1.7713410268  
 C,1.7408209819,3.2584698732,-1.8785280172  
 H,1.07752619,2.4903802892,1.8575115607  
 H,2.5054007745,3.1725819475,1.0810627604  
 H,2.3135455509,1.1376093957,-1.9082130937  
 H,3.3882313869,2.1228912743,-0.921120905  
 H,1.1780991605,4.861952737,0.2145275961  
 H,2.3948848715,4.1235133164,-1.7284695824  
 H,0.1025385893,-0.8794826607,1.2880773071  
 H,2.130292536,0.8470216402,0.5989599611  
 H,2.4970807839,-3.3263077514,1.8599691082  
 H,5.0999991277,-0.8626990058,0.5790502712

C,3.9527684919,-1.2959410788,3.159427005  
 H,4.8350558076,-0.6501746103,3.2497511011  
 H,4.2657896762,-2.3316416613,3.3237190422  
 H,3.2435009332,-1.0022477953,3.9382776289  
 C,3.3316237946,-1.0693956543,1.7737773779  
 O,2.7815307971,0.1142857236,1.6465380438  
 H,1.6432916577,3.1102260795,-2.9585534493  
 C,-0.6931918207,4.2209537103,1.0185268542  
 H,-1.3389734371,3.3398558945,1.1094265441  
 H,-0.4598913605,4.5632984557,2.0326755179  
 H,-1.2740114055,5.0088414231,0.5269004383  
 C,4.5354618705,-2.1773183156,-1.8290898066  
 H,5.4321465543,-1.5537110839,-1.9096168954  
 H,4.8571758561,-3.1970703997,-1.5870929013  
 H,4.0527765683,-2.2014146161,-2.8129405852  
 C,-1.2129218434,-0.7420559353,-1.3550050625  
 C,-2.4529783155,-0.7807563741,-0.6328758309  
 C,-1.2210401006,-1.1230571168,-2.6803578021  
 C,-2.6215486147,-0.4202948278,0.7245914334  
 C,-3.6105120048,-1.223610278,-1.3643546113  
 C,-2.4240361852,-1.5374266049,-3.3019406782  
 H,-0.3062191336,-1.1110871137,-3.2673378772  
 C,-3.8604139554,-0.4875124074,1.3463090248  
 H,-1.7986119659,-0.0744499678,1.3381831789  
 C,-4.8620510461,-1.2839442746,-0.7006964323  
 N,-3.5795401641,-1.5913815227,-2.6773433174  
 H,-2.4142038321,-1.8338873278,-4.3492158088  
 C,-4.9975145977,-0.9283478069,0.6206500667  
 O,-3.8908634603,-0.1121911534,2.6497731509  
 H,-5.7160665311,-1.6228481676,-1.2778823192  
 H,-5.9686551717,-0.9866164827,1.0971563655  
 C,-5.1308563702,-0.1629828443,3.3580230922  
 H,-4.9035129052,0.1743258162,4.3697130541  
 H,-5.8739141728,0.5063689989,2.9096006733  
 H,-5.5269042544,-1.1841305627,3.3952243402  
 Electronic energy = -1366.2593228  
 Zero-point electronic energy = -1365.640521  
 Thermal energy = -1365.611711  
 Enthalpy = -1365.610767  
 Free energy = -1365.699165  
 Free energy with quasiharmonic approximation = -1365.693288  
 Frequencies = -247.0779, 11.8704, 24.2565, 39.8313, 47.0457  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9400089  
 SCF (B3LYP/def2-TZVPP) = -1366.7730952  
 SCF (M06-2X/def2-TZVPP) = -1366.1958841  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.2032576  
  
 TS-1c C27H38N3O2(1+)  
 C,1.5334285604,-1.9407258085,-1.026968952  
 C,2.6688497661,-1.4335072975,-1.6790444407  
 C,3.9428111863,-2.6969347777,0.33701258  
 C,2.6371050707,-3.4403039351,0.683291978  
 C,1.6206407693,-3.3473110893,-0.5074114628  
 H,2.6445695149,-0.4364175026,-2.1093383932  
 H,4.5941874274,-2.6933062543,1.2213666568  
 H,2.8855215085,-4.5059095527,0.7647761759  
 H,0.6410704338,-3.7227611525,-0.1910815714  
 H,-1.4386297718,2.5108316468,0.312854406  
 N,0.5180498703,-1.1865152713,-0.5925512758  
 C,0.1239688977,0.1617407307,-1.043716888  
 C,0.3025970782,1.2411110188,0.0679321287

H,0.7815910196,0.4141673002,-1.8765249291  
 C,-1.2925187836,0.102447148,-1.6185904911  
 H,-0.0209417377,0.8038785173,1.0136449019  
 C,-0.4680495502,2.5608414874,-0.186729023  
 N,1.7532480074,1.6003533485,0.3120829938  
 C,-2.44894804,-0.2620017121,-0.8493578121  
 C,-1.4644914615,0.3753076558,-2.9590977919  
 C,0.3794128629,3.7515482537,0.3081240475  
 H,-0.6759638381,2.689769229,-1.2545635718  
 H,1.9714089118,-3.9897636958,-1.3214254936  
 C,1.8550573371,2.2602152859,1.6657501091  
 C,2.2994328033,2.5316269813,-0.7351135217  
 C,-2.4446446004,-0.5762767013,0.5312940503  
 C,-3.7020467331,-0.315603886,-1.5534184953  
 C,-2.7508032127,0.3009721491,-3.5469859649  
 H,-0.617223576,0.6466868346,-3.5830042794  
 C,0.9223983603,3.5024998976,1.7358405963  
 H,-0.2239614464,4.6642680515,0.2954380831  
 C,1.5804932258,3.8987137007,-0.6461012432  
 H,1.5993073869,1.4966040692,2.4044955757  
 H,2.9087969977,2.5121968162,1.8041484372  
 H,2.1644322683,2.0552771869,-1.708555119  
 H,3.3742246084,2.603487089,-0.5546426031  
 C,-3.6097169148,-0.9309128356,1.1984451293  
 H,-1.5416349777,-0.5408891222,1.1301730843  
 C,-4.8742705932,-0.6788944656,-0.8427246864  
 N,-3.8344805398,-0.0326296786,-2.8808477596  
 H,-2.8711526391,0.5231902832,-4.6057064725  
 H,1.5391867422,4.3688741049,2.0021936581  
 H,2.2664929004,4.6692157426,-0.2798347373  
 C,-4.842948962,-0.9828468089,0.4982100396  
 O,-3.4746013403,-1.2080489132,2.5189083136  
 H,-5.8048626423,-0.7090439378,-1.3998884934  
 H,-5.7574777752,-1.2575778012,1.0099010021  
 C,-4.6298888461,-1.5796536821,3.27370043  
 H,-4.2722912589,-1.7497902636,4.2895872889  
 H,-5.3765115943,-0.7775107693,3.2800793111  
 H,-5.0790061002,-2.5011590625,2.8863319  
 H,-0.1817776079,-1.6657130056,-0.0365278775  
 H,2.4043187141,0.6895487755,0.387624388  
 H,3.2234102749,-2.1473683268,-2.279671035  
 H,4.4801659616,-3.2473238647,-0.4450214526  
 C,5.0482107466,-0.6459754732,-0.7510310053  
 H,5.820903297,-0.5613595208,0.0240024816  
 H,4.8560039278,0.359842574,-1.1375985552  
 H,5.4399616151,-1.2708859642,-1.5589251527  
 C,3.7884272185,-1.2246425142,-0.094956597  
 O,3.1770904105,-0.449373553,0.7498448294  
 C,2.0109363731,-3.0159312135,2.0205606172  
 H,1.7492526911,-1.9560988616,2.0242454653  
 H,2.7214632992,-3.1802913822,2.8381107842  
 H,1.1171258689,-3.6141992593,2.2356577402  
 H,1.2455485583,4.2100196631,-1.6404628844  
 C,-0.1694301887,3.3687484515,2.805405778  
 H,-0.7905982067,4.2704120464,2.8364476777  
 H,-0.8315288718,2.5137432514,2.6260412915  
 H,0.2765193377,3.2375496253,3.7974561014  
 Electronic energy = -1366.2591893  
 Zero-point electronic energy = -1365.640482  
 Thermal energy = -1365.611608  
 Enthalpy = -1365.610664

Free energy = -1365.698829  
Free energy with quasiharmonic approximation = -1365.693372  
Frequencies = -349.6488, 22.2470, 29.3345, 35.3482, 45.2521  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9387219  
SCF (B3LYP/def2-TZVPP) = -1366.7714648  
SCF (M06-2X/def2-TZVPP) = -1366.1924225  
SCF (M06-2X-D3/def2-TZVPP) = -1366.1998882

TS-1c-primed C27H38N3O2(1+)  
C,0.9699893191,-2.1006254663,0.3685062297  
C,1.2129665747,-2.2430241149,-1.0078425265  
C,3.613075142,-3.1022237318,-0.1224392358  
C,3.0396679611,-3.2152103474,1.3039967953  
C,1.4724820699,-3.1954417353,1.2653467836  
H,0.8344320552,-1.4970236129,-1.7013921392  
H,4.7064316887,-3.0183748452,-0.0598579275  
H,3.3046293954,-4.2110454358,1.6805619823  
H,1.0744097004,-3.0977805789,2.2815226626  
H,-0.2659470017,3.2841496317,0.9092827019  
N,0.5935921747,-0.9552190852,0.9461015809  
C,-0.0965660733,0.2025264266,0.3417153337  
C,0.7899221531,1.4782480808,0.3064814894  
H,-0.3420666501,-0.0741425384,-0.6812266938  
C,-1.3901061563,0.4223636646,1.1256925637  
H,1.2827213565,1.5697567001,1.2786307912  
C,0.013414822,2.7825421478,-0.0195071214  
N,1.9321246092,1.3730195655,-0.6806740046  
C,-2.6553299661,-0.0295043053,0.6235272299  
C,-1.3545153386,1.0040927833,2.3770680287  
C,0.8835333303,3.6886158244,-0.916230504  
H,-0.9243506146,2.5530927195,-0.5391553606  
H,1.1174046626,-4.1503354757,0.864296268  
C,2.9587516048,2.4217276242,-0.3311587787  
C,1.483596161,1.5733263479,-2.1036206199  
C,-2.8484629734,-0.6610356474,-0.6264698337  
C,-3.7999370873,0.1837073866,1.4695416988  
C,-2.5462446637,1.1563939862,3.1261152357  
H,-0.4244234573,1.3632405818,2.8101454181  
C,2.3140485712,3.8374076916,-0.3429871852  
H,0.4163093975,4.6739778074,-1.0062406488  
C,0.9864186139,3.0239376974,-2.3009254348  
H,3.3597294505,2.15019002,0.6487225734  
H,3.7659593199,2.3163101269,-1.0591789254  
H,0.7039866069,0.8388388752,-2.3167859361  
H,2.3422436942,1.3287768686,-2.7325607629  
C,-4.1094089948,-1.0632795589,-1.0411589728  
H,-2.0246532653,-0.865260182,-1.3007946683  
C,-5.0751504865,-0.2378947609,1.0151985357  
N,-3.728521988,0.768669761,2.6986835803  
H,-2.5056660531,1.620091494,4.1100877779  
H,2.880372686,4.456963442,-1.0482013303  
H,1.6762323747,3.5820447843,-2.9420868146  
C,-5.2383032193,-0.8463284981,-0.2070652963  
O,-4.1725495004,-1.6582640152,-2.2595469783  
H,-5.9223001388,-0.0646612049,1.670742647  
H,-6.225965932,-1.1583562615,-0.5246223944  
C,-5.4399811688,-2.0886858075,-2.7575838393  
H,-5.8895503502,-2.8457811668,-2.1049662931  
H,-6.1302607554,-1.2452529371,-2.8748720454  
H,-5.2362339756,-2.5282793497,-3.7345219807  
H,0.5874671921,-0.9531816221,1.9608714727

H,2.4782932356,0.3915319739,-0.6075924281  
 H,1.1581068262,-3.2560479182,-1.3933296428  
 H,3.4013044401,-4.0248242843,-0.6764941973  
 C,3.4563183205,-2.0094573372,-2.4426220854  
 H,2.9904825111,-1.1964849549,-3.0079618743  
 H,3.1517600531,-2.9662187251,-2.8769335773  
 H,4.5436816094,-1.9107334573,-2.5555599757  
 C,3.1297528397,-1.8932940487,-0.9485791112  
 O,3.3256288501,-0.7265068684,-0.4085237841  
 C,3.6136767194,-2.1875033005,2.2910879639  
 H,3.4090935995,-1.164560092,1.9698018934  
 H,4.7015990566,-2.2974098567,2.3586636687  
 H,3.2036336285,-2.3462004294,3.29593239  
 H,0.0121686991,3.0198441938,-2.7993658909  
 C,2.3745988489,4.5265203693,1.026071299  
 H,1.8488747809,3.9608353865,1.8042295835  
 H,3.4137864864,4.6455277141,1.3519012873  
 H,1.9250026178,5.5241018807,0.9771093535  
 Electronic energy = -1366.2594218  
 Zero-point electronic energy = -1365.640188  
 Thermal energy = -1365.611592  
 Enthalpy = -1365.610648  
 Free energy = -1365.697574  
 Free energy with quasiharmonic approximation = -1365.693001  
 Frequencies = -353.8914, 21.4551, 38.6893, 44.9725, 53.9607  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9382158  
 SCF (B3LYP/def2-TZVPP) = -1366.7720408  
 SCF (M06-2X/def2-TZVPP) = -1366.1924713  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1996376

TS-1d C27H38N3O2(1+)  
 C,1.5235313036,-2.0250106833,0.3097607264  
 C,2.0049137851,-2.4218369984,1.5693192923  
 C,4.1541794484,-1.1191644788,0.4248034649  
 C,3.874437857,-2.3241989734,-0.4944154601  
 C,2.3691930381,-2.3649223886,-0.8848894776  
 H,1.3770427947,-2.2421637993,2.438879732  
 H,5.2081804613,-1.1465406446,0.7278278088  
 H,4.1032489836,-3.2413285822,0.0616569604  
 H,2.10260364,-3.3701168493,-1.2364641648  
 H,-1.4936063884,2.4686748677,-1.0645487666  
 N,0.5306010717,-1.1310352939,0.275755565  
 C,0.0921491458,-0.226143125,-0.797399604  
 C,0.1053759126,1.2332932549,-0.2693843936  
 H,0.8291645041,-0.2950492144,-1.5970888634  
 C,-1.2453208072,-0.6444828761,-1.4094148274  
 H,-0.4877438522,1.2708728996,0.6470873405  
 C,-0.4369773009,2.2801906436,-1.2717598657  
 N,1.4893025606,1.6608222658,0.1709534834  
 C,-2.4719448025,-0.7571631555,-0.671636848  
 C,-1.2689644281,-0.9389008464,-2.756386361  
 C,0.4129454803,3.5633792773,-1.1631302869  
 H,-0.3852624291,1.896039952,-2.2969217751  
 H,2.1852557264,-1.6887466798,-1.7252273048  
 C,1.3423144423,2.8721225539,1.0569985098  
 C,2.3748791158,2.014824518,-0.9907496839  
 C,-2.6248903589,-0.4967345045,0.7107205823  
 C,-3.6334060257,-1.1725754507,-1.4133022844  
 C,-2.4739336452,-1.3352375385,-3.3853856089  
 H,-0.3628414437,-0.8736009216,-3.3534376911  
 C,0.5782782487,4.0051974563,0.3115741128

H,-0.055393432,4.366708115,-1.739863928  
 C,1.8105134156,3.2518261299,-1.7314270278  
 H,0.8238468714,2.5397941255,1.9598400407  
 H,2.3538481453,3.1647990823,1.3466623277  
 H,2.4412810879,1.1410210251,-1.6420042343  
 H,3.3707140809,2.1867917754,-0.5757198276  
 C,-3.8517887646,-0.6308196119,1.3451758488  
 H,-1.8008434399,-0.1747047227,1.3358432687  
 C,-4.8724103813,-1.3026632915,-0.7361379453  
 N,-3.6180284453,-1.4517682902,-2.7482187034  
 H,-2.476016577,-1.5627993047,-4.4498329727  
 H,1.2178429346,4.8958202651,0.3105451994  
 H,2.4740122421,4.1126370737,-1.6011400815  
 C,-4.9928296051,-1.0416646869,0.6085121866  
 O,-3.8668093661,-0.3472534054,2.6720227596  
 H,-5.7293373463,-1.6181193433,-1.3222297631  
 H,-5.9548452722,-1.1510772847,1.0944445441  
 C,-5.0941130622,-0.4681943426,3.3932651042  
 H,-4.8556740459,-0.2006118225,4.4230973117  
 H,-5.8541990985,0.2196381986,3.0052665882  
 H,-5.4746774259,-1.4954786013,3.3628910828  
 H,0.0601563306,-0.999052865,1.163885638  
 H,2.0050324649,0.863416685,0.8260745995  
 H,2.5703553958,-3.3465517859,1.6164534377  
 H,4.0290341186,-0.1956434449,-0.1541350804  
 C,3.9978579968,-1.4347326035,2.9865410997  
 H,4.7821323559,-0.6979774096,3.2011403842  
 H,4.4692813509,-2.4169552142,2.8829203832  
 H,3.3088916397,-1.449203769,3.8348072278  
 C,3.2748060158,-0.9896992838,1.7098099997  
 O,2.5916037005,0.1152102261,1.8529007994  
 C,4.7573995165,-2.3112485577,-1.7470142859  
 H,4.5936334902,-1.4011173045,-2.3378642602  
 H,4.5462354345,-3.1731982603,-2.3898393528  
 H,5.8177687883,-2.3476122844,-1.4761797264  
 H,1.7510474891,3.0494151831,-2.8054501148  
 C,-0.7379922096,4.383125007,1.0025681649  
 H,-1.24559203,5.1858631962,0.456797448  
 H,-1.4311194464,3.5368678835,1.0738451059  
 H,-0.5494409558,4.739948834,2.0209724425  
 Electronic energy = -1366.2540911  
 Zero-point electronic energy = -1365.636229  
 Thermal energy = -1365.607323  
 Enthalpy = -1365.606379  
 Free energy = -1365.694271  
 Free energy with quasiharmonic approximation = -1365.689216  
 Frequencies = -349.5201, 24.8557, 32.6474, 38.4888, 53.7079  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9341401  
 SCF (B3LYP/def2-TZVPP) = -1366.7680043  
 SCF (M06-2X/def2-TZVPP) = -1366.1884226  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1957033  
  
 TS-1d-primed C27H38N3O2(1+)  
 C,-1.4150403288,-1.6975696451,-1.373288138  
 C,-2.5791890643,-1.9085266671,-2.1299577491  
 C,-3.466035548,-2.0591175485,0.4847969776  
 C,-2.4549148884,-3.2112251753,0.3277079657  
 C,-1.1226618508,-2.6832541003,-0.2767067429  
 H,-2.7778487066,-1.2420983436,-2.9657219279  
 H,-4.4115225075,-2.4720812937,0.857618724  
 H,-2.8740525971,-3.9431304965,-0.3731276135

H,-0.5451238713,-3.5196419984,-0.6912335672  
 H,1.0548269104,3.0883530584,0.0908082116  
 N,-0.8147086148,-0.5065809149,-1.466213963  
 C,0.1427146326,0.167157678,-0.5757154192  
 C,-0.4480634642,1.5366533103,-0.1549366911  
 H,0.2602500421,-0.4556458915,0.3064490928  
 C,1.4989486773,0.3463048426,-1.2605956236  
 H,-0.6861539052,2.0788939922,-1.0755217616  
 C,0.4908584653,2.4002485771,0.7243853295  
 N,-1.7777940358,1.4024777271,0.5546877898  
 C,2.7147488938,-0.1415807293,-0.6866046342  
 C,1.5634915812,0.9969489946,-2.4788609574  
 C,-0.3574198349,3.1490116523,1.7736355693  
 H,1.2286968973,1.771438104,1.2357534905  
 H,-0.5035993921,-2.2459100794,0.5125370306  
 C,-2.4745724491,2.7395525541,0.5058825408  
 C,-1.6106230511,0.9919421083,1.9906468921  
 C,2.8081477233,-0.818109992,0.5638946433  
 C,3.9173999691,0.0806263323,-1.4415100444  
 C,2.8037921653,1.1602684475,-3.1312875106  
 H,0.6726522701,1.3897940102,-2.9623869245  
 C,-1.5696150506,3.850118774,1.1133437253  
 H,0.2624284554,3.888584013,2.2893689502  
 C,-0.8888781437,2.1111842011,2.779782203  
 H,-2.7234478304,2.9244332189,-0.5421292576  
 H,-3.4135916684,2.6144422981,1.0492698784  
 H,-1.0551831505,0.0515213274,2.0082850706  
 H,-2.6128196889,0.7856659953,2.3726555717  
 C,4.0330625294,-1.2532911225,1.0379157774  
 H,1.9200794869,-0.9984309883,1.1547304257  
 C,5.1574636325,-0.3868288992,-0.9198621997  
 N,3.9456811933,0.7208723618,-2.6407265671  
 H,2.8450816968,1.6718072692,-4.0910511935  
 H,-2.1339941044,4.3400109081,1.9156657015  
 H,-1.5764383801,2.5856749394,3.4871413909  
 C,5.2197309068,-1.0340693812,0.2831183034  
 O,4.2291494501,-1.9019882025,2.2124043804  
 H,6.0482780089,-0.2066547546,-1.512346507  
 H,6.158913746,-1.3930813377,0.6912102787  
 C,3.1092134645,-2.157381816,3.0516613971  
 H,3.5044243813,-2.6704221534,3.9288024671  
 H,2.6254412197,-1.2226844534,3.3625407454  
 H,2.3760534731,-2.8027907844,2.5516501395  
 H,-1.1305112692,0.0601858373,-2.2470477615  
 H,-2.4930011805,0.6759382096,0.0155771665  
 H,-2.8830320526,-2.9358889583,-2.2990945374  
 H,-3.1056638611,-1.3747423839,1.2631175803  
 C,-5.1063314426,-1.5413745956,-1.4493296398  
 H,-5.2340585979,-2.6147448182,-1.619429473  
 H,-5.9069390848,-1.2017740306,-0.7801188045  
 H,-5.2116159173,-1.0072581483,-2.3970481157  
 C,-3.7673957372,-1.2021283704,-0.785253497  
 O,-3.5317659271,0.0795306069,-0.7054679746  
 C,-2.1974749089,-3.9386277279,1.6518093489  
 H,-1.8032296095,-3.2526302887,2.4125721476  
 H,-1.4741395674,-4.7516699274,1.5225090856  
 H,-3.1226680459,-4.3740539808,2.0434721111  
 H,-0.0662230745,1.686501525,3.3635135363  
 C,-1.1892282195,4.9308500374,0.0930019109  
 H,-0.5573915925,5.6958703035,0.5571114553  
 H,-0.6438592564,4.5241006232,-0.7665833134

H,-2.0856184003,5.4287261601,-0.2925168964  
Electronic energy = -1366.25455302  
Zero-point electronic energy = -1365.63659  
Thermal energy = -1365.60781  
Enthalpy = -1365.60686  
Free energy = -1365.69409  
Free energy with quasiharmonic approximation = -1365.689499  
Frequencies = -362.9918, 24.3180, 31.2520, 40.9306, 57.2431  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.93502  
SCF (B3LYP/def2-TZVPP) = -1366.768599  
SCF (M06-2X/def2-TZVPP) = -1366.189753  
SCF (M06-2X-D3/def2-TZVPP) = -1366.197366

TS-1e C27H38N3O2(1+)  
C,-0.2770925892,2.0104874294,0.1524326189  
C,-0.6130684758,3.1947705311,-0.5332360293  
C,-2.8872111112,2.9379973827,0.8166241325  
C,-2.2237529272,1.897049786,1.7262363709  
C,-0.6615682922,1.9327618815,1.5968976309  
H,-0.3012940911,3.2876979398,-1.5723216044  
H,-3.9762380228,2.7996251426,0.8593193624  
H,-2.5659144003,0.907674844,1.3974972276  
H,-0.2192454713,1.0780511311,2.1104158205  
H,-1.1178362774,-3.2100634111,0.9151409273  
N,0.0405137216,0.9364559478,-0.5816424939  
C,0.2021031087,-0.4988075792,-0.2506561296  
C,-1.1458380749,-1.2181253253,0.0140319741  
H,0.6042691932,-0.9226636444,-1.1762307753  
H,-1.5218271994,-0.920590161,0.9945361631  
C,-1.0289886989,-2.7662816113,-0.0793753228  
N,-2.2245792062,-0.7634056376,-0.9415931316  
C,-2.113192051,-3.3128507648,-1.0303681873  
H,-0.0395722382,-3.0498030627,-0.4563434544  
H,-0.2980848418,2.8382187301,2.0946756782  
C,-3.5457203412,-1.3345446611,-0.4946663204  
C,-1.9589174199,-1.1895913663,-2.3606822064  
C,-3.5266325058,-2.8866058028,-0.5680475459  
H,-2.0492825638,-4.4048779924,-1.0626618046  
C,-1.8646419084,-2.7326589704,-2.436154067  
H,-3.7139667282,-0.9762638184,0.524788385  
H,-4.307965617,-0.8833863133,-1.1332564878  
H,-1.0457641472,-0.6947174356,-2.6945051665  
H,-2.7779350014,-0.7805739232,-2.9548104105  
H,-4.2281207216,-3.2010775028,-1.3499754101  
H,-2.6042145806,-3.1201814304,-3.1436936037  
H,0.171012538,1.145141675,-1.5649815769  
H,-2.3430602765,0.3532628427,-0.9455741064  
H,-0.5374905481,4.1181298863,0.0330528591  
H,-2.6828316026,3.9466963891,1.19750301  
C,-2.9383522552,4.0686678042,-1.4874971226  
H,-2.5533766617,3.999763762,-2.5085981908  
H,-2.6291801547,5.0202316257,-1.0446715893  
H,-4.0343884427,4.0541794717,-1.5418698207  
C,-2.4848989718,2.852018116,-0.6733104667  
O,-2.660541155,1.7163050493,-1.289260371  
H,-0.878656427,-3.0369855217,-2.8024295896  
C,-3.9823218113,-3.5296451869,0.7473059092  
H,-3.3406641633,-3.2475800703,1.5906048007  
H,-5.0041172058,-3.2210196669,0.9947584262  
H,-3.9750400889,-4.6219073687,0.6685760554  
C,-2.6259666025,2.0696276529,3.19588308

H,-2.3140160263,3.0501977364,3.5741908628  
 H,-3.7123893984,1.9951823811,3.312069892  
 H,-2.1657324667,1.302602427,3.8293932788  
 C,1.26506554,-0.7539080724,0.8208475868  
 C,2.6430185407,-0.4792360013,0.5195223062  
 C,0.9693395948,-1.2719722591,2.0637246459  
 C,3.1048500633,0.0282795229,-0.7151025198  
 C,3.6056281844,-0.7570760809,1.5497170298  
 C,2.0025181693,-1.5042943499,3.0064784947  
 H,-0.0455460264,-1.5175844175,2.3569403073  
 C,4.4551761779,0.2548365861,-0.9405459669  
 H,2.4263904642,0.2628373948,-1.5267916818  
 C,4.9774340418,-0.5089330877,1.2917640575  
 N,3.2724733238,-1.2586951571,2.7731817522  
 H,1.75016936,-1.9090480921,3.9849054204  
 C,5.4037751525,-0.0159145375,0.0808330849  
 O,4.78030549,0.7385667528,-2.1657919226  
 H,5.6833952814,-0.7263670563,2.0865528229  
 H,6.459386336,0.1613276643,-0.0860482587  
 C,6.1533792569,0.9843261835,-2.4737093539  
 H,6.1610611131,1.3558847903,-3.4988437507  
 H,6.582592182,1.742819289,-1.8089725835  
 H,6.7459589551,0.064141591,-2.4156829508  
 Electronic energy = -1366.2563527  
 Zero-point electronic energy = -1365.637175  
 Thermal energy = -1365.608342  
 Enthalpy = -1365.607398  
 Free energy = -1365.695328  
 Free energy with quasiharmonic approximation = -1365.690181  
 Frequencies = -307.6000, 18.5188, 31.8910, 38.5559, 46.1539  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9374869  
 SCF (M06-2X/def2-TZVPP) = -1366.1930244  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.2003402  
  
 TS-1f C27H38N3O2(1+)  
 C,1.6522096809,-1.6209346717,-1.1840206367  
 C,2.7530108323,-0.9551156036,-1.7413651232  
 C,3.8645098577,-2.2929826525,0.4336566091  
 C,3.2533205798,-3.4463313058,-0.3943348927  
 C,1.8071258691,-3.0823456718,-0.8534223873  
 H,2.6588854241,0.0848921223,-2.0385918278  
 H,3.3424158483,-2.2408176449,1.394632419  
 H,1.0884126926,-3.3537189005,-0.0708798761  
 H,-1.6698619673,2.5032293103,0.3682012279  
 N,0.5769703026,-0.9933881535,-0.6989742042  
 C,0.0521525151,0.3337042878,-1.0820690588  
 C,0.1716737044,1.394626645,0.0551924126  
 H,0.6530356169,0.6706802249,-1.9283339505  
 C,-1.3731808981,0.1602807099,-1.6094564881  
 H,-0.0850698545,0.9090422949,0.9977590573  
 C,-0.7178834445,2.6477627743,-0.1488401189  
 N,1.590005657,1.8751481605,0.2678446888  
 C,-2.4561004143,-0.3524208819,-0.8181117642  
 C,-1.6232206578,0.4689142352,-2.9296308865  
 C,0.0339165652,3.8961720066,0.358751853  
 H,-0.9593317414,2.782775988,-1.2088999297  
 H,1.5370448384,-3.6720439927,-1.7397762468  
 C,1.6730302788,2.5112009596,1.634292553  
 C,2.0205588505,2.8736498511,-0.7693858833  
 C,-2.3658076772,-0.7202290782,0.5465784036  
 C,-3.722184299,-0.5099111748,-1.4822059184

C,-2.9172612856,0.2881159177,-3.4757991082  
 H,-0.8308051769,0.8469986038,-3.5697544063  
 C,0.6324741308,3.6586076478,1.7656075044  
 H,-0.6474853565,4.7519786764,0.3844261935  
 C,1.1955181949,4.1742789518,-0.616019402  
 H,1.5132828195,1.7097973797,2.3596951514  
 H,2.7023308978,2.8585622752,1.747190246  
 H,1.8843944576,2.4174303918,-1.7523740782  
 H,3.0925416462,3.0267125521,-0.6259489417  
 C,-3.4607876659,-1.2267092056,1.2343410114  
 H,-1.4502878427,-0.6067815956,1.1162733375  
 C,-4.8210595131,-1.0283442075,-0.7509669677  
 N,-3.9342256503,-0.1857499041,-2.7896749779  
 H,-3.1007650466,0.5418656858,-4.5182251356  
 H,1.1740548335,4.570462424,2.0437107223  
 H,1.8244038307,4.9860327566,-0.2360984916  
 C,-4.7061834995,-1.3845555579,0.5723247072  
 O,-3.2494915373,-1.5417329413,2.5359914354  
 H,-5.7636064892,-1.1357478035,-1.2777350847  
 H,-5.5656786659,-1.7791611288,1.1007000119  
 C,-4.3307797946,-2.0685234574,3.3079574275  
 H,-3.921547326,-2.240996699,4.3037437541  
 H,-5.1592613212,-1.3540612555,3.3731009713  
 H,-4.6914283372,-3.0165586535,2.8929783109  
 H,-0.0771908022,-1.5692623714,-0.1789386513  
 H,2.3289525656,1.0194794617,0.3155873531  
 H,3.3647297868,-1.5369714344,-2.4189284306  
 H,4.9117519502,-2.5359022768,0.6540202229  
 C,5.1071771079,-0.3262797747,-0.7376149544  
 H,5.8215735235,-0.1867012563,0.0835080192  
 H,4.957416665,0.6451891552,-1.2186494148  
 H,5.5467183985,-1.0221226363,-1.4587654273  
 C,3.7962054351,-0.8395543101,-0.125044985  
 O,3.1903143386,-0.0130027657,0.679631473  
 H,0.8131740753,4.4908099288,-1.591284317  
 C,-0.4120102299,3.3916318766,2.8570856609  
 H,-1.1209409239,4.2238504836,2.926394609  
 H,-0.9874865811,2.4769047285,2.673175857  
 H,0.0716297486,3.2842175203,3.8342131235  
 H,3.1366995437,-4.2910615929,0.2954027989  
 C,4.1606264688,-3.9633600124,-1.5247350837  
 H,5.1017976617,-4.3330720259,-1.1031690933  
 H,3.6838081273,-4.7973602695,-2.0522818778  
 H,4.4187279485,-3.2061544395,-2.2714605646  
 Electronic energy = -1366.2485768  
 Zero-point electronic energy = -1365.630287  
 Thermal energy = -1365.601323  
 Enthalpy = -1365.600379  
 Free energy = -1365.688831  
 Free energy with quasiharmonic approximation = -1365.683345  
 Frequencies = -369.7523, 20.9179, 33.0746, 43.0190, 48.0920  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9288166  
 SCF (M06-2X/def2-TZVPP) = -1366.1827702  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1898907  
  
 TS-1g C27H38N3O2(1+)  
 C,-0.2912600483,1.9638528188,-0.123972739  
 C,-0.7428213274,3.0010178476,-0.947893877  
 C,-2.9080494369,2.3815549963,0.7211382022  
 C,-1.8099509866,2.8098195523,1.7215248036  
 C,-0.4391194646,2.1388942586,1.3608900768

H,-0.6011536709,2.91427477,-2.0225200024  
 H,-3.1498377754,1.3275693543,0.9047551711  
 H,-2.0980214865,2.3877292268,2.6921490452  
 H,-0.3386247415,1.1865870163,1.8792757827  
 H,-1.320814334,-3.0017007501,1.5123499956  
 N,-0.0119663006,0.78390394,-0.7024477814  
 C,0.1460775081,-0.5864973975,-0.1633545313  
 C,-1.2107280231,-1.225365161,0.2363262957  
 H,0.514899518,-1.1552206623,-1.0240845866  
 H,-1.5906728533,-0.7242083637,1.1308157053  
 C,-1.1123467295,-2.7634354828,0.4660899259  
 N,-2.2749500524,-0.9686877414,-0.8064560608  
 C,-2.0932267719,-3.4963803066,-0.4707453674  
 H,-0.0924818258,-3.1099686629,0.2682629909  
 H,0.3853290107,2.7681617513,1.7193498119  
 C,-3.5878253144,-1.5031954168,-0.2979033006  
 C,-1.9657091426,-1.6207410268,-2.1264419157  
 C,-3.5512101129,-3.052275256,-0.202931584  
 H,-1.9995313318,-4.5762175499,-0.3188656971  
 C,-1.7334694767,-3.1366812671,-1.9244073489  
 H,-3.7599356556,-1.0400883341,0.6784079152  
 H,-4.3597001114,-1.1369082421,-0.9784239264  
 H,-1.1042983556,-1.113879006,-2.5643434981  
 H,-2.8204337099,-1.4066206321,-2.7712609371  
 H,-4.1660857729,-3.4601448442,-1.0146685456  
 H,-2.3511800681,-3.7058377237,-2.6257747525  
 H,0.0225690685,0.8319786906,-1.714263261  
 H,-2.4350463181,0.1527655938,-1.0129366209  
 H,-0.6634558045,4.0100568635,-0.565085293  
 H,-3.8247130549,2.9408451845,0.9471051951  
 C,-3.2464513561,3.7443229901,-1.4654322937  
 H,-4.3361375106,3.6131156447,-1.4699831616  
 H,-2.9152309822,3.8330412391,-2.5031242583  
 H,-3.0159070459,4.6677896068,-0.9267716976  
 C,-2.6328913554,2.5044117619,-0.8095765004  
 O,-2.7662187235,1.4161080517,-1.5108606247  
 H,-0.6898364681,-3.3979682158,-2.1297377325  
 C,-4.1363927778,-3.5597428164,1.1193340039  
 H,-4.1344381449,-4.6543334002,1.1485938461  
 H,-3.5719988084,-3.1971596018,1.9864442758  
 H,-5.1731730432,-3.225543326,1.2380830669  
 C,-1.723113522,4.3292905877,1.9446776171  
 H,-2.6808212498,4.7044846686,2.3219618751  
 H,-0.9572982578,4.564088476,2.6923675724  
 H,-1.4865211322,4.8969384965,1.0401659033  
 C,1.2370863417,-0.6926346602,0.9046805723  
 C,2.6057774507,-0.4630912788,0.5328973928  
 C,0.9750754098,-1.0325194227,2.2146416755  
 C,3.0350316835,-0.1358102221,-0.7726460757  
 C,3.5945558505,-0.5888320895,1.5683211989  
 C,2.0317854743,-1.1298606604,3.1541941738  
 H,-0.0319843485,-1.232883994,2.5635494518  
 C,4.3776130217,0.0643270728,-1.0599923241  
 H,2.3360611523,-0.0235508582,-1.5926762484  
 C,4.9578650149,-0.3726465282,1.2446517014  
 N,3.2944149444,-0.9152871667,2.8579228653  
 H,1.8055292461,-1.3957333493,4.1852346396  
 C,5.3519719081,-0.0529234473,-0.0335803564  
 O,4.6696269317,0.3708581549,-2.3493640578  
 H,5.6840629002,-0.4726424406,2.0446854029  
 H,6.4021275081,0.104522264,-0.2484937661

C,6.0321467357,0.5811559584,-2.7221284131  
H,6.0123359139,0.8030342492,-3.789609088  
H,6.4674775571,1.4301444715,-2.1824919792  
H,6.6363946343,-0.3166782535,-2.5484079473  
Electronic energy = -1366.2450308  
Zero-point electronic energy = -1365.626834  
Thermal energy = -1365.598034  
Enthalpy = -1365.597090  
Free energy = -1365.684496  
Free energy with quasiharmonic approximation = -1365.679846  
Frequencies = -368.1295, 24.7027, 38.5841, 43.8530, 49.3145  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9267439  
SCF (M06-2X/def2-TZVPP) = -1366.1818658  
SCF (M06-2X-D3/def2-TZVPP) = -1366.1890549

TS-1h C27H38N3O2(1+)

C,-0.5392756038,1.94859888,0.4720413919  
C,-1.4207461491,1.734928646,1.5485166792  
C,-2.9027663632,3.5690992841,0.2965694422  
C,-1.7234527948,3.8781178595,-0.6336341895  
C,-0.3861961109,3.3626795772,-0.0111718673  
H,-1.5211958556,0.7371091765,1.9598168623  
H,-2.8238988291,4.1388837705,1.2314338805  
H,-1.8906882103,3.3171195142,-1.560508147  
H,-0.1262823934,3.9962241821,0.8448617165  
H,-0.9610070758,-3.3747307461,0.9849399829  
N,-0.0864402319,0.9789647813,-0.3270573406  
C,0.1286809378,-0.4722261932,-0.0685219562  
C,-1.1297218839,-1.3437341191,0.181309786  
H,0.5440217044,-0.8285064342,-1.0137569795  
C,1.2151734284,-0.6643580727,0.9935787971  
H,-1.5369641265,-1.1410050446,1.1723238595  
C,-0.7861028147,-2.8582295771,0.0373738541  
N,-2.2682118013,-1.0242925912,-0.7510614934  
C,2.5893715793,-0.4448238737,0.6334101455  
C,0.9392201784,-1.0168109546,2.2967680736  
C,-1.6325548009,-3.4738560817,-1.0951495988  
H,0.2772085137,-2.9867679101,-0.19001686  
H,0.4253077104,3.4513881662,-0.7420135725  
C,-3.4403540041,-1.9040025829,-0.4054991478  
C,-1.905138966,-1.2320889066,-2.1919733231  
C,3.0311297167,-0.0824301365,-0.65939819  
C,3.5720307445,-0.6137200172,1.6676156811  
C,1.9915175375,-1.1502080553,3.2378535967  
H,-0.0714061886,-1.2081056178,2.6401900453  
C,-3.1404319821,-3.3837545622,-0.7610280413  
H,-1.3426755632,-4.5195424707,-1.2384560728  
C,-1.3743990896,-2.6738396672,-2.3883564545  
H,-3.625987205,-1.7724338582,0.6646237349  
H,-4.3028799485,-1.5024220079,-0.9425394733  
H,-1.1814003364,-0.4648422416,-2.4735510423  
H,-2.8149264276,-1.0388900588,-2.7645478509  
C,4.377933012,0.1004289143,-0.9384607932  
H,2.3422374952,0.0623186975,-1.4846064918  
C,4.9405475005,-0.417400872,1.3530978252  
N,3.2595684886,-0.9591790681,2.9495629034  
H,1.7563063803,-1.4273085478,4.2639260742  
H,-3.6902696709,-3.637004135,-1.6759695016  
H,-1.8799102698,-3.144637849,-3.2371157008  
C,5.3462607312,-0.0691134233,0.0857574655  
O,4.6775842777,0.441822746,-2.2173109175

H,5.661821059,-0.5535577949,2.152249547  
 H,6.4001766817,0.0721458017,-0.1218492299  
 C,6.0460347059,0.6169314297,-2.5877154103  
 H,6.6197818552,-0.3051432583,-2.4398509855  
 H,6.0316771041,0.8681297887,-3.6487716823  
 H,6.5103162564,1.4359603041,-2.0265154553  
 H,0.4042878108,1.3078053759,-1.1505653139  
 H,-2.6283894386,0.0595833789,-0.5858128248  
 H,-1.4282717473,2.5103930756,2.3081267934  
 H,-3.8331550561,3.8866159035,-0.1932457349  
 C,-4.0728143838,1.7188396006,1.6656035435  
 H,-3.9259145853,2.2882922181,2.5883021865  
 H,-4.0486602207,0.6489956986,1.8982927356  
 H,-5.0702548064,1.9501753578,1.2710714392  
 C,-3.0475708752,2.0637889036,0.5813455045  
 O,-3.0874348746,1.3346687561,-0.5038782678  
 C,-1.6074038609,5.3694769587,-0.9644107093  
 H,-1.4452459894,5.9667175018,-0.0586825711  
 H,-2.5225783345,5.7309189089,-1.4454714491  
 H,-0.7723358051,5.5621264367,-1.6477683114  
 H,-0.3033476611,-2.6657049603,-2.6194663301  
 C,-3.6074801891,-4.343298999,0.3386626929  
 H,-3.0947407468,-4.1608699897,1.2903296422  
 H,-4.6829820772,-4.2341871008,0.5182004823  
 H,-3.4229300604,-5.3831618151,0.049452917  
 Electronic energy = -1366.2569824  
 Zero-point electronic energy = -1365.638768  
 Thermal energy = -1365.610053  
 Enthalpy = -1365.609108  
 Free energy = -1365.696285  
 Free energy with quasiharmonic approximation = -1365.691762  
 Frequencies = -450.2943, 26.1465, 34.9661, 42.4469, 50.2614  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9364044  
 SCF (M06-2X/def2-TZVPP) = -1366.1920162  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1990385

TS-1i C27H38N3O2(1+)  
 C,1.6099131308,-1.9091684501,0.2064254571  
 C,2.1969537017,-2.2543487279,1.4333126789  
 C,4.1700924241,-0.858942202,0.0499995286  
 C,3.8877867573,-2.0593275601,-0.8843840491  
 C,2.3440961676,-2.284450297,-1.0483505976  
 H,1.6436658475,-2.044601579,2.3458670802  
 H,5.2512404265,-0.8045570972,0.2292750116  
 H,4.2528209182,-1.7715788936,-1.8777762615  
 H,2.1468645837,-3.3428922952,-1.2592198952  
 H,-1.689753124,2.4564595032,-0.919508688  
 N,0.6063239042,-1.0243623854,0.2286733947  
 C,0.0818358614,-0.1440188019,-0.8262984385  
 C,0.0349379845,1.3074146728,-0.2772608219  
 H,0.7984604698,-0.1651675921,-1.647905034  
 C,-1.2483844633,-0.6288494026,-1.4038049827  
 H,-0.4910711262,1.2911790026,0.6804391684  
 C,-0.6427655823,2.3390715085,-1.2104743406  
 N,1.4195380528,1.8153195684,0.074571816  
 C,-2.4399510137,-0.8310799513,-0.6289090199  
 C,-1.3022398853,-0.8928850423,-2.7563267953  
 C,0.1327691912,3.6708968796,-1.1310061037  
 H,-0.6465716333,1.9838296575,-2.2470244865  
 H,1.9710399387,-1.7304677105,-1.9126323872  
 C,1.2627413124,2.9960427971,0.9995555188

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C,2.1935594738,2.2462635573,-1.1411502835
C,-2.5587067606,-0.6101943207,0.7630716719
C,-3.6002052565,-1.2990033069,-1.3403766372
C,-2.5030857608,-1.347497884,-3.3535492967
H,-0.4248897051,-0.7581365043,-3.3841051697
C,0.3777196659,4.0925309012,0.3386816047
H,-0.4255838892,4.454500904,-1.6520377837
C,1.4998061939,3.4589416349,-1.807633158
H,0.8327254487,2.6102995266,1.9273542067
H,2.2726321127,3.3448903468,1.2261616559
H,2.2647025968,1.3891057278,-1.8137899246
H,3.2047174599,2.4748888123,-0.7969972732
C,-3.7512293319,-0.8332078904,1.4363330268
H,-1.7308534771,-0.257066817,1.3650025592
C,-4.8044730084,-1.5177086262,-0.624597605
N,-3.6150534066,-1.5476845806,-2.6813771111
H,-2.5288762565,-1.5508779279,-4.4225754946
H,0.9593005987,5.0215290844,0.3138277252
H,2.1176933012,4.3566652161,-1.7059047621
C,-4.8918220359,-1.2945113341,0.7294904478
O,-3.7340358703,-0.5834510976,2.7701241722
H,-5.6618430407,-1.8704624687,-1.1883559328
H,-5.8274186465,-1.4726086966,1.2456592513
C,-4.9223964479,-0.8001652169,3.5327773545
H,-4.6616902384,-0.542134096,4.5596887358
H,-5.7391646192,-0.1539254409,3.19146966
H,-5.2380992726,-1.8488549341,3.4902859917
H,0.2226107812,-0.8606957469,1.1525233513
H,2.019348478,1.044690934,0.6648589448
H,2.7738050596,-3.1699470711,1.4669101434
H,3.9087267917,0.0597024253,-0.4863056721
C,4.3075061291,-1.1971075791,2.6216614884
H,5.085951988,-0.4347258248,2.7524919395
H,4.7973259767,-2.1635776216,2.4709174355
H,3.711606053,-1.2284091962,3.5374943406
C,3.4385075871,-0.7791828182,1.4298083399
O,2.7332716684,0.2967874147,1.6468049573
C,4.6639063026,-3.3349188905,-0.5135501918
H,4.4361645725,-3.7148015023,0.4865120732
H,5.7406793965,-3.1360599743,-0.5471097315
H,4.4520894359,-4.1372802785,-1.2291219661
H,1.3721741627,3.2736423744,-2.8788001854
C,-0.9058780123,4.374388284,1.1296516577
H,-1.4935954703,5.1609420011,0.6441888907
H,-1.545175334,3.4886693269,1.2213578767
H,-0.6673792382,4.7145535725,2.1433909239
Electronic energy = -1366.2478643
Zero-point electronic energy = -1365.629129
Thermal energy = -1365.600340
Enthalpy = -1365.599396
Free energy = -1365.687376
Free energy with quasiharmonic approximation = -1365.681989
Frequencies = -311.9929, 15.6135, 31.4999, 40.6197, 45.5410
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9284692
SCF (M06-2X/def2-TZVPP) = -1366.1820787
SCF (M06-2X-D3/def2-TZVPP) = -1366.1892804

TS-1j C27H38N3O2(1+)
C,-0.4219652389,1.9601697188,-0.1306635379
C,-1.1757995459,2.0824496817,1.0591142752
C,-2.781138186,3.0913975041,-0.8948814597

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C,-1.5683754261,4.0328579595,-1.0454272454  
 C,-0.2439335747,3.1999778469,-0.9657275487  
 H,-1.2334381595,1.2317683703,1.7284438279  
 H,-3.7064687138,3.676783093,-0.9675494691  
 H,-1.6119462867,4.431187087,-2.0661021991  
 H,0.5560623607,3.8047743893,-0.5193837658  
 H,-1.1552190098,-3.2241108966,1.3597037014  
 N,-0.0818997604,0.8011950004,-0.6977346631  
 C,0.1016563217,-0.5620270962,-0.1204319197  
 C,-1.1922606948,-1.331464925,0.2563292263  
 H,0.5440911459,-1.1132440384,-0.9545924708  
 C,1.144087302,-0.5468804669,1.0009949159  
 H,-1.6006647696,-0.9388488713,1.1876208264  
 C,-0.908632671,-2.8597508911,0.3586623957  
 N,-2.3149641292,-1.1177306362,-0.7257542862  
 C,2.5335510479,-0.3913513792,0.6661469128  
 C,0.8123362983,-0.6647734273,2.3334190921  
 C,-1.7261179374,-3.6034137996,-0.7187204239  
 H,0.1585137231,-3.0573388672,0.2141440651  
 H,0.0958695033,2.9279691016,-1.9721186909  
 C,-3.5081405847,-1.9269747054,-0.2732453436  
 C,-1.9491141074,-1.5265018924,-2.1179850094  
 C,3.0337528701,-0.2750687991,-0.6504492916  
 C,3.4689885125,-0.3589467968,1.7564631507  
 C,1.8216807874,-0.6181640196,3.3280548431  
 H,-0.2123993363,-0.7988730302,2.6611207576  
 C,-3.2414533001,-3.441457979,-0.4533210424  
 H,-1.45437815,-4.6635743572,-0.7170938179  
 C,-1.4085517111,-2.9803450027,-2.0948802722  
 H,-3.68635863,-1.6510882541,0.7683135836  
 H,-4.3621383171,-1.5716744079,-0.8540812452  
 H,-1.2275519954,-0.8100990196,-2.5158254303  
 H,-2.8578765445,-1.43335947,-2.7169355103  
 C,4.3918218234,-0.1337547474,-0.8975075863  
 H,2.3838513334,-0.3003673328,-1.5181165201  
 C,4.8501000678,-0.2105664921,1.4727454518  
 N,3.10058326,-0.4680841126,3.0649746804  
 H,1.5415035638,-0.7081241228,4.3759869147  
 H,-3.7673506835,-3.7827539171,-1.3539812368  
 H,-1.8740522885,-3.5611791989,-2.8967694919  
 C,5.3126646897,-0.0987323718,0.1823764763  
 O,4.7502925166,-0.034045113,-2.2026576949  
 H,5.534007146,-0.1903966676,2.3149252733  
 H,6.3746473214,0.0116384002,-0.0011454506  
 C,6.1334615031,0.0979710633,-2.5344951679  
 H,6.7103798266,-0.7686829043,-2.1920554228  
 H,6.1694375609,0.1494799718,-3.6231183595  
 H,6.5594177371,1.0156275676,-2.1126702861  
 H,0.3103443391,0.8945174832,-1.6273567242  
 H,-2.6708598592,-0.0366562372,-0.5661307988  
 H,-1.0125737033,3.0175914759,1.586053821  
 H,-2.7866161412,2.4011827454,-1.7475692887  
 C,-3.624570895,2.8579678601,1.5450848661  
 H,-3.5524139064,2.2368793738,2.4426388874  
 H,-4.6825308364,2.9216617243,1.2649089352  
 H,-3.2665125886,3.8657678706,1.7718232995  
 C,-2.876048807,2.1961852347,0.3758446406  
 O,-3.3015486437,0.9715841159,0.1521228197  
 C,-1.5678245028,5.2544056676,-0.1118325692  
 H,-1.4546355451,4.9972662224,0.9458119342  
 H,-2.5043965121,5.8127097191,-0.2168917104

H,-0.7463357694,5.9311811837,-0.3724818625  
H,-0.3275676731,-2.9974419543,-2.2750911566  
C,-3.7736443892,-4.2593770956,0.7280972723  
H,-3.2844209321,-3.9877966085,1.6705750385  
H,-4.8496149933,-4.0975204023,0.857992292  
H,-3.6156171115,-5.3300751253,0.5607217939  
Electronic energy = -1366.2439952  
Zero-point electronic energy = -1365.625965  
Thermal energy = -1365.597147  
Enthalpy = -1365.596203  
Free energy = -1365.684032  
Free energy with quasiharmonic approximation = -1365.678932  
Frequencies = -429.2878, 16.3313, 35.7947, 41.3067, 49.8552  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9236949  
SCF (M06-2X/def2-TZVPP) = -1366.1798786  
SCF (M06-2X-D3/def2-TZVPP) = -1366.1869379

TS-1k C27H38N3O2(1+)  
C,-0.174855365,2.0225020539,0.1069399658  
C,-0.5300963205,3.1715024691,-0.6289660376  
C,-2.4976413115,3.4074027474,1.0789875321  
C,-1.7677379035,2.4820121567,2.0734968181  
C,-0.3095185781,2.0947591574,1.596698338  
H,-0.3708694393,3.1459016945,-1.7063232084  
H,-3.5648767292,3.4237582157,1.3373812584  
H,-1.6075618923,3.0520586388,2.9954104938  
H,0.0148290519,1.1788561413,2.0902474225  
H,-1.417497363,-3.1790161998,1.00378662  
N,0.0173628991,0.8929977151,-0.5865144984  
C,0.1531968791,-0.5354106839,-0.2160192803  
C,-1.2128303506,-1.1944909861,0.1089068508  
H,0.515300972,-0.9964661163,-1.1420628878  
H,-1.5379931963,-0.8617846964,1.0951795176  
C,-1.1796395,-2.7479737335,0.027551304  
N,-2.3044988184,-0.6983285506,-0.8146669108  
C,-2.1731054754,-3.2367922585,-1.0474280322  
H,-0.1710000448,-3.0918270989,-0.2243345864  
H,0.3688310088,2.8902268531,1.9247253653  
C,-3.6174694063,-1.3117050787,-0.3855659363  
C,-2.0572962986,-1.0479012058,-2.2590355794  
C,-3.6232924544,-2.8326183087,-0.6882646453  
H,-2.1000362683,-4.3246272284,-1.1406381794  
C,-1.804938538,-2.5677443549,-2.3858082549  
H,-3.7230731572,-1.1110746524,0.6834544611  
H,-4.4042475656,-0.7637962186,-0.9076620467  
H,-1.2231091695,-0.4462192414,-2.6218649089  
H,-2.9453254915,-0.7195246849,-2.8018707107  
H,-4.2376224279,-3.0032842587,-1.5811794066  
H,-2.4091995972,-2.9762712053,-3.2009849542  
H,0.0637321771,1.0511157296,-1.586864479  
H,-2.4068938025,0.3897314065,-0.7249082824  
H,-0.2909653474,4.1288164546,-0.1763690418  
H,-2.1366110978,4.4358012976,1.1939521382  
C,-2.8986173794,4.1412139104,-1.3412276617  
H,-2.7291167363,3.8641460864,-2.3856321714  
H,-2.4260144909,5.107564366,-1.1395053562  
H,-3.9809852391,4.2509822175,-1.196772997  
C,-2.4049563998,3.0174063396,-0.4183565271  
O,-2.8044036742,1.8311883467,-0.7814684879  
H,-0.7565506157,-2.7674345921,-2.6317251111  
C,-4.2429881942,-3.6377836496,0.4589236904

H,-3.670878883,-3.5384976835,1.3886043967  
 H,-5.2652467789,-3.3002561051,0.6632471896  
 H,-4.2894856043,-4.7013470816,0.2029934641  
 C,-2.6291202987,1.2695195253,2.4572094782  
 H,-3.0007688548,0.7539798586,1.5699723414  
 H,-2.0824163676,0.5651087086,3.0954980388  
 H,-3.5074216006,1.6041270645,3.0198358275  
 C,1.2382838333,-0.7982197561,0.8296578791  
 C,2.6117922834,-0.5453588942,0.4914706136  
 C,0.967553936,-1.3158606162,2.0784532469  
 C,3.0476299139,-0.0477636711,-0.7562861342  
 C,3.5972126498,-0.8381387883,1.4954562336  
 C,2.0221190505,-1.5637153869,2.9932476087  
 H,-0.042182927,-1.5484803916,2.3978514594  
 C,4.394842855,0.1550720208,-1.0195674565  
 H,2.3498692105,0.1965272889,-1.5481371229  
 C,4.96529912,-0.6122022794,1.199841288  
 N,3.2889401347,-1.3352230777,2.7272313337  
 H,1.7897790051,-1.9661083047,3.9775600506  
 C,5.3664925903,-0.1287814165,-0.0236297212  
 O,4.6936598248,0.6295335602,-2.2550633645  
 H,5.6891559425,-0.8398898913,1.9754283521  
 H,6.4200470895,0.0302974965,-0.2196454031  
 C,6.0621700265,0.8406264651,-2.6059250093  
 H,6.0475428616,1.2074265161,-3.6327009833  
 H,6.5297889451,1.5913012208,-1.9585152121  
 H,6.6332946943,-0.093725376,-2.5611599909  
 Electronic energy = -1366.2446778  
 Zero-point electronic energy = -1365.624688  
 Thermal energy = -1365.595969  
 Enthalpy = -1365.595025  
 Free energy = -1365.681767  
 Free energy with quasiharmonic approximation = -1365.677796  
 Frequencies = -286.9425, 24.7348, 43.5467, 46.4746, 58.7571  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9270371  
 SCF (M06-2X/def2-TZVPP) = -1366.1824849  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.18684

TS-11 C27H38N3O2(1+)  
 C,-0.2527796347,2.0006506022,-0.1936991043  
 C,-0.6697603122,3.0450746896,-1.030895362  
 C,-2.8718309025,2.5308439479,0.5863886053  
 C,-1.7569697727,3.0015765658,1.5380740867  
 C,-0.4616215015,2.1801209498,1.2839629197  
 H,-0.4849683169,2.9610129467,-2.0992277002  
 H,-3.1385240262,1.4954827506,0.8376707634  
 H,-1.543164933,4.0553047425,1.3223456201  
 H,-0.5201926834,1.2198028967,1.7984734307  
 H,-1.3482493524,-2.9393307263,1.4651136135  
 N,0.0285865152,0.8175994501,-0.7582379854  
 C,0.1604119826,-0.547387138,-0.1980720549  
 C,-1.2101165803,-1.168564137,0.1838030401  
 H,0.5402384,-1.1321356205,-1.0431353713  
 H,-1.5977317162,-0.6642080545,1.0728663163  
 C,-1.1281164697,-2.706659547,0.4199719889  
 N,-2.2570856623,-0.9017878019,-0.8717544174  
 C,-2.1085986324,-3.4314579346,-0.5232545806  
 H,-0.1100101752,-3.064122328,0.2322699141  
 H,0.4037188103,2.7038449989,1.7103303573  
 C,-3.5812304257,-1.4190071892,-0.3774803282  
 C,-1.9387892067,-1.562974963,-2.1840659765

C,-3.5633130022,-2.9681017188,-0.2703056022  
 H,-2.0298766188,-4.5118073815,-0.3663332313  
 C,-1.7301710942,-3.0817469728,-1.9747718412  
 H,-3.7625513444,-0.9457096385,0.5924950815  
 H,-4.340434035,-1.050814497,-1.0711882744  
 H,-1.0641483523,-1.069984446,-2.6120046827  
 H,-2.7808235341,-1.3392044721,-2.8422978887  
 H,-4.1767074965,-3.3749584613,-1.0836879118  
 H,-2.3488068658,-3.6450165568,-2.6801508528  
 H,0.0886502593,0.8564832716,-1.7691912633  
 H,-2.404051232,0.2337622651,-1.0910073857  
 H,-0.5960416885,4.0544436327,-0.6416540057  
 H,-3.7731291652,3.1289286313,0.7702026459  
 C,-3.1372520682,3.806576723,-1.6482185923  
 H,-4.2277561878,3.6885716868,-1.6829457649  
 H,-2.7726474524,3.8656042936,-2.6766732977  
 H,-2.9103660818,4.7409648611,-1.1259630357  
 C,-2.5602781392,2.5786326575,-0.9392359766  
 O,-2.6981393858,1.4686939077,-1.6098634906  
 H,-0.6882108955,-3.3583532806,-2.1687236819  
 C,-4.1638892746,-3.4593545166,1.0512434236  
 H,-4.1747366629,-4.5536937985,1.0885694972  
 H,-3.6013309741,-3.0970801177,1.9197668593  
 H,-5.1975521842,-3.1124273072,1.1603997246  
 C,-2.1745384213,2.9050197373,3.0093354367  
 H,-1.3671408565,3.2358016128,3.6721142196  
 H,-3.049987782,3.5317842669,3.2087145711  
 H,-2.4319889942,1.8733096064,3.2801712037  
 C,1.2280621245,-0.6426982471,0.8940083006  
 C,2.6061607586,-0.4291945366,0.5474020004  
 C,0.9355346641,-0.9542529403,2.2043683525  
 C,3.0666798326,-0.1318558712,-0.754774463  
 C,3.5711205667,-0.5381033094,1.6069936346  
 C,1.9708589933,-1.0385310015,3.1686517178  
 H,-0.0799723198,-1.1413091769,2.5357922608  
 C,4.4164150541,0.0565048318,-1.0155299862  
 H,2.3887934959,-0.0359278339,-1.5944114796  
 C,4.9424663074,-0.3352819858,1.3098189069  
 N,3.2407878107,-0.8362810895,2.8960864608  
 H,1.7206377508,-1.2822869987,4.199601611  
 C,5.3669714131,-0.0440108453,0.0345297455  
 O,4.7387817066,0.334769487,-2.3040927782  
 H,5.649876205,-0.4224147603,2.1279742175  
 H,6.4224764653,0.1034287623,-0.1602202468  
 C,6.1095204431,0.5401414631,-2.648400039  
 H,6.1149459297,0.7405185839,-3.7202926305  
 H,6.5303647009,1.400664542,-2.1155494217  
 H,6.7110022236,-0.3526621632,-2.4423098222  
 Electronic energy = -1366.2514759  
 Zero-point electronic energy = -1365.633455  
 Thermal energy = -1365.604817  
 Enthalpy = -1365.603873  
 Free energy = -1365.690561  
 Free energy with quasiharmonic approximation = -1365.686240  
 Frequencies = -439.4366, 23.4873, 37.9024, 47.0127, 53.1431  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9326835  
 SCF (M06-2X/def2-TZVPP) = -1366.1885999  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1898962  
  
 TS-1m C27H38N3O2(1+)  
 C,-2.2021593676,1.2465090833,-0.3901025345

C,-2.2544352145,0.196021814,-1.3195831734  
 C,-3.5444989397,-0.9377816445,0.8503235901  
 C,-4.3737260029,0.3115154458,0.4940421216  
 C,-3.4554707842,1.5519821159,0.3869228993  
 H,-1.3824273774,-0.0223911135,-1.9283877901  
 H,-3.177096719,-0.8389410069,1.8782120394  
 H,-4.8435350842,0.1520264564,-0.4850608178  
 H,-3.1884841509,1.9100543201,1.3903744489  
 H,3.2339812432,2.0845606289,0.2634874341  
 N,-1.0667557022,1.8014729009,0.0357278581  
 C,0.2425213987,1.8703177582,-0.6481685966  
 C,1.3359747477,1.0353834277,0.0738905769  
 H,0.1006668112,1.4664659099,-1.6483497205  
 H,1.246063575,1.2315768588,1.1456025536  
 C,2.7832557371,1.3426092182,-0.3989664984  
 N,1.121347321,-0.4555169116,-0.0499099979  
 C,3.6008013354,0.0343390206,-0.4254383058  
 H,2.7776248806,1.7874478452,-1.4010221387  
 H,-3.9923671379,2.3737236034,-0.106578376  
 C,1.9334545835,-1.1391455963,1.0206147148  
 C,1.5345867752,-0.9846786714,-1.3942858141  
 C,3.435228209,-0.7511054589,0.8979622265  
 H,4.6580490283,0.2640502808,-0.5903002878  
 C,3.0636570869,-0.8379956338,-1.5748885511  
 H,1.4988756517,-0.8439325648,1.9794244125  
 H,1.7623995682,-2.2109462672,0.8979131297  
 H,0.976872224,-0.4372434489,-2.1572326876  
 H,1.2004124775,-2.0240527413,-1.4317138905  
 H,4.0141517071,-1.6769579218,0.7984569201  
 H,3.5472137783,-1.8201592899,-1.5644507854  
 H,-1.1457238222,2.4240670883,0.8340140165  
 H,0.0348800597,-0.7679237473,0.166081973  
 H,-3.1898629675,0.075474113,-1.8552685361  
 H,-4.2037594824,-1.8143075195,0.8265892592  
 C,-2.4408472992,-2.4126812958,-0.9748585641  
 H,-2.48474236,-3.3239915171,-0.3651120164  
 H,-1.5806144012,-2.5003540617,-1.6456743358  
 H,-3.3560262854,-2.3564562148,-1.5725236539  
 C,-2.2829252597,-1.2245715054,-0.0159514551  
 O,-1.1683049956,-1.1789112459,0.66310833  
 H,3.2850000639,-0.3792461109,-2.5434387812  
 C,3.958012544,-0.0107959819,2.1353475478  
 H,3.4081355253,0.9173065618,2.3304318058  
 H,5.0159400285,0.2467095348,2.0154271835  
 H,3.8671601388,-0.6397421994,3.027672342  
 C,0.621785375,3.3480320321,-0.7511707081  
 C,0.4862105757,4.075111688,-1.9798340226  
 C,1.0454744481,4.0337408181,0.3697863415  
 C,0.0433265149,3.520521179,-3.202683564  
 C,0.8273914884,5.4731064342,-1.9446806871  
 C,1.348427349,5.414270051,0.2885618992  
 H,1.1638131326,3.5365955308,1.3294356959  
 C,-0.0581464881,4.2950658773,-4.3487258056  
 H,-0.2439660091,2.4791271248,-3.2930762342  
 C,0.7166932022,6.2357484738,-3.1348620519  
 H,1.6856663245,5.9428131313,1.1783545501  
 C,0.2864482003,5.6724027276,-4.3131102694  
 H,0.983161046,7.2862557181,-3.082081602  
 H,0.2116552852,6.2828881087,-5.2051044722  
 O,-0.4969610283,3.6536553816,-5.4616579305  
 C,-0.6425342945,4.3904829734,-6.6761896376

H,0.3167569538,4.7998791406,-7.0130743549  
H,-1.0073561251,3.6728511799,-7.4117488378  
H,-1.3723253119,5.2009120069,-6.5661240055  
N,1.2506547691,6.1162471002,-0.8198773032  
C,-5.4984840048,0.5565378044,1.5065778376  
H,-6.1795797658,-0.3001387122,1.5442917692  
H,-5.0954699798,0.7088246824,2.5151838832  
H,-6.0874169533,1.4415132628,1.2396039355  
Electronic energy = -1366.2552644  
Zero-point electronic energy = -1365.638177  
Thermal energy = -1365.609060  
Enthalpy = -1365.608116  
Free energy = -1365.697428  
Free energy with quasiharmonic approximation = -1365.691348  
Frequencies = -428.8143, 18.1932, 26.2374, 36.9631, 43.2304  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9340071  
SCF (M06-2X/def2-TZVPP) = -1366.1889642  
SCF (M06-2X-D3/def2-TZVPP) = -1366.1959043

TS-1n C27H38N3O2(1+)  
C,-0.5545802785,2.0118215526,0.6063887166  
C,-1.4677588339,1.7567927159,1.6475434763  
C,-2.9014993023,3.652981365,0.4257372949  
C,-1.6654624496,4.0571077006,-0.403577552  
C,-0.3617116005,3.451301618,0.2226056479  
H,-1.5941214743,0.7431669085,2.0102896401  
H,-2.8871130067,4.1789937891,1.388238521  
H,-1.5530307136,5.1440618965,-0.3076158995  
H,-0.1155117025,4.0071337323,1.1335200996  
H,-0.9121704467,-3.3183983136,0.9440938251  
N,-0.0894360213,1.0803674582,-0.2310854596  
C,0.132220159,-0.3808730266,-0.0356952144  
C,-1.1160457068,-1.2697159582,0.1986864023  
H,0.53493534,-0.6970841209,-0.9999220432  
C,1.2325050182,-0.6073413946,1.0051277113  
H,-1.5157912874,-1.1022747436,1.1988391828  
C,-0.7606330416,-2.7759372921,0.0071811955  
N,-2.2668854505,-0.9342662189,-0.713545092  
C,2.6062368112,-0.4113964438,0.6292420009  
C,0.9649615386,-0.9589406339,2.3104992828  
C,-1.621533033,-3.3697390966,-1.1258746847  
H,0.2993090961,-2.8875314715,-0.2436500826  
H,0.4776540556,3.5742837591,-0.4704520986  
C,-3.4312478014,-1.8282545041,-0.3766174474  
C,-1.9192434373,-1.1027869303,-2.1637009295  
C,3.04197549,-0.0534418693,-0.6673314048  
C,3.5965962598,-0.5987061407,1.6535877125  
C,2.0245611656,-1.1142387331,3.2394154477  
H,-0.0453194102,-1.1309289147,2.6646270074  
C,-3.124819152,-3.2978273109,-0.7669427207  
H,-1.3273721117,-4.4097712594,-1.2985491878  
C,-1.387210695,-2.5374754596,-2.4034273851  
H,-3.60886398,-1.7192660566,0.6974964573  
H,-4.2999298407,-1.4200219144,-0.8982798093  
H,-1.2011896622,-0.3253771319,-2.4314537622  
H,-2.8360347014,-0.8967026184,-2.7203332592  
C,4.3889826682,0.1104645357,-0.9575894033  
H,2.3501167285,0.0990217588,-1.489018566  
C,4.9648823565,-0.4219634,1.3269707533  
N,3.2923441807,-0.9429937082,2.9377111238  
H,1.7959675069,-1.390992609,4.2670891055

H,-3.6866773049,-3.5365278634,-1.6784537803  
 H,-1.9050821949,-2.9893055742,-3.2549945858  
 C,5.364115831,-0.075587583,0.0572239605  
 O,4.6824876463,0.4499820151,-2.2382817618  
 H,5.6911146187,-0.5714082593,2.119228088  
 H,6.4180510565,0.0510227741,-0.1594771984  
 C,6.0500028071,0.6097831613,-2.6189117622  
 H,6.6140297964,-0.3192199721,-2.4773056433  
 H,6.0304662034,0.863413491,-3.6792829884  
 H,6.5281103449,1.4220919039,-2.0595088727  
 H,0.4248516783,1.4477053706,-1.0233223938  
 H,-2.6302259436,0.1341152333,-0.5228411896  
 H,-1.48333221,2.4958955631,2.442652555  
 H,-3.8062442008,3.9854242731,-0.0999346773  
 C,-4.1139968157,1.8016319708,1.7407712007  
 H,-3.9627839059,2.3428040001,2.679540159  
 H,-4.1221175028,0.7257094332,1.944036585  
 H,-5.1000474041,2.0704267285,1.3414734218  
 C,-3.0673414066,2.1398749559,0.671042009  
 O,-3.1173446858,1.4133956754,-0.4148702362  
 C,-1.7832651346,3.7419549349,-1.902923332  
 H,-1.8935815885,2.6703187711,-2.0799746587  
 H,-0.9054605236,4.1149981878,-2.4447783237  
 H,-2.665321005,4.2360016894,-2.3248038106  
 H,-0.3201806477,-2.5197520147,-2.6515011209  
 C,-3.5679162338,-4.2832893134,0.3195882366  
 H,-3.0421532333,-4.1165044997,1.2669960705  
 H,-4.6413113164,-4.1859222392,0.5173706055  
 H,-3.3805099586,-5.3156043291,0.0062048416  
 Electronic energy = -1366.2524541  
 Zero-point electronic energy = -1365.634452  
 Thermal energy = -1365.605612  
 Enthalpy = -1365.604668  
 Free energy = -1365.693754  
 Free energy with quasiharmonic approximation = -1365.687433  
 Frequencies = -414.1142, 5.5859, 31.9211, 40.0821, 49.7745  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9323207  
 SCF (M06-2X/def2-TZVPP) = -1366.187358  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1945648

TS-1o C27H38N3O2(1+)  
 C,1.6491593753,-1.7450730895,1.4385369751  
 C,3.0281815289,-1.8736850682,1.8373521533  
 C,3.3628824779,-3.1620493013,-0.3324296949  
 C,1.8446758427,-3.379827193,-0.5153614792  
 C,1.0228474806,-2.9066024044,0.7472981605  
 H,3.412612976,-1.0396005462,2.4285899598  
 H,3.7832290066,-3.9724792303,0.2765910371  
 H,1.6631176291,-4.4586059294,-0.5760985849  
 H,1.0295395419,-3.7228295044,1.4802437158  
 H,-0.8711763224,3.0202870939,0.2394164703  
 N,1.1221511681,-0.5373382658,1.4902854057  
 C,0.0542277888,0.0691010855,0.6673264462  
 C,0.6160395763,1.446356578,0.2211054571  
 H,-0.0804788786,-0.5752678438,-0.2000115678  
 H,0.9607572864,1.939918129,1.1364248276  
 C,-0.351316937,2.4090852965,-0.5023718382  
 N,1.8604279605,1.2986422923,-0.6283515887  
 C,0.4718556007,3.2682747595,-1.4915759908  
 H,-1.12092213,1.8582912913,-1.0534262645  
 H,-0.0221713121,-2.7241598041,0.4854464105

C,2.6610507887,2.5654223492,-0.4898739516  
 C,1.5183661806,1.0853618721,-2.0827440986  
 C,1.7746350858,3.7988332629,-0.8399815707  
 H,-0.1340838268,4.1077736792,-1.8452180345  
 C,0.8738981505,2.3606567758,-2.6685342134  
 H,3.0297847499,2.6023296836,0.5391503788  
 H,3.5244794087,2.4629036646,-1.1503269726  
 H,0.8453690472,0.228968876,-2.132608944  
 H,2.4493517246,0.7947291515,-2.5715919751  
 H,2.3022435143,4.3750279456,-1.6086675113  
 H,1.5738236614,2.8810988152,-3.3305984533  
 H,1.6677699414,0.1305595575,2.0289036847  
 H,2.4973684885,0.405024515,-0.3342642361  
 H,3.2852705061,-2.8313659948,2.2875655541  
 H,3.8466849767,-3.2236771424,-1.3144927156  
 C,5.2711994172,-1.7405555416,0.5896974603  
 H,5.8093200762,-1.7746273784,-0.3644780391  
 H,5.6210267496,-2.5692349159,1.2157167933  
 H,5.5192527235,-0.7933053178,1.0796520976  
 C,3.7595743819,-1.79527895,0.2966889779  
 O,3.3347108875,-0.7304458992,-0.40099011  
 H,-0.0004535111,2.0910904604,-3.2693064917  
 C,1.5478859543,4.7356404208,0.3538721018  
 H,1.031976145,4.2450686635,1.1875482229  
 H,2.5036086994,5.1124230056,0.7345763074  
 H,0.9457444376,5.6003330073,0.0550678065  
 C,1.3154626429,-2.7578962466,-1.8146143545  
 H,0.2265055433,-2.8609282218,-1.8977586065  
 H,1.597245355,-1.7067164062,-1.8752358935  
 H,1.7608626592,-3.2650728331,-2.6776007289  
 C,-1.2599792198,0.2131178423,1.4254813224  
 C,-2.5172751286,-0.0650974101,0.7958122524  
 C,-1.2629983811,0.6429990882,2.7357037066  
 C,-2.6731812826,-0.5239336128,-0.5338731584  
 C,-3.6967901524,0.1409131625,1.5934706843  
 C,-2.4877160767,0.8071151192,3.4257276167  
 H,-0.3379633699,0.8521523445,3.2659076699  
 C,-3.9304323691,-0.7665053112,-1.0678616157  
 H,-1.8249273396,-0.7081482131,-1.1845987092  
 C,-4.96657718,-0.1159971119,1.0165923297  
 N,-3.6647053773,0.5725329485,2.8856458282  
 H,-2.4795615302,1.1464134839,4.4598883063  
 C,-5.0933135713,-0.5563055789,-0.2797284628  
 O,-3.955686405,-1.2032244982,-2.3521711922  
 H,-5.8403557763,0.0484332758,1.6386001721  
 H,-6.0784069877,-0.742309615,-0.6904992826  
 C,-5.2144544945,-1.4767357709,-2.9695176707  
 H,-4.9775256668,-1.8111610435,-3.9800096705  
 H,-5.7545017376,-2.2706346348,-2.440999164  
 H,-5.8378221722,-0.5766536681,-3.0213434569  
 Electronic energy = -1366.2485765  
 Zero-point electronic energy = -1365.629947  
 Thermal energy = -1365.601543  
 Enthalpy = -1365.600599  
 Free energy = -1365.686962  
 Free energy with quasiharmonic approximation = -1365.682272  
 Frequencies = -63.8093, 19.4529, 30.5398, 44.6634, 50.6621  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.9302227  
 SCF (M06-2X/def2-TZVPP) = -1366.188101  
 SCF (M06-2X-D3/def2-TZVPP) = -1366.1955928

TS-1p C27H38N3O2(1+)

C,-0.4515745877,1.915194169,0.2717502831  
C,-1.2771114336,1.8050646514,1.3962831016  
C,-2.7537005142,3.6855283281,0.0093560035  
C,-1.3325267556,4.2857735086,0.127228098  
C,-0.2534898202,3.2834400135,-0.3302789147  
H,-1.4235876757,0.8370459417,1.8597357424  
H,-1.1445936528,4.5099518267,1.1848219571  
H,0.7401171656,3.6568903404,-0.0464469205  
H,-1.1017529565,-3.3598859174,1.0574698278  
N,-0.0663584371,0.8761953273,-0.4736659995  
C,0.1019602669,-0.5581345288,-0.117388686  
C,-1.197894724,-1.3557105197,0.1754671065  
H,0.5126089617,-0.9908492758,-1.032508643  
H,-1.5710770143,-1.1030857637,1.1680751732  
C,-0.9392601996,-2.8918440849,0.0828516486  
N,-2.3332547579,-0.999968007,-0.7427021387  
C,-1.8654136408,-3.504844765,-0.9866761828  
H,0.1054635687,-3.0883024308,-0.1816069582  
H,-0.2534186179,3.196428555,-1.4255417318  
C,-3.5464653411,-1.7842601779,-0.3293352697  
C,-2.0164121344,-1.3009837664,-2.1765141306  
C,-3.3513993657,-3.2994389703,-0.6068592592  
H,-1.6495937553,-4.5732853925,-1.0862223778  
C,-1.6054931207,-2.7874511146,-2.3260951505  
H,-3.7025061859,-1.5854044501,0.7361362653  
H,-4.396483102,-1.3611362986,-0.8706156309  
H,-1.2357900615,-0.6097395626,-2.5003415839  
H,-2.9156005433,-1.056741523,-2.7471205179  
H,-3.949948383,-3.5687069232,-1.4860486747  
H,-2.1829703932,-3.2564883205,-3.1288218226  
H,0.3272911591,1.1225253764,-1.37468293  
H,-2.6353660459,0.167508665,-0.6439101709  
H,-1.2645835115,2.62568618,2.1043103867  
C,-3.9453934653,1.882913248,1.4484212992  
H,-3.7822255098,2.4653252437,2.3595395623  
H,-3.9611660278,0.8183912275,1.7003986158  
H,-4.9335883706,2.1435691631,1.0471629393  
C,-2.9143897873,2.1848723984,0.3598856154  
O,-2.9441481163,1.4162116372,-0.7002372831  
H,-0.5484206479,-2.8729846768,-2.6024517984  
C,-3.8342651676,-4.1644386028,0.5622964672  
H,-4.8940471924,-3.9789428801,0.7708001714  
H,-3.7224476793,-5.2288436618,0.329861192  
H,-3.2765272221,-3.9592203913,1.4836477394  
H,-3.0962742223,3.7729284111,-1.0280598985  
H,-3.432539972,4.2852698251,0.626701989  
C,1.1709727495,-0.7240472269,0.9668449006  
C,2.5539649611,-0.5383738878,0.6202688716  
C,0.8723028776,-1.025065707,2.2778819882  
C,3.0214972317,-0.2377997607,-0.6792842026  
C,3.5178031616,-0.6733431912,1.6772162359  
C,1.9077424326,-1.1355232559,3.2402620602  
H,-0.145541551,-1.1901771172,2.6130558072  
C,4.3742577114,-0.0734218381,-0.9404638429  
H,2.3497266036,-0.129727034,-1.5235414345  
C,4.8929424626,-0.499320311,1.3796661616  
H,1.6530270164,-1.3724852391,4.2717587914  
C,5.3233744135,-0.2051783744,0.1068150231  
H,5.5988450407,-0.6083069623,2.1965174129  
H,6.3816950694,-0.0790264768,-0.0876482973

N,3.1818425101,-0.9660627305,2.9664970034  
O,4.6995539831,0.213006138,-2.2268716127  
C,6.0738853287,0.3910293077,-2.5722005307  
H,6.0815808989,0.6036148792,-3.6417435147  
H,6.5155780631,1.2354162928,-2.030416886  
H,6.6551642483,-0.5175813155,-2.3778734958  
C,-1.214230948,5.6074340313,-0.6408142855  
H,-1.9617398189,6.3270179093,-0.2901909679  
H,-0.2253199388,6.0592075866,-0.5033575823  
H,-1.373025517,5.4569822519,-1.7154461143  
Electronic energy = -1366.2485904  
Zero-point electronic energy = -1365.632557  
Thermal energy = -1365.603335  
Enthalpy = -1365.602390  
Free energy = -1365.691238  
Free energy with quasiharmonic approximation = -1365.685947  
Frequencies = -788.8873, 18.4919, 33.8573, 40.8731, 44.3360  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.928572  
SCF (M06-2X/def2-TZVPP) = -1366.1843588  
SCF (M06-2X-D3/def2-TZVPP) = -1366.1913511

TS-2a C29H42N3O2(1+)

C,1.7381196326,-0.6130801633,-1.4508654597  
C,2.4886117285,0.4247757183,-2.0241275485  
C,4.3423644429,-0.4948433524,-0.2832411921  
C,3.4671493181,-1.728423067,-0.0079359233  
C,2.4423897028,-1.9096402394,-1.1769635621  
H,2.0093473102,1.3710856001,-2.2589168586  
H,5.0191806208,-0.3303922713,0.563069911  
H,2.8919048928,-1.525016612,0.9052099417  
H,1.7212583239,-2.6954421903,-0.9365275048  
H,-2.6674812006,1.9241185423,0.7332403078  
N,0.5539765315,-0.439852909,-0.8545158472  
C,-0.4182071969,0.652287743,-1.0426745225  
C,-0.5914012271,1.5363469457,0.2306589119  
H,-0.0305131099,1.2792039528,-1.8477282833  
C,-1.7355393617,0.0626504193,-1.5511855079  
H,-0.6238089681,0.8755947307,1.0976164836  
C,-1.8541022315,2.434342019,0.211247912  
N,0.603409209,2.4265281267,0.4985522198  
C,-2.5244849524,-0.8806857181,-0.8092401185  
C,-2.1694320129,0.4251078326,-2.8085491951  
C,-1.52226732,3.7980070588,0.8517681932  
H,-2.198768603,2.5949149174,-0.816085347  
H,2.9815948717,-2.2213614456,-2.0788476632  
C,0.538744107,2.8879137054,1.9339237128  
C,0.6384824551,3.6286021877,-0.4025845203  
C,-2.2204259177,-1.3610752197,0.4882458984  
C,-3.7103847201,-1.3774011433,-1.4544902111  
C,-3.3640257672,-0.1188306637,-3.3399886649  
H,-1.5982134953,1.127168577,-3.4097615083  
C,-0.8058635932,3.6190232897,2.2116652368  
H,-2.4425106319,4.3734811725,0.9909724215  
C,-0.571525891,4.5459873151,-0.1023372737  
H,0.6698294889,1.9980459732,2.5547445744  
H,1.4083853269,3.5307041358,2.0878709229  
H,0.6409445165,3.2743028244,-1.4353930963  
H,1.5978961839,4.1199630472,-0.2248990223  
C,-3.0308091024,-2.2906990558,1.1263670403  
H,-1.3573806387,-1.0171070148,1.0471241051  
C,-4.5191336213,-2.322656905,-0.7735863286

N,-4.1122202108,-0.9894797187,-2.6985316705  
 H,-3.6966367361,0.1806773398,-4.3321448239  
 H,-0.5706299656,4.6214849391,2.5881689471  
 H,-0.2377521384,5.4846984611,0.3513603342  
 C,-4.1980340409,-2.7783954209,0.4835317426  
 O,-2.6294177028,-2.6743710369,2.363595463  
 H,-5.407709531,-2.6774267136,-1.28538442  
 H,-4.8374609048,-3.5027391992,0.9735420047  
 C,-3.4128678961,-3.6275271495,3.0844201688  
 H,-2.8937650899,-3.7753273055,4.0318276302  
 H,-4.4226669082,-3.2482778206,3.2777940453  
 H,-3.4717179282,-4.5817073417,2.5486435033  
 H,0.1883981753,-1.2463156812,-0.3594452898  
 H,1.5737959498,1.8519427381,0.4199990666  
 H,3.2356323153,0.1254439488,-2.7520770593  
 H,4.9725654521,-0.6616229962,-1.1669546815  
 C,4.3782820798,1.9887196833,-0.9539156155  
 H,5.0942440497,2.2695615499,-0.1707404686  
 H,3.7469532696,2.8603139091,-1.1525960376  
 H,4.940126761,1.7424000841,-1.8596712864  
 C,3.5466524544,0.8142680246,-0.4274367533  
 O,2.7393492734,1.0672400648,0.5595527339  
 H,-1.0865272214,4.8016897616,-1.0335927944  
 C,-1.653739019,2.9121510643,3.2769402019  
 H,-2.5890793846,3.4554227333,3.4498518257  
 H,-1.9108904387,1.8849428713,2.9931608704  
 H,-1.1150648048,2.8649451123,4.2297650258  
 C,4.2911104975,-3.0251292579,0.2159022956  
 C,3.3967611345,-4.2535261598,0.4616146169  
 C,5.2825820171,-2.8781702649,1.3837451383  
 H,4.8727749977,-3.209506199,-0.700706767  
 H,2.769659861,-4.5028520421,-0.4003893841  
 H,4.0129526316,-5.1336192177,0.6746504138  
 H,2.7396648793,-4.094748808,1.3268761781  
 H,6.0452203724,-2.1167613059,1.1954472792  
 H,4.7603059635,-2.6116713052,2.3116778258  
 H,5.8040586861,-3.825585205,1.5580671067  
 Electronic energy = -1444.8872177  
 Zero-point electronic energy = -1444.212095  
 Thermal energy = -1444.180389  
 Enthalpy = -1444.179445  
 Free energy = -1444.274058  
 Free energy with quasiharmonic approximation = -1444.267495  
 Frequencies = -361.5337, 22.3796, 26.2626, 38.8188, 39.9997  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1445.6088117  
 SCF (B3LYP/def2-TZVPP) = -1445.4303536  
 SCF (M06-2X/def2-TZVPP) = -1444.8113499  
 SCF (M06-2X-D3/def2-TZVPP) = -1444.8193124  
  
 TS-2b C29H42N3O2(1+)  
 C,1.5079289664,-1.0292975583,1.8198152285  
 C,2.737275762,-1.0496281337,2.515262477  
 C,3.5789727884,-2.0636008209,0.2059670406  
 C,2.1229322438,-2.2852282098,-0.2335028369  
 C,1.160575478,-2.2318746731,1.0017438739  
 H,2.969536187,-0.1969901675,3.1518949649  
 H,3.9364962814,-2.9228699219,0.7850987836  
 H,1.8568937154,-1.4425310594,-0.8841245688  
 H,1.3206933789,-3.1188525624,1.6210285738  
 H,-1.1076748919,3.3258456282,-0.4135321622  
 N,0.9133398307,0.1497049936,1.6370260857

C,-0.0972881273,0.5558542191,0.6471590043  
 C,0.4240751852,1.8323950409,-0.0618382346  
 H,-0.1800184736,-0.2514946061,-0.0771655497  
 H,0.7404726274,2.5228531703,0.7265930279  
 C,-0.5785068054,2.5612742793,-0.9870131676  
 N,1.6871102929,1.5627925495,-0.8540590907  
 C,0.200515389,3.1682735001,-2.1754142706  
 H,-1.3402778582,1.8709794155,-1.3666724556  
 H,0.114029158,-2.2384388133,0.6883258275  
 C,2.413399969,2.8722035489,-1.040239203  
 C,1.384653804,0.9687690931,-2.2046163676  
 C,1.4682671887,3.9202915883,-1.6968492098  
 H,-0.4478947607,3.8520633613,-2.7311478287  
 C,0.6531772166,2.0096281036,-3.083295789  
 H,2.7656894061,3.1769606129,-0.0518877472  
 H,3.2927364424,2.652050691,-1.6488581363  
 H,0.7788797151,0.0762729459,-2.0415425192  
 H,2.3404437773,0.6468329237,-2.6237732142  
 H,1.9692082158,4.3018616436,-2.5942020119  
 H,1.3149520308,2.3807156743,-3.8727173032  
 H,1.2855988968,0.9052559857,2.2029300821  
 H,2.3902176394,0.8960010065,-0.2908215849  
 H,3.0342259248,-2.0046558589,2.9391973672  
 H,4.2112216135,-2.0024320054,-0.6902495449  
 C,5.2199140745,-0.7501846946,1.6718349118  
 H,5.9734113553,-0.7029218917,0.8755536935  
 H,5.4180487787,-1.6380379096,2.2801768129  
 H,5.3300232563,0.1461484603,2.2884756063  
 C,3.8317244643,-0.7674445097,1.0164648228  
 O,3.5100557279,0.3730717541,0.4628836212  
 H,-0.2060082033,1.5420139327,-3.5741923186  
 C,1.1845519123,5.1219811398,-0.7862251489  
 H,0.706219467,4.835556387,0.157856011  
 H,2.1155579634,5.6424155986,-0.5362901591  
 H,0.5269777183,5.8400548619,-1.2878393724  
 C,-1.4568451299,0.7993952343,1.2993286003  
 C,-2.6521837998,0.1805859764,0.8077434868  
 C,-1.5538355292,1.6382392751,2.3896937461  
 C,-2.7145282827,-0.6945768097,-0.3032704941  
 C,-3.8705466884,0.4838181553,1.5112120526  
 C,-2.8089602438,1.8682791144,3.0007703181  
 H,-0.6784217049,2.1300695894,2.8060498911  
 C,-3.9157285507,-1.2578852828,-0.7079791485  
 H,-1.8357558797,-0.9589524494,-0.8816872632  
 C,-5.0810366276,-0.1091969287,1.0708825522  
 N,-3.9305845092,1.3174037362,2.5875488873  
 H,-2.8739089317,2.5321446705,3.8609457428  
 C,-5.1154435731,-0.9599935594,-0.0085502007  
 O,-3.852609145,-2.0830365357,-1.7840977733  
 H,-5.9849712994,0.1338727293,1.6197541988  
 H,-6.0570432891,-1.3971849629,-0.3180680985  
 C,-5.0508938697,-2.700730037,-2.2560317608  
 H,-4.7502594314,-3.306551353,-3.1114244942  
 H,-5.494697034,-3.3475985052,-1.490587157  
 H,-5.7846903108,-1.9533824424,-2.5793458483  
 C,1.9264110501,-3.568051381,-1.0907582405  
 C,0.5499012638,-3.5963227865,-1.7754048941  
 C,2.1755502843,-4.8837209395,-0.3353767802  
 H,2.6822434001,-3.499666132,-1.8864118182  
 H,0.3658115315,-2.6828815536,-2.3548176741  
 H,0.4845278464,-4.4417276977,-2.4689268984

H,-0.2672804295,-3.709850058,-1.0528957224  
H,3.1582286806,-4.9102248062,0.1465570873  
H,1.4146674038,-5.0638451961,0.4335834288  
H,2.131308077,-5.7270677775,-1.0330037468  
Electronic energy = -1444.8841914  
Zero-point electronic energy = -1444.208019  
Thermal energy = -1444.176574  
Enthalpy = -1444.175630  
Free energy = -1444.268720  
Free energy with quasiharmonic approximation = -1444.263271  
Frequencies = -258.9828, 20.0764, 32.4755, 44.6909, 49.5129  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1445.6086561  
SCF (B3LYP/def2-TZVPP) = -1445.4277112  
SCF (M06-2X/def2-TZVPP) = -1444.8124344  
SCF (M06-2X-D3/def2-TZVPP) = -1444.8209362

TS-2c C29H42N3O2(1+)  
C,1.6749027529,-1.1637884152,-1.6205297468  
C,2.6325952323,-0.32058471,-2.204888918  
C,4.2819429793,-1.7080003262,-0.5934441914  
C,3.1617748003,-2.7306968164,-0.305874797  
C,2.0614794835,-2.6018824904,-1.4220408055  
H,2.3904490896,0.7192011141,-2.405129001  
H,5.0469351467,-1.7665734897,0.1894131335  
H,3.6064819591,-3.7251662498,-0.4509226188  
H,1.1909584878,-3.2186365253,-1.1823031215  
H,-1.8960291217,2.1444989391,0.9709943525  
N,0.5843841375,-0.7285328221,-0.9790889756  
C,-0.0658979766,0.5911003163,-1.0738460245  
C,0.0112125904,1.3829014964,0.2700500012  
H,0.4830199057,1.1538459929,-1.8296661837  
C,-1.4820693819,0.4121413723,-1.6232677028  
H,-0.1007044709,0.6680687433,1.0872524116  
C,-1.0316339826,2.5197165767,0.4175142589  
N,1.3821366875,1.9839904383,0.5049477724  
C,-2.5122799542,-0.3247091037,-0.9476685601  
C,-1.7702109106,0.9427867483,-2.8628125616  
C,-0.3768599197,3.7288406622,1.1164588081  
H,-1.4057239991,2.8324812057,-0.5630394128  
H,2.4752019775,-2.9783232878,-2.3626900854  
C,1.5081818516,2.326153832,1.9694008443  
C,1.6177415241,3.2236103148,-0.3127212628  
C,-2.3794111758,-0.9300340327,0.3254307226  
C,-3.7688579854,-0.4557977784,-1.6348708444  
C,-3.0505843349,0.7621393896,-3.4403758844  
H,-1.0186673159,1.498567085,-3.4169000449  
C,0.3742565044,3.298859801,2.3999794382  
H,-1.1433433517,4.4686177691,1.3669020458  
C,0.6446846884,4.3402151912,0.1382047856  
H,1.4809025785,1.3786106546,2.5128634506  
H,2.5055870697,2.7523245176,2.0985301498  
H,1.489641795,2.962141166,-1.3655537507  
H,2.6669244061,3.4916715914,-0.1690482801  
C,-3.4242667006,-1.6388925155,0.9032647124  
H,-1.4698685085,-0.8512835751,0.9105519182  
C,-4.8161537012,-1.1856097405,-1.0173489721  
N,-4.0190967465,0.0876765054,-2.8603870952  
H,-3.2641777746,1.1902547059,-4.4180845567  
H,0.8434901892,4.1982278283,2.8156617741  
H,1.194109643,5.1546557389,0.6211233768  
C,-4.6602562861,-1.7694112799,0.2180366311

O,-3.1761558808,-2.1696525039,2.1261476912  
 H,-5.7528277235,-1.2675938955,-1.5589401814  
 H,-5.4810172963,-2.3209141197,0.6604142632  
 C,-4.2036394956,-2.9171000142,2.7804788695  
 H,-3.7739792797,-3.2333750342,3.7313692377  
 H,-5.0885729459,-2.2984990294,2.9681997955  
 H,-4.4863675784,-3.8004259145,2.1966931634  
 H,0.0295053065,-1.4394510419,-0.5152533784  
 H,2.1951098117,1.2363597682,0.3169093687  
 H,3.2493687446,-0.77375967,-2.9739853675  
 H,4.7830075852,-1.9877860192,-1.5283969446  
 C,4.9094142081,0.7004836015,-1.2520772469  
 H,5.7133333077,0.7910890042,-0.5102750377  
 H,4.4983754135,1.7013078714,-1.4194697138  
 H,5.3443595085,0.3326515073,-2.1860981539  
 C,3.8414561578,-0.2354858786,-0.6738719334  
 O,3.1874674004,0.2098608975,0.3571463198  
 H,0.1345431764,4.765464148,-0.7317589124  
 C,-0.5294678161,2.7055434654,3.4878875033  
 H,-1.3152337717,3.4152655713,3.7681251628  
 H,-1.0155566503,1.776827391,3.1678047073  
 H,0.0510670302,2.4783861194,4.3888170058  
 C,2.5623229867,-2.7252050959,1.1311604486  
 C,3.6384963502,-2.5732173338,2.2179759832  
 C,1.7532951868,-4.0090483916,1.3940585566  
 H,1.8944501907,-1.8602466804,1.2208337121  
 H,4.1016209742,-1.5839472062,2.1824698055  
 H,3.1926088502,-2.6987765198,3.2114266893  
 H,4.4245603551,-3.3329780744,2.1145441449  
 H,0.9374091519,-4.1638889785,0.6786415665  
 H,2.4018376391,-4.8932808713,1.3486111814  
 H,1.3042958113,-3.9813169101,2.3932017136  
 Electronic energy = -1444.8831071  
 Zero-point electronic energy = -1444.207292  
 Thermal energy = -1444.175806  
 Enthalpy = -1444.174861  
 Free energy = -1444.268567  
 Free energy with quasiharmonic approximation = -1444.262438  
 Frequencies = -346.3838, 21.2859, 27.0156, 34.0379, 43.6891  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1445.6059162  
 SCF (B3LYP/def2-TZVPP) = -1445.4245309  
 SCF (M06-2X/def2-TZVPP) = -1444.8079732  
 SCF (M06-2X-D3/def2-TZVPP) = -1444.8165612  
  
 TS-3a C32H40N3O2(1+)  
 C,1.1927514106,-0.8010837434,-0.4690670294  
 C,1.1063530017,-0.503856739,-1.8405358811  
 C,3.6779322795,0.2102377849,-1.4946781783  
 C,3.6471554477,-0.4242758872,-0.0942634277  
 C,2.4601924096,-1.4430038522,0.0173593263  
 H,0.1945743616,-0.0666012709,-2.2384507021  
 H,4.4922996509,0.9456384685,-1.5277189551  
 H,3.4431572626,0.3870487037,0.6121378012  
 H,2.3677620591,-1.7901768021,1.0519054388  
 H,-2.7417377295,2.3760143505,1.8156708511  
 N,0.3829079151,-0.2838128301,0.4582942799  
 C,-0.9753889889,0.2728632936,0.2989642568  
 C,-1.0327559621,1.7971561579,0.598136337  
 H,-1.2659833087,0.1063942996,-0.7358456949  
 C,-1.9064180455,-0.514762583,1.2215152034  
 H,-0.4615717028,1.9740754921,1.5137099355

C,-2.4710037815,2.3605581938,0.7578654138  
 N,-0.3288855893,2.632953715,-0.4476137177  
 C,-2.8517223437,-1.464472519,0.7121771437  
 C,-1.8091677876,-0.3584628091,2.5897934958  
 C,-2.5416824842,3.7684410257,0.1312800979  
 H,-3.1996407455,1.7088946064,0.2618262242  
 H,2.6760369922,-2.3176625975,-0.6038809286  
 C,-0.0518390682,3.9947965069,0.1371144036  
 C,-1.1463827002,2.7935216994,-1.7000540888  
 C,-3.0560024677,-1.7465612719,-0.6581137417  
 C,-3.6411462729,-2.1742191953,1.6844238595  
 C,-2.6347397622,-1.1166543185,3.4541323519  
 H,-1.1096380263,0.347249283,3.0317006257  
 C,-1.37329952,4.6580578884,0.6208044327  
 H,-3.4966727796,4.2373308654,0.3873741988  
 C,-2.4241916274,3.6103537838,-1.3958661765  
 H,0.6664581281,3.8477167494,0.9477587882  
 H,0.448407562,4.5678179803,-0.6469166298  
 H,-1.3760797801,1.7965432857,-2.0818614676  
 H,-0.4955712058,3.2805943093,-2.4295342702  
 C,-3.9948576693,-2.6815209835,-1.067460092  
 H,-2.4843053688,-1.2566014203,-1.4380388916  
 C,-4.5946815603,-3.1212135459,1.2322942289  
 N,-3.521681396,-1.9910097404,3.0297677937  
 H,-2.5507270807,-0.9827767535,4.5311083292  
 H,-1.4688495487,5.6249381231,0.1127453519  
 H,-2.3776790327,4.591631149,-1.8787790296  
 C,-4.7765035852,-3.3766192242,-0.1065610156  
 O,-4.100545655,-2.8692688297,-2.4076360739  
 H,-5.1783656088,-3.6414225366,1.9846512729  
 H,-5.5134376018,-4.1069484361,-0.4190617753  
 C,-5.0352747459,-3.8290525513,-2.9018062568  
 H,-4.9341860531,-3.8041826854,-3.9872690656  
 H,-4.8025519664,-4.8362902633,-2.537622126  
 H,-6.0628045548,-3.564930458,-2.6263092868  
 H,0.6418868503,-0.4650699951,1.4228288766  
 H,0.6883842094,2.2141544579,-0.7226872942  
 H,1.5632541366,-1.22587909,-2.5099169121  
 H,3.8951522613,-0.5394250563,-2.264372599  
 C,2.2812428135,1.4119126079,-3.2915415819  
 H,3.0225934877,2.2047029653,-3.4540505483  
 H,1.2938093886,1.8315344864,-3.5074524228  
 H,2.4847228253,0.6009992437,-3.9970193088  
 C,2.3817108902,0.9686879991,-1.8292876759  
 O,2.020982075,1.836577013,-0.9285283826  
 H,-3.3017855451,3.0939266825,-1.7967163894  
 C,-1.3802275582,4.9292991817,2.1308391416  
 H,-2.320013766,5.402468169,2.4352885991  
 H,-1.2599117523,4.0140444034,2.7225217733  
 H,-0.5630940538,5.6060057338,2.4040924205  
 C,4.9597414347,-1.0808714713,0.3013075809  
 C,5.6547501897,-0.6326143324,1.4319666756  
 C,5.5075299822,-2.1368684063,-0.4426296743  
 C,6.8645213075,-1.2179458012,1.8112822096  
 H,5.2474139602,0.1874312249,2.0193738824  
 C,6.715449668,-2.7249267275,-0.067001799  
 H,4.9927541525,-2.5045009644,-1.3274658006  
 C,7.3985624741,-2.2670002137,1.0622980169  
 H,7.3881552069,-0.8527210879,2.6905595103  
 H,7.1243296112,-3.5402769262,-0.6575196592  
 H,8.3395403768,-2.7246379643,1.3543444216

Electronic energy = -1557.9985997  
Zero-point electronic energy = -1557.327692  
Thermal energy = -1557.295466  
Enthalpy = -1557.294522  
Free energy = -1557.391889  
Free energy with quasiharmonic approximation = -1557.383811  
Frequencies = -370.1742, 13.6070, 24.8700, 29.6297, 36.0746  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1558.7666378  
SCF (B3LYP/def2-TZVPP) = -1558.5806293  
SCF (M06-2X/def2-TZVPP) = -1557.9261726  
SCF (M06-2X-D3/def2-TZVPP) = -1557.9339692

TS-3b C32H40N3O2(1+)

C,1.3289760959,-0.4596693583,-2.0904604445  
C,2.2964767217,-1.2137110114,-2.7933934975  
C,3.8289461451,-0.4997844852,-0.7505177164  
C,2.7837186262,0.5528423397,-0.335885731  
C,1.7750379763,0.8424306778,-1.5062717951  
H,1.9647150794,-2.1359892181,-3.2678974707  
H,4.5167803347,-0.0733160711,-1.4898859286  
H,2.2052063067,0.1236272443,0.488250027  
H,2.2904214914,1.4077625206,-2.2877539934  
H,-2.9264176986,-2.2884700533,0.9805976467  
N,0.2242155104,-1.0841854395,-1.6855611273  
C,-0.7479168345,-0.7208407091,-0.6421008758  
C,-0.8952007989,-1.9387781881,0.3076711777  
H,-0.3346372368,0.124196251,-0.0946658212  
H,-1.0924258264,-2.8083277092,-0.3281937951  
C,-2.0104108033,-1.8435189294,1.3761687089  
N,0.4056523499,-2.2707057049,1.0095931277  
C,-1.5277441226,-2.5614904362,2.6559693117  
H,-2.2465490901,-0.7998504124,1.610605146  
H,0.9500181506,1.4640462334,-1.1497309716  
C,0.3460640056,-3.7111811062,1.4568166585  
C,0.6358925276,-1.3918471203,2.2103310539  
C,-0.9208073676,-3.9492156125,2.3294616637  
H,-2.3643212875,-2.6783427945,3.3510714765  
C,-0.4238658521,-1.6974248744,3.2938668775  
H,0.3609670046,-4.3204042688,0.5496133611  
H,1.2751903785,-3.9038499757,1.9973335926  
H,0.589479807,-0.3546685445,1.8737493045  
H,1.6587255571,-1.5829835053,2.5419384124  
H,-0.5913073935,-4.3855102934,3.2797210915  
H,0.0312174201,-2.2243593042,4.1385915054  
H,0.0715837791,-1.9929498618,-2.1108420728  
H,1.2816666373,-2.1981228818,0.3145297943  
H,3.0037196173,-0.6461455514,-3.3913203906  
H,4.4336051751,-0.7535185562,0.1297485155  
C,4.3037183296,-2.7081327063,-1.9588066569  
H,5.0017767942,-3.04329958,-1.1817140675  
H,4.8752575727,-2.1864720903,-2.7327963968  
H,3.8335855751,-3.5962662225,-2.3902693373  
C,3.238117245,-1.8236863202,-1.2963604814  
O,2.4224870743,-2.493209667,-0.5224183507  
H,-0.839398191,-0.7619756738,3.6810465717  
C,-1.9101726381,-4.9337046481,1.6926624187  
H,-2.276135827,-4.5933877583,0.7168929895  
H,-1.4382727069,-5.9109349903,1.5436021533  
H,-2.7801711128,-5.0797461667,2.3418446918  
C,-2.09431051,-0.3296137776,-1.2500913401  
C,-2.7973262516,0.8496807325,-0.8405838646

C,-2.6617758154,-1.1260205542,-2.2224454717  
 C,-2.3508242878,1.755391878,0.150843181  
 C,-4.048246921,1.115615342,-1.5002250559  
 C,-3.904858447,-0.7711689634,-2.7971315254  
 H,-2.1660126846,-2.0266359699,-2.5750440666  
 C,-3.0892598654,2.8827042536,0.4797900963  
 H,-1.4233944083,1.6059444055,0.6926303048  
 C,-4.7767217174,2.2783845639,-1.1420890824  
 N,-4.5801128239,0.3068311048,-2.4594320229  
 H,-4.3432815699,-1.4070600491,-3.5640062778  
 C,-4.3189845425,3.1472803109,-0.1798763003  
 O,-2.5633935576,3.6776289399,1.4458658148  
 H,-5.7149730951,2.4585447769,-1.6565774054  
 H,-4.9002891129,4.0268121973,0.0694603967  
 C,-3.2620822158,4.8646799161,1.8238837591  
 H,-2.6537206854,5.3268567745,2.6019222025  
 H,-3.3591401833,5.5564269338,0.9793536403  
 H,-4.2543898129,4.6327401272,2.2274155698  
 C,3.404155692,1.8465829364,0.1696293263  
 C,4.2182922394,2.637388645,-0.6552422881  
 C,3.1718669146,2.2757734781,1.4824288165  
 C,4.7835304277,3.820170339,-0.1793517108  
 H,4.4200520692,2.3303145469,-1.6788201516  
 C,3.7366375504,3.4588871569,1.9636463623  
 H,2.5454051776,1.6767612989,2.1404989352  
 C,4.5446187093,4.2354201572,1.1329085214  
 H,5.4125653556,4.4171466205,-0.8338182578  
 H,3.5449564664,3.7712488065,2.9864754678  
 H,4.9860434048,5.1561256057,1.503452071  
 Electronic energy = -1557.9947696  
 Zero-point electronic energy = -1557.322770  
 Thermal energy = -1557.290846  
 Enthalpy = -1557.289902  
 Free energy = -1557.386080  
 Free energy with quasiharmonic approximation = -1557.378527  
 Frequencies = -249.3140, 14.8196, 18.7222, 23.3819, 38.4965  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1558.7657564  
 SCF (B3LYP/def2-TZVPP) = -1558.5771102  
 SCF (M06-2X/def2-TZVPP) = -1557.9261738  
 SCF (M06-2X-D3/def2-TZVPP) = -1557.9346758  
  
 TS-3c C32H40N3O2(1+)  
 C,-1.4423272645,0.4421178472,-2.1120723865  
 C,-2.4559155651,-0.4572213106,-2.472900054  
 C,-3.9818645931,1.4955463473,-1.3190701397  
 C,-2.7832773408,2.4682555713,-1.4121179538  
 C,-1.6982394604,1.8914780678,-2.3973879229  
 H,-2.3191624156,-1.525032432,-2.3268263324  
 H,-4.6663337635,1.8404462914,-0.5334507798  
 H,-3.1657846683,3.3581994325,-1.9274557043  
 H,-0.7815472583,2.4848309647,-2.3366117431  
 H,1.812278809,-2.162572896,1.4952623755  
 N,-0.4252168198,0.151742605,-1.2931137813  
 C,0.1486101822,-1.1722376504,-0.9904304533  
 C,-0.0235064765,-1.5605210631,0.5104460255  
 H,-0.4051254496,-1.8925157835,-1.5939421896  
 C,1.5920667615,-1.219374462,-1.4939467621  
 H,0.0820871407,-0.6530818377,1.1059744701  
 C,0.9515581854,-2.6471992293,1.027843921  
 N,-1.4319197966,-2.0297683528,0.8195979899  
 C,2.6453304336,-0.3917220536,-0.9774509622

C,1.8875536423,-2.0710954489,-2.537264051  
 C,0.2077849092,-3.5756624087,2.0105913132  
 H,1.3444244776,-3.2438401279,0.1980738099  
 H,-2.0789577239,1.9750619559,-3.4196652287  
 C,-1.651090801,-1.933682195,2.3109468093  
 C,-1.6793043661,-3.4435737736,0.3689136926  
 C,2.5077311162,0.5336888602,0.0848577425  
 C,3.9344335605,-0.5243646739,-1.6019452446  
 C,3.1980881443,-2.1238771026,-3.0712094134  
 H,1.1193215793,-2.7080218222,-2.9675114007  
 C,-0.5746656152,-2.7602243999,3.0690311851  
 H,0.9249294209,-4.2357615299,2.5079180676  
 C,-0.8012544932,-4.4110810882,1.1980032597  
 H,-1.6235812391,-0.869705439,2.5589889672  
 H,-2.6669668291,-2.2907600074,2.4935675116  
 H,-1.4579119429,-3.4984890025,-0.6990495766  
 H,-2.7491137015,-3.6262862074,0.4910481119  
 C,3.5812673825,1.2983410595,0.5222874705  
 H,1.5706376191,0.6766998561,0.611130884  
 C,5.0097123702,0.2715902754,-1.1320786822  
 N,4.1908483651,-1.3826416322,-2.6302302797  
 H,3.41674449,-2.8036804336,-3.8927107844  
 H,-1.0966002765,-3.4792682903,3.7110143024  
 H,-1.4221938432,-5.0148828821,1.8674569345  
 C,4.8507088087,1.1641135844,-0.0981049702  
 O,3.3263292268,2.144304178,1.5504760279  
 H,5.9706893575,0.1492862944,-1.6209239259  
 H,5.6940941373,1.755960398,0.2366629797  
 C,4.3813173856,2.9660057014,2.0532546072  
 H,3.9369428846,3.5505713878,2.859290946  
 H,5.2026732862,2.3601725804,2.4526479629  
 H,4.7629412815,3.6427413673,1.2802601905  
 H,0.1447166784,0.9385111949,-1.000626255  
 H,-2.1798734815,-1.349536927,0.3808336711  
 H,-3.0082172809,-0.2090012994,-3.3733711493  
 H,-4.5371551299,1.5652464787,-2.2620893661  
 C,-4.8720257943,-0.9130678515,-1.4236865743  
 H,-5.7055880617,-0.7038961648,-0.7406629756  
 H,-4.5908626878,-1.9622035035,-1.2910828738  
 H,-5.2223480021,-0.7590882713,-2.4484218977  
 C,-3.7043138507,0.0017468265,-1.0312264156  
 O,-3.1281887324,-0.2740609552,0.0943620896  
 H,-0.2782312828,-5.1029025149,0.5306531089  
 C,0.3117059883,-1.8922919144,3.9714771221  
 H,1.0512891381,-2.5079917558,4.494635917  
 H,0.8536610251,-1.1218460671,3.4110130198  
 H,-0.2932928555,-1.3827023523,4.7294592349  
 C,-2.1642720142,2.9935498458,-0.1146431561  
 C,-2.3976703123,2.4492096599,1.155424559  
 C,-1.338706562,4.1287673277,-0.2040766166  
 C,-1.8156329244,3.0185436445,2.2930538803  
 H,-3.018192872,1.5663599679,1.2490540012  
 C,-0.7510996355,4.6920143083,0.9273331367  
 H,-1.1641318517,4.5896995911,-1.1748780275  
 C,-0.9883999626,4.1359277813,2.1866894963  
 H,-2.0177799105,2.5846106188,3.2693635137  
 H,-0.1209542632,5.5716385923,0.8269330947  
 H,-0.5412886164,4.5763246499,3.0736526266  
 Electronic energy = -1557.9917312  
 Zero-point electronic energy = -1557.319275  
 Thermal energy = -1557.287319

Enthalpy = -1557.286374  
Free energy = -1557.382099  
Free energy with quasiharmonic approximation = -1557.374704  
Frequencies = -311.4020, 18.9769, 23.0973, 29.7005, 42.9665  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1558.7630049  
SCF (B3LYP/def2-TZVPP) = -1558.5714653  
SCF (M06-2X/def2-TZVPP) = -1557.9204763  
SCF (M06-2X-D3/def2-TZVPP) = -1557.9298523

TS-13a C17H31N2O1(1+)  
C,2.3105861338,-1.2208084499,-0.6159533453  
C,2.4002217437,-0.0374916886,-1.36782013  
C,3.6374905149,0.8541061376,0.8528126975  
C,3.6747107488,-0.5831228109,1.3863214034  
C,3.4998784943,-1.6032006212,0.2164851851  
H,1.5700404636,0.2554124397,-2.0048987143  
H,3.7296054178,1.5487639097,1.6990138843  
H,2.8158555355,-0.7013375065,2.0576645012  
H,3.3987516408,-2.6179381493,0.6181247683  
H,-3.0574074439,-2.2059790016,-0.1791541382  
N,1.1628964217,-1.8541144386,-0.360530325  
C,-0.1323566323,-1.6920299498,-1.0172199463  
C,-1.225389363,-1.0373492881,-0.1510367408  
H,0.0098508708,-1.1647478427,-1.9620953988  
H,-1.1216055963,-1.4314659517,0.8640909966  
C,-2.6491889239,-1.3279996732,-0.6877738458  
N,-1.0813807066,0.4579138685,0.009538544  
C,-3.5319874845,-0.0798832752,-0.4846295754  
H,-2.6130878204,-1.5715346632,-1.7571822563  
H,4.3980770058,-1.5841976313,-0.4108878886  
C,-1.931163759,0.8918283608,1.1766568656  
C,-1.5110889818,1.2069660545,-1.2203956314  
C,-3.4107056124,0.4592956229,0.9618038702  
H,-4.5764410855,-0.3223419612,-0.7028939217  
C,-3.02985958,1.0123502351,-1.448903492  
H,-1.4877605604,0.4451079042,2.0702696223  
H,-1.8168008282,1.9751149675,1.2562116931  
H,-0.9150435308,0.8418607733,-2.059516433  
H,-1.2383190859,2.2524368716,-1.0586134907  
H,-4.0338729779,1.3592082136,1.0210939963  
H,-3.5669630043,1.9494750519,-1.2706472551  
H,1.2048896581,-2.5985705148,0.327278863  
H,-0.0145637394,0.7276282592,0.2832104259  
H,3.3720077209,0.17272653,-1.8028200476  
H,4.4932464403,1.0438318735,0.1919063826  
C,2.3436590766,2.5336500243,-0.6123645737  
H,3.2087870657,2.6308033665,-1.2746865497  
H,2.3857423357,3.3410852161,0.1299268478  
H,1.4297148027,2.6696946474,-1.1989188407  
C,2.3175947823,1.2032655281,0.1443685844  
O,1.251351432,0.9493341349,0.8445222195  
H,-3.2182775899,0.7245896326,-2.4878847901  
C,-3.905068897,-0.5145461417,2.0393035665  
H,-3.3127383879,-1.4364433904,2.076591848  
H,-3.8516706901,-0.0507666838,3.0303849534  
H,-4.9485761406,-0.7943382298,1.8587364772  
H,-0.4948359352,-2.6939822622,-1.2714651643  
C,4.9607736256,-0.8854127636,2.1626640385  
H,5.0664604393,-0.2059971152,3.0152904123  
H,4.9606808511,-1.9107307659,2.550063653  
H,5.8464138253,-0.7660276029,1.5264991649

Electronic energy = -851.0159161  
Zero-point electronic energy = -850.546460  
Thermal energy = -850.527426  
Enthalpy = -850.526482  
Free energy = -850.591679  
Free energy with quasiharmonic approximation = -850.590192  
Frequencies = -363.5775, 43.9404, 61.2955, 75.5114, 101.1248  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -851.4501479

TS-13b C17H31N2O1(1+)  
C,-2.2657901745,-0.9872147869,-1.0416852606  
C,-3.1105899377,0.11846034,-1.2988202208  
C,-3.0967108399,0.3087636689,1.3388920748  
C,-2.4861718885,-1.094691872,1.4466282207  
C,-2.6379236054,-1.8787624853,0.1004075045  
H,-2.8675884071,0.7412927868,-2.1589155914  
H,-4.1901817239,0.2307583909,1.2802995882  
H,-3.6898762766,-2.1601857564,-0.0197264814  
H,3.2082562113,-1.2288148878,-1.6524115755  
N,-1.0485308617,-0.9808978998,-1.5800469789  
C,0.1772137717,-1.6585344416,-1.1617566998  
C,1.2792982559,-0.631482089,-0.8608677854  
H,-0.0292366746,-2.3030404995,-0.3063972458  
H,1.2909964219,0.0810692363,-1.6922138234  
C,2.6880249014,-1.2433575689,-0.6909394157  
N,0.9729145794,0.2159281145,0.3528423488  
C,3.4479386273,-0.441110508,0.3888862592  
H,2.6186510352,-2.2943406283,-0.384794198  
H,-2.0570587732,-2.8047528244,0.1284541316  
C,1.8215454527,1.4614490502,0.2819560376  
C,1.2761375175,-0.5157521077,1.6327186522  
C,3.3251158002,1.0839237028,0.1422121895  
H,4.5023865593,-0.7322913243,0.3964052878  
C,2.8009285817,-0.7524184271,1.7520361353  
H,1.4487945146,2.0423236349,-0.5646895222  
H,1.6122773038,2.0291034699,1.191071636  
H,0.7206263539,-1.4550696281,1.619802285  
H,0.8738090716,0.0944567549,2.444090789  
H,3.8686817215,1.5815493358,0.9537380965  
H,3.2292138066,-0.1110557409,2.5291376254  
H,-0.9104681063,-0.2846707808,-2.3061297067  
H,-0.0970151314,0.5722302868,0.3181881426  
H,-4.1764625673,-0.0508103163,-1.1738317269  
H,-2.8688935708,0.8654845025,2.2577985327  
C,-3.3937401249,2.4295525482,-0.0706632798  
H,-3.2512243781,3.0876066147,0.7955741391  
H,-4.464703675,2.233059888,-0.1816658839  
H,-3.0275634417,2.9582276921,-0.9552053042  
C,-2.5695690679,1.1547259666,0.1548571682  
O,-1.2764929549,1.3606002812,0.0869440814  
H,2.9934350935,-1.7891125893,2.0454541726  
C,3.9414227631,1.5605607022,-1.1793541266  
H,3.4469730543,1.1275741838,-2.0566304061  
H,3.8693446414,2.6502042658,-1.2664298666  
H,5.0023887792,1.2926232933,-1.2289633045  
H,-1.4143337327,-0.9756503508,1.6421290449  
H,0.5341920583,-2.3010271616,-1.974863737  
C,-3.0894216847,-1.9082365375,2.5974696774  
H,-2.6286870807,-2.9001949609,2.6707187753  
H,-2.9402146311,-1.3964581428,3.5541067299  
H,-4.1677351969,-2.0474715649,2.4565760753

Electronic energy = -851.0110948  
Zero-point electronic energy = -850.541486  
Thermal energy = -850.522457  
Enthalpy = -850.521513  
Free energy = -850.586653  
Free energy with quasiharmonic approximation = -850.585070  
Frequencies = -248.9716, 37.2509, 63.4273, 77.7946, 110.0739  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -851.4470851

TS-13c C17H31N2O1(1+)  
C,2.3296232734,-1.1993427692,-0.6086800715  
C,2.3962117484,-0.0036127556,-1.3398383346  
C,3.650646448,0.8519438139,0.9003694256  
C,3.7871110925,-0.6107572577,1.3695388592  
C,3.5504669519,-1.5934842455,0.1710779379  
H,1.5517660912,0.3010359972,-1.9516380639  
H,3.7285127125,1.5141401963,1.773232038  
H,4.8347955142,-0.7590192109,1.6595530646  
H,3.475127206,-2.621292046,0.5429329612  
H,-3.0299231849,-2.2157911853,-0.0732639431  
N,1.1924827764,-1.8489119531,-0.3420489861  
C,-0.1134577319,-1.6996486663,-0.9804940912  
C,-1.2019559806,-1.0397141785,-0.1120729564  
H,0.0109428365,-1.1869552393,-1.9363978582  
H,-1.0774423446,-1.4081659201,0.9102464673  
C,-2.6293598735,-1.3603381878,-0.6245939672  
N,-1.0760240154,0.4614870351,0.0111030435  
C,-3.5190367358,-0.1098410605,-0.4724701389  
H,-2.5987494749,-1.6549813214,-1.6814415646  
H,4.4143267965,-1.5487908996,-0.499710977  
C,-1.9308112518,0.9207531386,1.1642505529  
C,-1.5070352728,1.1743202758,-1.2399160583  
C,-3.4081819029,0.4808933672,0.955027242  
H,-4.5608246251,-0.3666383019,-0.6870332351  
C,-3.0210234157,0.949537458,-1.4747356549  
H,-1.4890687644,0.4966045627,2.0693786854  
H,-1.8174714347,2.0058832613,1.2177670742  
H,-0.899377789,0.7966700926,-2.0644451227  
H,-1.2498813674,2.2269563678,-1.1003501979  
H,-4.0324891696,1.3816130625,0.9793621603  
H,-3.5726092687,1.8856181464,-1.3418973087  
H,1.2581230788,-2.6071190295,0.3277891933  
H,-0.0203157103,0.7441386286,0.2841155069  
H,3.3582911272,0.2233217143,-1.7877190284  
H,4.4906615193,1.1034841735,0.2414672903  
C,2.3776025301,2.55557914,-0.5474313497  
H,3.2423141636,2.6493802213,-1.2107504123  
H,2.4326967406,3.3532349132,0.204679157  
H,1.4634311737,2.7120461044,-1.1291282385  
C,2.3282214935,1.2155687102,0.1960411937  
O,1.2458722505,0.9755264129,0.8730512421  
H,-3.1946541365,0.616512653,-2.5026352927  
C,-3.9062238496,-0.4547812731,2.0638013829  
H,-3.308829836,-1.3709976417,2.1385194088  
H,-3.8617596779,0.0454046286,3.0374399625  
H,-4.9471942443,-0.7464348014,1.8870944265  
H,-0.4723225499,-2.7078259287,-1.2143564953  
C,2.9228011643,-0.9614325225,2.5907482904  
H,3.1048084761,-1.9958568262,2.907577625  
H,3.1778534579,-0.309402187,3.4332700611  
H,1.8593412249,-0.8261782067,2.3840569045

Electronic energy = -851.0117775  
Zero-point electronic energy = -850.542231  
Thermal energy = -850.523170  
Enthalpy = -850.522226  
Free energy = -850.587703  
Free energy with quasiharmonic approximation = -850.585868  
Frequencies = -343.3320, 38.6427, 52.6235, 76.1163, 90.5589  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -851.4464642

TS-13d C17H31N2O1(1+)  
C,-2.2308291641,-1.0581710896,-0.9198838667  
C,-3.0622195116,0.0083607835,-1.301954995  
C,-2.6558184468,0.4469873715,1.3976184043  
C,-3.3674970566,-0.9163067954,1.3065300982  
C,-2.6275169898,-1.8403197801,0.3007783693  
H,-2.8137757758,0.5494745328,-2.2120867099  
H,-3.2303034196,1.0986450253,2.0675001511  
H,-4.3834261302,-0.749975431,0.9276979571  
H,-3.2859527975,-2.6650869012,-0.0020350282  
H,2.5860568582,-2.3698902279,-0.1027124545  
N,-1.0182530438,-1.1397948962,-1.475746517  
C,0.2130985355,-1.7682197311,-1.002146194  
C,1.3278595287,-0.7271313358,-0.8196293313  
H,0.019663693,-2.3208958065,-0.0831910555  
H,1.3925396815,-0.1510211974,-1.7489037737  
C,2.7070830003,-1.3544778492,-0.5004375546  
N,1.0020359173,0.3033613291,0.2359397942  
C,3.4236994716,-0.4767506255,0.5467969156  
H,3.2894633713,-1.4454439864,-1.4215697955  
H,-1.7632909606,-2.3028539197,0.7880155558  
C,1.9319202739,1.4750476602,0.0538501228  
C,1.1699321656,-0.2442018547,1.6242112147  
C,3.4168123864,1.0129790229,0.1226792337  
H,4.4546662095,-0.8201078062,0.6753843731  
C,2.6563582899,-0.6001649685,1.877166858  
H,1.6780605343,1.9287575405,-0.9077619694  
H,1.6780168556,2.1949154488,0.8351155788  
H,0.5176406355,-1.1138278496,1.7245772388  
H,0.7984949472,0.5220673917,2.30837968  
H,3.9064442148,1.575667145,0.9263069384  
H,3.0884732751,0.0725100999,2.6248335555  
H,-0.8897707173,-0.5459399139,-2.2894887191  
H,-0.0664039078,0.7372741078,0.0818407698  
H,-4.1271384353,-0.0985913167,-1.1256752214  
H,-1.6782273083,0.3058431652,1.8758200255  
C,-3.3852290301,2.3698540395,-0.1723180414  
H,-3.2507883929,2.7935885349,-1.1708528717  
H,-3.1501826738,3.1521828539,0.5604516235  
H,-4.4310045103,2.0768723423,-0.0381209047  
C,-2.4122891695,1.2080220781,0.057056133  
O,-1.1736536393,1.4973287134,-0.2432469075  
H,2.7355852283,-1.6172491542,2.2738716292  
C,4.1845963137,1.2993547968,-1.1738251155  
H,5.2254727679,0.9688101769,-1.0891561247  
H,3.7422193085,0.7962808968,-2.0416269855  
H,4.1927334845,2.3738642972,-1.3869827657  
H,0.5588531607,-2.4952369601,-1.746087251  
C,-3.4942039576,-1.5957680447,2.6741054968  
H,-4.0692017497,-0.9726728584,3.3670396407  
H,-4.0049622406,-2.5616190861,2.5896924182  
H,-2.50861476,-1.7733240979,3.1219423074

Electronic energy = -851.0060927  
Zero-point electronic energy = -850.536927  
Thermal energy = -850.518064  
Enthalpy = -850.517120  
Free energy = -850.581581  
Free energy with quasiharmonic approximation = -850.580395  
Frequencies = -395.6444, 48.2847, 66.7456, 87.0887, 105.3261  
SCF (B3LYP-D3(BJ)/def2-TZVPP) = -851.4416962

Enamine formation TS-a C27H38N3O2(1+)  
C,2.2065753611,0.5310518507,-0.387576525  
C,0.9602944601,-0.1678162213,0.0934083439  
C,0.3979177726,-1.2507747086,-0.6179835177  
H,2.0655737485,0.7456160569,-1.4544387709  
H,2.3248466414,1.4963929305,0.1210878787  
H,-0.9169714695,-0.7567071333,-0.8085619294  
H,0.9631235312,-1.5813353253,-1.485535666  
H,0.036365094,-2.0871416869,-0.0134612695  
N,0.3592183218,0.3486929602,1.1691478172  
C,-2.8683036949,-1.7361945696,-0.2941993795  
C,-4.3654609026,-1.4848376658,0.0100606002  
H,-2.7163571304,-2.3309261695,-1.1988226174  
N,-2.1541220438,-0.4356726422,-0.5049556275  
C,-4.5462157104,0.0194916657,0.2861067748  
H,-4.6781139542,-2.0774058202,0.8756509103  
H,-4.9892039242,-1.7942816998,-0.8352713938  
C,-2.1115060237,0.3955290729,0.7679394861  
C,-2.8713633635,0.3566099031,-1.5503581714  
C,-3.5319552354,0.4179284166,1.3807733431  
H,-5.5644359712,0.2205415515,0.6331386853  
C,-4.2844803142,0.7830418089,-1.0376172318  
H,-1.8585914322,1.3980309077,0.4190283713  
C,-0.9606875569,-0.0627071801,1.7140849965  
H,-2.2464906519,1.221798568,-1.7937329932  
H,-2.9305448389,-0.2714497725,-2.4432360472  
H,-3.7357412788,1.4117366596,1.7882872255  
H,-3.6102138756,-0.2847326432,2.2182738765  
H,-5.024270931,0.4266505878,-1.7644354173  
C,-4.4475523786,2.3044029612,-0.9270678561  
H,-5.4546063223,2.5608562839,-0.5801992371  
H,-4.3017605641,2.7797545644,-1.9036575918  
H,-3.7312564819,2.756128009,-0.2307473767  
H,-2.3708479449,-2.263023439,0.5237656008  
H,-0.9615627291,-1.1556258626,1.7685109708  
H,0.8104115719,1.1272189895,1.6353614549  
C,3.4880872043,-0.3248002002,-0.2105996231  
H,3.343228898,-1.2694792752,-0.7466378808  
C,4.6813569106,0.3908121046,-0.8613288668  
H,4.4038873028,0.7901590779,-1.849303966  
H,4.9920290186,1.2644404745,-0.2710866939  
C,7.1890626635,0.1790783516,-1.4581070962  
H,7.5825550803,0.7030524831,-0.5773269756  
H,7.9245028519,-0.5544478023,-1.7939627425  
H,7.0309650739,0.9361044374,-2.2349776041  
C,5.8916519661,-0.5142275759,-1.0958890392  
O,5.8090410387,-1.7267643229,-1.0106878114  
C,3.7613161828,-0.6475657295,1.2653614652  
H,4.6644727854,-1.255899175,1.3602496084  
H,3.9029831491,0.2694240668,1.8524869463  
H,2.9375275335,-1.2130069059,1.7152458607  
C,-1.0930140298,0.4348542222,3.1486441026

C,-1.0285245347,1.8212689844,3.5187373802  
 C,-1.2689609656,-0.4970060292,4.14944438  
 C,-0.8490343071,2.8985491765,2.6168687462  
 C,-1.1512878234,2.1208857285,4.9203976466  
 C,-1.3873516185,-0.0859264485,5.4993422881  
 H,-1.3135140264,-1.5572697592,3.9163176038  
 C,-0.7918733573,4.2125384268,3.0616170693  
 H,-0.7579030196,2.7429659183,1.5483280511  
 C,-1.0889146868,3.4735260789,5.3412107724  
 H,-1.5283268334,-0.832834364,6.2782948359  
 C,-0.9128839204,4.5024072042,4.4456174801  
 H,-1.1859017052,3.669702091,6.403982943  
 H,-0.8696575201,5.5245528929,4.80223122  
 N,-1.330116194,1.1710184137,5.8821520619  
 O,-0.6181906304,5.1555272062,2.1015187353  
 C,-0.5651488395,6.5320321815,2.480930275  
 H,-0.4308234622,7.0863679471,1.551554343  
 H,-1.4972194846,6.8490802449,2.962271633  
 H,0.2817794711,6.7294669967,3.147880275  
 Electronic energy = -1366.25502618  
 Zero-point electronic energy = -1365.64199  
 Thermal energy = -1365.61137  
 Enthalpy = -1365.61043  
 Free energy = -1365.70466  
 Free energy with quasiharmonic approximation = -1365.697240  
 Frequencies = -1396.7272, 20.0713, 24.3697, 32.4336, 33.8299, 39.4456  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.92625911

Enamine formation TS-b C27H38N3O2(1+)  
 C,-1.9395228225,1.4476185992,-0.0613272675  
 C,-0.8995800042,0.3592663999,0.0345356569  
 C,-0.4635038342,-0.1471621539,1.2789821503  
 H,-1.605896183,2.2671121594,0.5884386763  
 H,-1.9818336017,1.8516503948,-1.0814147956  
 H,0.9221525982,0.0976777444,1.1641868776  
 H,-0.9853207875,0.2380472251,2.1509255598  
 H,-0.3094769642,-1.228543474,1.3278126676  
 N,-0.3296918547,-0.0288366294,-1.110715911  
 C,2.6507785304,-1.3205391206,1.4181368211  
 C,4.1407019162,-1.5648488593,1.0759587363  
 H,2.4782961401,-1.2040290334,2.4912407475  
 N,2.166006749,-0.0644982387,0.760843435  
 C,4.5216136941,-0.6160246979,-0.0760168171  
 H,4.292169279,-2.6090158593,0.7844387027  
 H,4.7754152643,-1.3781506372,1.9488131865  
 C,2.1420375022,-0.1991814997,-0.7535526121  
 C,3.0851255927,1.0611216028,1.1113637327  
 C,3.4861852841,-0.8167202754,-1.2062172667  
 H,5.5245601779,-0.851521038,-0.4449987376  
 C,4.492013891,0.834605891,0.470868785  
 H,2.0853685131,0.8307333659,-1.1096008829  
 C,0.850761721,-0.9222438714,-1.2428367799  
 H,2.6200374503,1.9882075021,0.7615437704  
 H,3.1326078678,1.1053668021,2.2026949243  
 H,3.8038822607,-0.3503462499,-2.142782825  
 H,3.3785461629,-1.8882400613,-1.4111546499  
 H,5.236079564,0.8887268975,1.2745892648  
 C,4.8588311247,1.9040669031,-0.5659577315  
 H,5.8544585365,1.7143875228,-0.9818280955  
 H,4.8750984739,2.8981149519,-0.1051633311  
 H,4.151270394,1.9411703194,-1.4024468475

H,2.0176661432,-2.1432283414,1.0767117681  
 H,0.6718215832,-1.7932900298,-0.6049907623  
 H,-0.6760040027,0.3747329219,-1.9730364406  
 C,-3.3549475714,1.0120985848,0.3966679707  
 H,-3.2765412602,0.5970519557,1.4073136667  
 C,-3.9336384857,-0.087701196,-0.5068344968  
 H,-4.2020892948,0.3118123744,-1.4952475015  
 H,-3.1873637598,-0.8738199247,-0.7024710441  
 C,-5.9609167735,-1.6576735087,-0.8575561895  
 H,-5.3158732316,-2.3095657705,-1.4586175482  
 H,-6.681305749,-2.2576043754,-0.2982800617  
 H,-6.5013290716,-1.0092120881,-1.5593386378  
 C,-5.144609802,-0.8053022857,0.0923659919  
 O,-5.423131213,-0.7074614993,1.2741183561  
 C,-4.2775418334,2.2382546562,0.4536011882  
 H,-3.8817893881,2.9990236121,1.1356221401  
 H,-4.3881473824,2.6977332464,-0.536750553  
 H,-5.270123774,1.9532152329,0.8122147598  
 C,0.9277791045,-1.4438060913,-2.6727870527  
 C,1.0397204238,-0.5931819402,-3.8252065433  
 C,0.8651619842,-2.8061856937,-2.8750081263  
 C,1.1116800923,0.8212279718,-3.7924165852  
 C,1.069012882,-1.2457894776,-5.1072603739  
 C,0.9165310003,-3.3404072816,-4.1853773886  
 H,0.7686717139,-3.4867308754,-2.0335867755  
 C,1.205559496,1.568032332,-4.959292598  
 H,1.1076344811,1.3760488599,-2.8613269172  
 C,1.1665802561,-0.4533931062,-6.2791426593  
 H,0.8699147087,-4.418278668,-4.3287421914  
 C,1.2318577587,0.9190412414,-6.2210951028  
 H,1.1879591353,-0.9730399014,-7.2314475758  
 H,1.3049253907,1.4938159834,-7.1364626306  
 N,1.0109894238,-2.5986110094,-5.2672285784  
 O,1.2681234668,2.9132135033,-4.7979017608  
 C,1.3667967368,3.7481041582,-5.9536394827  
 H,1.408750951,4.7692082439,-5.5735219014  
 H,2.2779468477,3.534012945,-6.5235163877  
 H,0.490236637,3.6364813985,-6.6020268483  
 Electronic energy = -1366.2544219  
 Zero-point electronic energy = -1365.640976  
 Thermal energy = -1365.61043  
 Enthalpy = -1365.609487  
 Free energy = -1365.703853  
 Free energy with quasiharmonic approximation = -1365.695899  
 Frequencies = -1404.6224, 13.3084, 23.4104, 29.1559, 35.6589, 44.2306  
 SCF (B3LYP-D3(BJ)/def2-TZVPP) = -1366.92571178