# Supporting Information (SI)

# Feruloylmonotropeins: promising natural antioxidants in *Paederia scandens*

Nguyen Quang Trung,[1,2*] Nguyen Thi Thu Thanh,[3] Nguyen Thi Hoa,[3] Adam Mechler,[5] Quan V. Vo[4*]

[1]The University of Danang – University of Science and Education, Da Nang 550000, Vietnam.
[2]Quality assurance and Testing center 2, Da Nang 550000, Vietnam.
[3]Le Thanh Phuong High School, An My, Phu Yen 621640, Vietnam
[4]The University of Danang – University of Technology and Education, Danang 550000, Vietnam.
[5]Department of Biochemistry and Chemistry, La Trobe University, Victoria 3086, Australia.
*Corresponding authors: nqtrung.quatest2@gmail.com; vvquan@ute.udn.vn;

## Table of Contents

**Table S1.** The method to calculate rate constant following the conventional transition state theory

The rate constant ($k$) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):[1-5]

$$k = \sigma\kappa\frac{k_B T}{h}e^{-(\Delta G^{\neq})/RT} \quad (1)$$

Where: σ is the reaction symmetry number ,[6,7]

κ contains the tunneling corrections calculated using the Eckart barrier,[8]

$k_B$ is the Boltzmann constant,

$h$ is the Planck constant,

$\Delta G^{\neq}$ is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.[9-12] The free energy of reaction $\Delta G^{\neq}$ for the SET pathway was computed following the equations (2,3).

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{SET}^{0}}{\lambda}\right)^2 \quad (2)$$

$$\lambda \approx \Delta E_{SET} - \Delta G_{SET}^{0} \quad (3)$$

where $\Delta G_{SET}$ is the Gibbs energy of reaction, $\Delta E_{SET}$ is the non-adiabatic energy difference between reactants and vertical products for SET.[13,14]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[15]. The apparent rate constants ($k_{app}$) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[16] the steady-state Smoluchowski rate constant ($k_D$) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).[15,17]

$$k_{app} = \frac{k_{TST} k_D}{k_{TST} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

where $R_{AB}$ is the reaction distance, $N_A$ is the Avogadro constant, and $D_{AB} = D_A + D_B$ ($D_{AB}$ is the mutual diffusion coefficient of the reactants A and B),[16,18] where $D_A$ or $D_B$ is estimated using the Stokes–Einstein formulation (6).[19,20]

$$D_{A\ or\ B} = \frac{k_B T}{6\pi\eta a_{A\ or\ B}} \quad (6)$$

η is the viscosity of the solvents (i.e. $\eta(H_2O) = 8.91\times10^{-4}$ Pa s, η(pentyl ethanoate) = $8.62\times10^{-4}$ Pa s) and $a$ is the radius of the solute.

The kinetic study requires different considerations. Water and pentyl ethanoate are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body.[15,21-23] Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno,[24] adjusted with the free volume theory according to the Benson correction[15,25-27] to reduce over-penalizing entropy losses in solution. For the species that have multiple conformers, all of these were investigated and the conformer with the lowest electronic energy was included in the analysis.[22,23] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy.[23,28] All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex. The kinetic calculations were performed by the *Eyringpy* code[29,30]

**Table S2: The Cartesian coordinates and energies of FMT, ANION, DIANION, TSs in the studied media (G: gas phase; P: pentyl ethanoate; H: water)**

| Name | | | | 6-FMT-G |
|---|---|---|---|---|
| Cartesian Coordinates | | | | Energy |
| C | 3.23396500 | -1.79783900 | 0.63228400 | Zero-point correction= 0.564368 (Hartree/Particle) |
| C | 1.81284900 | -2.33312700 | 0.29583200 | Thermal correction to Energy= 0.601146 |
| C | 2.08366000 | -3.76379500 | -0.13015200 | Thermal correction to Enthalpy= 0.602090 |
| C | 3.38426900 | -4.03953400 | -0.22351400 | Thermal correction to Gibbs Free Energy= 0.494663 |
| C | 4.25453400 | -2.85987600 | 0.13068000 | Sum of electronic and zero-point Energies= -2060.607379 |
| C | 3.46281300 | -0.41671000 | 0.04954000 | Sum of electronic and thermal Energies= -2060.570601 |
| O | 3.12949100 | -0.37268400 | -1.34608300 | Sum of electronic and thermal Enthalpies= -2060.569656 |
| C | 1.84842900 | -0.72907800 | -1.60286900 | Sum of electronic and thermal Free Energies= -2060.677083 |
| C | 1.14999600 | -1.56421700 | -0.82417200 | |
| O | 2.64080700 | 0.45427000 | 0.77736700 | |
| C | 2.32984800 | 2.66930600 | 1.51957800 | |
| C | 2.52567700 | 1.76001500 | 0.31272000 | |
| O | 1.38859200 | 1.80136600 | -0.53918000 | |
| C | 1.05754200 | 3.09639300 | -1.01918800 | |
| C | 0.71195700 | 4.00214000 | 0.16701300 | |
| C | 1.93171600 | 4.06459000 | 1.06855400 | |
| O | 3.54304900 | 2.69184400 | 2.23287600 | |
| O | 1.69434300 | 4.82206600 | 2.23442400 | |
| O | 0.41721500 | 5.32017600 | -0.23047800 | |
| C | -0.06200200 | 2.92765200 | -2.02963800 | |
| O | -1.19711700 | 2.27126100 | -1.45869400 | |
| C | 5.30056800 | -3.17874100 | 1.19854700 | |
| O | 5.04375600 | -2.42567500 | -0.97913800 | |
| O | 6.23659300 | -4.12008100 | 0.73369100 | |
| C | -2.18217100 | 3.05725000 | -0.94855100 | |
| C | -3.32973900 | 2.31902100 | -0.42085100 | |
| C | -3.40409300 | 0.97556600 | -0.47390100 | |
| C | -4.45466300 | 0.10383100 | 0.03347500 | |
| O | -2.09003800 | 4.27287600 | -0.93169500 | |
| C | -5.66378600 | 0.56614700 | 0.56441200 | |
| C | -6.61493200 | -0.33067900 | 1.03818000 | |
| C | -6.36500700 | -1.69786800 | 0.98929300 | |
| C | -5.15144200 | -2.17513200 | 0.45815300 | |
| C | -4.20682800 | -1.28341500 | -0.02003400 | |
| O | -7.28781100 | -2.57071100 | 1.45039100 | |
| O | -5.03546800 | -3.53259500 | 0.47163000 | |
| C | -3.81542300 | -4.08200300 | -0.00821700 | |
| C | -0.28920900 | -1.77260200 | -1.07591100 | |
| O | -0.89562900 | -2.77561700 | -0.77699900 | |
| O | -0.94633300 | -0.74009700 | -1.65923600 | |
| H | 3.32985200 | -1.69814800 | 1.71906800 | |
| H | 1.16043700 | -2.30551700 | 1.17557000 | |
| H | 1.26563100 | -4.44292200 | -0.34886800 | |
| H | 3.82205500 | -4.98622500 | -0.52486000 | |
| H | 4.50878300 | -0.09882600 | 0.07865600 | |
| H | 1.46084900 | -0.25344900 | -2.49889400 | |
| H | 1.51823400 | 2.24430100 | 2.13001700 | |
| H | 3.42478700 | 2.05760500 | -0.25349800 | |
| H | 1.91452100 | 3.53878700 | -1.55715600 | |

| | | | |
|---|---|---|---|
| H | -0.12314100 | 3.56042800 | 0.73115400 |
| H | 2.76547000 | 4.50757500 | 0.49640900 |
| H | 3.46289200 | 3.37485600 | 2.91765300 |
| H | 1.33642400 | 5.68035100 | 1.95517900 |
| H | -0.51504800 | 5.33655500 | -0.51518700 |
| H | 0.27242600 | 2.27266300 | -2.83887000 |
| H | -0.35146400 | 3.89633100 | -2.44356800 |
| H | 5.79378700 | -2.23965500 | 1.49848500 |
| H | 4.81366200 | -3.61338400 | 2.07597800 |
| H | 4.46697500 | -2.24169900 | -1.73639400 |
| H | 6.57132800 | -3.78786000 | -0.11468300 |
| H | -4.09109900 | 2.94983900 | 0.02576600 |
| H | -2.58233400 | 0.44522600 | -0.94320900 |
| H | -5.87237400 | 1.63101200 | 0.60289500 |
| H | -7.56043700 | 0.00757700 | 1.44937900 |
| H | -3.26618300 | -1.64065600 | -0.43352700 |
| H | -6.93843000 | -3.47092200 | 1.33475000 |
| H | -3.91258100 | -5.16188400 | 0.09699500 |
| H | -3.65726000 | -3.82023700 | -1.05947300 |
| H | -2.96696000 | -3.71889200 | 0.57970000 |
| H | -0.47357200 | 0.10221200 | -1.51805000 |

| **Name** | | | **10-FMT-G** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | -2.78418700 | 0.56122800 | -0.53206600 |
| C | -4.11214400 | -0.00116600 | -1.09802800 |
| C | -5.16963700 | 0.89948200 | -0.49936200 |
| C | -4.63985100 | 1.97579800 | 0.07600400 |
| C | -3.12749200 | 1.96487800 | 0.07483600 |
| C | -2.17279600 | -0.31823500 | 0.54534700 |
| O | -2.10527400 | -1.69633700 | 0.13456700 |
| C | -3.23988400 | -2.21539200 | -0.36421700 |
| C | -4.24623800 | -1.48616300 | -0.87479900 |
| O | -0.86060500 | 0.09499800 | 0.74353800 |
| C | 0.94250900 | 0.74777900 | 2.15796100 |
| C | -0.36998000 | -0.05072800 | 2.07652300 |
| O | -0.26891200 | -1.39109600 | 2.45282400 |
| C | 0.90356700 | -2.17239300 | 2.17516000 |
| C | 2.18630700 | -1.33770600 | 2.13242300 |
| C | 1.98707900 | -0.05363100 | 2.91041800 |
| O | 0.78397900 | 1.98364700 | 2.82358700 |
| O | 3.22520000 | 0.62330700 | 2.93434400 |
| O | 3.22672900 | -2.13671800 | 2.65748000 |
| C | 0.72121000 | -3.02325600 | 0.92638100 |
| O | 0.71783200 | -2.26363300 | -0.26722700 |
| C | -2.55403200 | 3.07133600 | -0.81718000 |
| O | -2.70848400 | 2.11215500 | 1.42239000 |
| O | -1.17662000 | 2.83438100 | -1.17139900 |
| C | -0.22505000 | 3.14523500 | -0.29142100 |
| C | 1.13655200 | 2.79756200 | -0.71296600 |
| C | 1.40508200 | 1.66148300 | -1.37948700 |
| O | -0.46856200 | 3.65544700 | 0.79828800 |
| C | 2.75477200 | 1.16651900 | -1.65714900 |
| C | 3.81266300 | 2.03861200 | -1.92902900 |
| C | 5.09477500 | 1.54667100 | -2.15778500 |

Zero-point correction= 0.565120 (Hartree/Particle)
Thermal correction to Energy= 0.601579
Thermal correction to Enthalpy= 0.602523
Thermal correction to Gibbs Free Energy= 0.497076
Sum of electronic and zero-point Energies= -2060.611523
Sum of electronic and thermal Energies= -2060.575063
Sum of electronic and thermal Enthalpies= -2060.574119
Sum of electronic and thermal Free Energies= -2060.679566

| | | | |
|---|---|---|---|
| C | 5.33078200 | 0.17993500 | -2.09344500 |
| C | 4.27259000 | -0.70503200 | -1.80876300 |
| C | 2.98914600 | -0.22164700 | -1.61005000 |
| O | 6.57515900 | -0.30414600 | -2.30628900 |
| H | -2.02982100 | 0.64132900 | -1.32103300 |
| H | -4.12498300 | 0.15163000 | -2.18808300 |
| H | -6.22863200 | 0.68720200 | -0.60139400 |
| H | -5.18288600 | 2.78405900 | 0.55633300 |
| H | -2.75026200 | -0.29366900 | 1.47693800 |
| H | -3.26444600 | -3.30054700 | -0.33392400 |
| H | 1.32047700 | 0.90497700 | 1.13990500 |
| H | -1.10672900 | 0.38686200 | 2.75906200 |
| H | 0.99100100 | -2.84313300 | 3.03788300 |
| H | 2.42192500 | -1.05626800 | 1.09368500 |
| H | 1.64566000 | -0.27043100 | 3.93453500 |
| H | 0.47176800 | 2.66420600 | 2.20038800 |
| H | 3.05637200 | 1.52457500 | 3.25329100 |
| H | 4.00048500 | -1.55902100 | 2.76220600 |
| H | -0.20386900 | -3.60612200 | 1.02034300 |
| H | 1.56523700 | -3.71932300 | 0.86088000 |
| H | -0.12806900 | -1.78674500 | -0.29908600 |
| H | -3.07469200 | 3.07824200 | -1.77650600 |
| H | -2.64602800 | 4.05069100 | -0.33715200 |
| H | -1.95394500 | 2.72445100 | 1.47116800 |
| H | 1.92248000 | 3.40418900 | -0.27147800 |
| H | 0.57264200 | 1.01641600 | -1.66168300 |
| H | 3.62789200 | 3.10708700 | -1.99330800 |
| H | 5.92475200 | 2.20707200 | -2.38681600 |
| H | 2.17336000 | -0.90220000 | -1.37450100 |
| H | 6.54590600 | -1.27034100 | -2.19984600 |
| C | -5.40215500 | -2.24309200 | -1.38781800 |
| O | -5.59005000 | -3.43283200 | -1.26577900 |
| O | -6.27468200 | -1.44600200 | -2.05020000 |
| H | -6.99453200 | -2.01935500 | -2.36641000 |
| O | 4.64822800 | -2.01483800 | -1.76368800 |
| C | 3.70785300 | -2.94301800 | -1.24074500 |
| H | 2.80514200 | -2.98376800 | -1.85799500 |
| H | 4.20917100 | -3.91040500 | -1.24598600 |
| H | 3.43447500 | -2.66866400 | -0.21537400 |

| **Name** | **6-FMT-C5-H-OOH-G** |
|---|---|
| Cartesian Coordinates | Energy |

| | | | |
|---|---|---|---|
| C | 3.14031100 | -1.53118100 | 0.27097900 |
| C | 1.80964400 | -2.09040500 | -0.25030200 |
| C | 2.10719700 | -3.48729200 | -0.65776200 |
| C | 3.41762400 | -3.76120800 | -0.56959400 |
| C | 4.22606500 | -2.55448700 | -0.15038100 |
| C | 3.36724700 | -0.10521100 | -0.19813800 |
| O | 3.03773000 | 0.05965500 | -1.58806500 |
| C | 1.76611000 | -0.28192600 | -1.88602900 |
| C | 1.09046900 | -1.24097600 | -1.22918700 |
| O | 2.53222300 | 0.69021100 | 0.59441100 |
| C | 2.17473800 | 2.82836700 | 1.51192300 |
| C | 2.37881100 | 2.02522200 | 0.23373700 |
| O | 1.23112900 | 2.09503700 | -0.60207300 |

Zero-point correction= 0.575080 (Hartree/Particle)
Thermal correction to Energy= 0.615289
Thermal correction to Enthalpy= 0.616234
Thermal correction to Gibbs Free Energy= 0.500323
Sum of electronic and zero-point Energies= -2211.414574
Sum of electronic and thermal Energies= -2211.374364
Sum of electronic and thermal Enthalpies= -2211.373420
Sum of electronic and thermal Free Energies= -2211.489331

| | | | |
|---|---|---|---|
| C | 0.83083700 | 3.40946000 | -0.96107500 |
| C | 0.47320300 | 4.19399100 | 0.30532100 |
| C | 1.71033200 | 4.23732600 | 1.18374900 |
| O | 3.40537800 | 2.84418400 | 2.19515000 |
| O | 1.46865700 | 4.88792300 | 2.41127900 |
| O | 0.10898800 | 5.52517000 | 0.02647900 |
| C | -0.30495600 | 3.27310600 | -1.95884300 |
| O | -1.39160600 | 2.51252600 | -1.42358700 |
| C | 5.21359700 | -2.84121800 | 0.97643900 |
| O | 5.05187100 | -2.08993900 | -1.22157500 |
| O | 6.18971400 | -3.77186500 | 0.57286200 |
| C | -2.39667900 | 3.20185200 | -0.81888800 |
| C | -3.48456000 | 2.36454100 | -0.31396500 |
| C | -3.49413600 | 1.02746800 | -0.47207100 |
| C | -4.47161300 | 0.06225200 | 0.01035800 |
| O | -2.36387200 | 4.41514500 | -0.70538900 |
| C | -5.67867700 | 0.41325600 | 0.62456400 |
| C | -6.55181600 | -0.56995400 | 1.07651900 |
| C | -6.22361100 | -1.91295700 | 0.92516800 |
| C | -5.01130700 | -2.27836900 | 0.30937000 |
| C | -4.14705700 | -1.30032300 | -0.15083800 |
| O | -7.06898300 | -2.86963300 | 1.36792000 |
| O | -4.81202200 | -3.62371200 | 0.22852500 |
| C | -3.57593400 | -4.06132800 | -0.32050200 |
| C | -0.33113200 | -1.49873000 | -1.53978400 |
| O | -0.87115300 | -2.57064900 | -1.40011900 |
| O | -1.03871700 | -0.43626900 | -1.99049300 |
| H | 3.10149700 | -1.49731700 | 1.36799800 |
| H | 1.32613800 | -4.15982100 | -0.99893000 |
| H | 3.89919100 | -4.70244500 | -0.81706300 |
| H | 4.41090700 | 0.21612500 | -0.13800300 |
| H | 1.36508900 | 0.28771100 | -2.71922000 |
| H | 1.39759700 | 2.32136200 | 2.10388500 |
| H | 3.26262200 | 2.39159300 | -0.31579900 |
| H | 1.65283400 | 3.93681800 | -1.47657700 |
| H | -0.32677900 | 3.66735900 | 0.84680800 |
| H | 2.51159400 | 4.76012300 | 0.63286600 |
| H | 3.30850400 | 3.44286400 | 2.95259900 |
| H | 1.06411900 | 5.74724600 | 2.20975300 |
| H | -0.83067600 | 5.52154200 | -0.23286800 |
| H | 0.03925200 | 2.70946200 | -2.83045600 |
| H | -0.65183200 | 4.25824600 | -2.27903700 |
| H | 5.67253900 | -1.89147400 | 1.29439700 |
| H | 4.68294800 | -3.27286600 | 1.82925000 |
| H | 4.51181400 | -1.96153400 | -2.01691400 |
| H | 6.59159600 | -3.42731000 | -0.24041100 |
| H | -4.25563800 | 2.91606800 | 0.21356400 |
| H | -2.67009100 | 0.58087500 | -1.01769600 |
| H | -5.94628200 | 1.45847400 | 0.74640200 |
| H | -7.49430400 | -0.31861400 | 1.55189900 |
| H | -3.21115000 | -1.57149300 | -0.63396800 |
| H | -6.66929100 | -3.73668300 | 1.18273000 |
| H | -3.59986000 | -5.14968400 | -0.27817100 |
| H | -3.46970600 | -3.72860300 | -1.35785900 |
| H | -2.73381400 | -3.67860900 | 0.26526700 |

| | | | | |
|---|---|---|---|---|
| H | -0.62033000 | 0.40743300 | -1.73153700 | |
| O | 1.72566000 | -3.19391000 | 2.48232500 | |
| H | 1.53293200 | -4.12654400 | 2.27912800 | |
| O | 0.65451200 | -2.51224800 | 1.93882500 | |
| H | 1.06428700 | -2.22096800 | 0.81157100 | |
| **Name** | | | | **6-FMT-O24-H-OOH-G** |
| Cartesian Coordinates | | | | Energy |
| C | 3.16544700 | -2.24018100 | 0.59218700 | Zero-point correction= 0.575766 (Hartree/Particle) |
| C | 1.70564400 | -2.49399100 | 0.11900700 | Thermal correction to Energy= 0.615475 |
| C | 1.75794700 | -3.92441400 | -0.38384700 | Thermal correction to Enthalpy= 0.616419 |
| C | 2.99364800 | -4.42348800 | -0.40017500 | Thermal correction to Gibbs Free Energy= 0.501047 |
| C | 4.02335300 | -3.44048300 | 0.09765800 | Sum of electronic and zero-point Energies= -2211.420636 |
| C | 3.67878900 | -0.89414500 | 0.11901400 | Sum of electronic and thermal Energies= -2211.380927 |
| O | 3.47503800 | -0.71863600 | -1.29156400 | Sum of electronic and thermal Enthalpies= -2211.379983 |
| C | 2.17744500 | -0.82375100 | -1.66121300 | Sum of electronic and thermal Free Energies= -2211.495355 |
| C | 1.28153700 | -1.55790200 | -0.98963200 | |
| O | 2.96097800 | 0.07040700 | 0.83945400 | |
| C | 2.99510600 | 2.25881100 | 1.71011100 | |
| C | 3.11341000 | 1.39853700 | 0.45813400 | |
| O | 2.06546800 | 1.69326800 | -0.45836000 | |
| C | 2.00336400 | 3.05276700 | -0.86407700 | |
| C | 1.73772700 | 3.93613800 | 0.35932900 | |
| C | 2.88206400 | 3.72683500 | 1.33469300 | |
| O | 4.13976500 | 2.02011600 | 2.49287700 | |
| O | 2.69757700 | 4.44411800 | 2.53449300 | |
| O | 1.70810600 | 5.30597000 | 0.03545600 | |
| C | 0.94939700 | 3.14972900 | -1.95139200 | |
| O | -0.32153500 | 2.66646000 | -1.50188600 | |
| C | 4.90077800 | -3.99969900 | 1.21742500 | |
| O | 4.96896500 | -3.09614500 | -0.91713400 | |
| O | 5.69057700 | -5.07054700 | 0.76261700 | |
| C | -1.19024600 | 3.57299900 | -0.99163500 | |
| C | -2.48553800 | 3.00651500 | -0.59496900 | |
| C | -2.78393400 | 1.70627400 | -0.77209200 | |
| C | -4.00528300 | 1.01021700 | -0.39013200 | |
| O | -0.90372300 | 4.74978700 | -0.86762400 | |
| C | -5.14349500 | 1.66528400 | 0.12757200 | |
| C | -6.25717700 | 0.93985000 | 0.48350500 | |
| C | -6.29891700 | -0.46797600 | 0.32044600 | |
| C | -5.12909400 | -1.12661500 | -0.18327600 | |
| C | -4.00928500 | -0.38634400 | -0.54086000 | |
| O | -7.39447900 | -1.12852600 | 0.56608500 | |
| O | -5.21100300 | -2.47421100 | -0.26080000 | |
| C | -4.15646100 | -3.16495000 | -0.93085100 | |
| C | -0.14661000 | -1.47839400 | -1.34824000 | |
| O | -0.95055300 | -2.36280600 | -1.16034800 | |
| O | -0.55594600 | -0.30727200 | -1.89684000 | |
| H | 3.18639400 | -2.21488000 | 1.68721900 | |
| H | 0.99779100 | -2.39882100 | 0.94976900 | |
| H | 0.85553600 | -4.43389300 | -0.70700300 | |
| H | 3.28315200 | -5.41598400 | -0.73154400 | |
| H | 4.75769700 | -0.76903200 | 0.24527100 | |
| H | 1.95359700 | -0.23972500 | -2.54911200 | |
| H | 2.08011300 | 1.95294300 | 2.24052500 | |

| | | | |
|---|---|---|---|
| H | 4.08901400 | 1.55969700 | -0.03108700 |
| H | 2.96116700 | 3.36480600 | -1.31644000 |
| H | 0.80054500 | 3.62035500 | 0.84157600 |
| H | 3.81928700 | 4.04523700 | 0.84602700 |
| H | 4.13054700 | 2.65951000 | 3.22290700 |
| H | 2.52833100 | 5.37050900 | 2.29849600 |
| H | 0.81420600 | 5.51112500 | -0.29293600 |
| H | 1.22293300 | 2.49954400 | -2.78666100 |
| H | 0.85951400 | 4.17897100 | -2.30637200 |
| H | 5.52513200 | -3.18296900 | 1.61525200 |
| H | 4.27096300 | -4.38289700 | 2.02511900 |
| H | 4.50058200 | -2.78715400 | -1.70768400 |
| H | 6.15541700 | -4.76046400 | -0.03100000 |
| H | -3.15656900 | 3.72534800 | -0.13657700 |
| H | -2.03868000 | 1.07240000 | -1.24069000 |
| H | -5.14460400 | 2.74493000 | 0.24078400 |
| H | -7.15044500 | 1.41502500 | 0.87555300 |
| H | -3.12119600 | -0.87717600 | -0.93255500 |
| H | -4.46420500 | -4.20928400 | -0.95644900 |
| H | -4.03896300 | -2.78304200 | -1.94965700 |
| H | -3.20767800 | -3.05897300 | -0.39693100 |
| H | 0.05451100 | 0.41802800 | -1.66425000 |
| O | -5.57296200 | -2.22435500 | 2.49946900 |
| H | -5.13786500 | -2.69753500 | 1.76069500 |
| O | -6.88531900 | -2.56562700 | 2.36075000 |
| H | -7.23155200 | -1.95232700 | 1.37447900 |

| **Name** | | | **10-FMT-C5-H-OOH-G** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 2.61888400 | -0.37426900 | 0.02942400 |
| C | 3.96990800 | 0.13506300 | -0.48220600 |
| C | 5.00122600 | -0.52731500 | 0.34363700 |
| C | 4.46469600 | -1.49550600 | 1.09913200 |
| C | 2.95589800 | -1.55993100 | 0.98918400 |
| C | 1.84281700 | 0.71343500 | 0.74559600 |
| O | 1.75148100 | 1.90068300 | -0.07660300 |
| C | 2.87519700 | 2.32209500 | -0.66987100 |
| C | 3.98951500 | 1.57198800 | -0.82153400 |
| O | 0.54064500 | 0.27697400 | 0.94124600 |
| C | -1.37261900 | -0.06671500 | 2.32202000 |
| C | -0.08526700 | 0.75192000 | 2.13554700 |
| O | -0.26378000 | 2.13530900 | 2.11351400 |
| C | -1.43656600 | 2.74189800 | 1.54655300 |
| C | -2.69088700 | 1.87152600 | 1.67705200 |
| C | -2.49608500 | 0.84594600 | 2.77461900 |
| O | -1.22984100 | -1.08380200 | 3.29098900 |
| O | -3.70658200 | 0.13335700 | 2.90673300 |
| O | -3.77824200 | 2.73722000 | 1.93161600 |
| C | -1.18801500 | 3.19368200 | 0.11464400 |
| O | -1.07394900 | 2.11573700 | -0.79457900 |
| C | 2.50037500 | -2.87986800 | 0.35837800 |
| O | 2.43608200 | -1.37605300 | 2.29585200 |
| O | 1.14410000 | -2.81519400 | -0.12697700 |
| C | 0.14363400 | -2.95225000 | 0.73933000 |
| C | -1.19622600 | -2.82723600 | 0.15530300 |

Zero-point correction= 0.576179 (Hartree/Particle)
Thermal correction to Energy= 0.616040
Thermal correction to Enthalpy= 0.616984
Thermal correction to Gibbs Free Energy= 0.502502
Sum of electronic and zero-point Energies= -2211.427619
Sum of electronic and thermal Energies= -2211.387759
Sum of electronic and thermal Enthalpies= -2211.386815
Sum of electronic and thermal Free Energies= -2211.501296

| | | | |
|---|---|---|---|
| C | -1.46495500 | -1.95590800 | -0.83216100 |
| O | 0.32154200 | -3.13953900 | 1.94073200 |
| C | -2.81171800 | -1.65727200 | -1.32338500 |
| C | -3.80175400 | -2.64151100 | -1.39137500 |
| C | -5.08393400 | -2.32651700 | -1.83314700 |
| C | -5.38965700 | -1.01978800 | -2.18912800 |
| C | -4.40076200 | -0.01997800 | -2.11284900 |
| C | -3.11590300 | -0.33501600 | -1.70093000 |
| O | -6.63508700 | -0.70556800 | -2.61220600 |
| H | 1.99141700 | -0.70353700 | -0.80671100 |
| H | 4.08288100 | -0.45635400 | -1.58716100 |
| H | 6.05444200 | -0.27554700 | 0.28235100 |
| H | 4.99834600 | -2.14891900 | 1.78233100 |
| H | 2.31600900 | 1.01560700 | 1.68733600 |
| H | 2.80996900 | 3.34340400 | -1.03273800 |
| H | -1.66253800 | -0.49332500 | 1.35311900 |
| H | 0.59503200 | 0.55911100 | 2.97248000 |
| H | -1.60274200 | 3.63144300 | 2.16478100 |
| H | -2.86685800 | 1.31699000 | 0.74128400 |
| H | -2.23396200 | 1.34094100 | 3.72264900 |
| H | -0.80961700 | -1.87129900 | 2.89951800 |
| H | -3.52311100 | -0.65090000 | 3.44898000 |
| H | -4.54513100 | 2.17606300 | 2.13201000 |
| H | -0.29061800 | 3.82473600 | 0.08651500 |
| H | -2.04579000 | 3.79446400 | -0.20838700 |
| H | -0.22234600 | 1.68155900 | -0.62126000 |
| H | 3.09455700 | -3.07956700 | -0.53512600 |
| H | 2.59431100 | -3.70668300 | 1.06964700 |
| H | 1.71315500 | -2.00952700 | 2.45283300 |
| H | -1.98474800 | -3.33245700 | 0.70643100 |
| H | -0.64347900 | -1.36983800 | -1.24500000 |
| H | -3.56107800 | -3.66750100 | -1.12812500 |
| H | -5.86026500 | -3.08080900 | -1.90940300 |
| H | -2.35530600 | 0.43880600 | -1.62407500 |
| H | -6.65997600 | 0.24857800 | -2.79801000 |
| C | 5.14015800 | 2.21860000 | -1.47753800 |
| O | 5.21463700 | 3.38283700 | -1.79776000 |
| O | 6.15297500 | 1.34688300 | -1.70152700 |
| H | 6.85874600 | 1.84955500 | -2.14467400 |
| O | -4.83968900 | 1.21803400 | -2.47948500 |
| C | -3.97368600 | 2.31438700 | -2.22506100 |
| H | -3.04041000 | 2.22137300 | -2.78934300 |
| H | -4.51632000 | 3.20416200 | -2.54278000 |
| H | -3.74388500 | 2.37632700 | -1.15534600 |
| O | 4.80813800 | -2.35922800 | -2.10245900 |
| H | 5.72364700 | -2.15099200 | -2.36225900 |
| O | 4.07882500 | -1.30198000 | -2.58399800 |

| **Name** | | | **10-FMT-O24-H-OOH-G** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 3.06174600 | -0.03735000 | -0.86602500 |
| C | 4.25279000 | 0.89308000 | -1.20521900 |
| C | 5.43998300 | -0.04294100 | -1.24958700 |
| C | 5.06874700 | -1.32053800 | -1.23854300 |
| C | 3.57636200 | -1.50302600 | -1.07529000 |

Zero-point correction= 0.576618 (Hartree/Particle)
Thermal correction to Energy= 0.615889
Thermal correction to Enthalpy= 0.616834
Thermal correction to Gibbs Free Energy= 0.504160
Sum of electronic and zero-point Energies= -2211.424833

| | | | |
|---|---|---|---|
| C | 2.56645100 | 0.12282500 | 0.56071400 |
| O | 2.34720200 | 1.50564300 | 0.89502400 |
| C | 3.36517700 | 2.34039100 | 0.61708000 |
| C | 4.32867000 | 2.08357100 | -0.28282800 |
| O | 1.33239500 | -0.50845000 | 0.65770500 |
| C | -0.16844700 | -2.01632700 | 1.72996400 |
| C | 1.03319300 | -1.07499200 | 1.93383900 |
| O | 0.85880000 | -0.09550200 | 2.91253100 |
| C | -0.40693400 | 0.54678400 | 3.12765200 |
| C | -1.59592800 | -0.32929000 | 2.73037000 |
| C | -1.20023400 | -1.78894100 | 2.81740500 |
| O | 0.20271600 | -3.37903800 | 1.74917800 |
| O | -2.36145700 | -2.55594000 | 2.58194600 |
| O | -2.66843000 | 0.00015200 | 3.58822200 |
| C | -0.45064800 | 1.92027800 | 2.47307900 |
| O | -0.51679100 | 1.86117700 | 1.06046400 |
| C | 2.93730500 | -2.10557100 | -2.33136900 |
| O | 3.38472700 | -2.33699400 | 0.05644100 |
| O | 1.51124200 | -1.88661800 | -2.38449800 |
| C | 0.70979200 | -2.68023900 | -1.67939100 |
| C | -0.71777700 | -2.33029000 | -1.76595800 |
| C | -1.13450200 | -1.05394500 | -1.72955200 |
| O | 1.11938600 | -3.61157700 | -0.99579700 |
| C | -2.53868100 | -0.65495900 | -1.61160000 |
| C | -3.56618100 | -1.40963000 | -2.21540600 |
| C | -4.88203600 | -1.02914100 | -2.07291300 |
| C | -5.23585800 | 0.08957700 | -1.27902600 |
| C | -4.18131600 | 0.85116200 | -0.67693400 |
| C | -2.85198300 | 0.48689100 | -0.86016800 |
| O | -6.48790100 | 0.37418800 | -1.05950900 |
| H | 2.20466200 | 0.18180500 | -1.51038100 |
| H | 4.11029300 | 1.29523000 | -2.21992300 |
| H | 6.45668600 | 0.32420500 | -1.34125000 |
| H | 5.72554900 | -2.18376400 | -1.28596400 |
| H | 3.28112300 | -0.27054700 | 1.29328000 |
| H | 3.32848200 | 3.26570200 | 1.18397200 |
| H | -0.64691000 | -1.76542600 | 0.77587600 |
| H | 1.90119700 | -1.65825700 | 2.25998800 |
| H | -0.46262900 | 0.68366900 | 4.21415000 |
| H | -1.88192200 | -0.12794100 | 1.68540700 |
| H | -0.77890000 | -2.01829400 | 3.80833400 |
| H | 0.43811700 | -3.66306900 | 0.84841900 |
| H | -2.08604200 | -3.48161200 | 2.48573600 |
| H | -3.35336900 | -0.67707300 | 3.46007600 |
| H | 0.42188100 | 2.50091500 | 2.79807500 |
| H | -1.35579800 | 2.43429200 | 2.81619100 |
| H | 0.36594900 | 1.60486300 | 0.74507200 |
| H | 3.31227500 | -1.59420600 | -3.21959300 |
| H | 3.14512700 | -3.17776000 | -2.40283600 |
| H | 2.65746500 | -2.96096300 | -0.10886300 |
| H | -1.40402200 | -3.16561300 | -1.65556800 |
| H | -0.38844800 | -0.26034100 | -1.69117600 |
| H | -3.31043000 | -2.27233800 | -2.82377200 |
| H | -5.69262800 | -1.58009000 | -2.53852200 |
| H | -2.05331700 | 1.05610100 | -0.38846700 |

Sum of electronic and thermal Energies= -2211.385562
Sum of electronic and thermal Enthalpies= -2211.384618
Sum of electronic and thermal Free Energies= -2211.497292

| | | | |
|---|---|---|---|
| C | 5.35160800 | 3.13172200 | -0.45628000 |
| O | 5.48370800 | 4.12100000 | 0.22823400 |
| O | 6.16273200 | 2.87603700 | -1.51017100 |
| H | 6.79467800 | 3.61408700 | -1.56501100 |
| O | -4.58108900 | 1.92776700 | 0.04091300 |
| C | -3.66693500 | 2.46379000 | 0.99905100 |
| H | -2.78421100 | 2.89421500 | 0.51647700 |
| H | -4.22315200 | 3.23637300 | 1.52879900 |
| H | -3.36076700 | 1.67991200 | 1.70068100 |
| O | -5.57214700 | 2.74670300 | -2.41413900 |
| H | -5.10547300 | 2.97852800 | -1.58431600 |
| O | -6.84839600 | 2.50185300 | -1.99977400 |
| H | -6.75522000 | 1.46683900 | -1.39743700 |

| **Name** | | | **6-FMT-P** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 3.23396500 | -1.79783900 | 0.63228400 |
| C | 1.81284900 | -2.33312700 | 0.29583200 |
| C | 2.08366000 | -3.76379500 | -0.13015200 |
| C | 3.38426900 | -4.03953400 | -0.22351400 |
| C | 4.25453400 | -2.85987600 | 0.13068000 |
| C | 3.46281300 | -0.41671000 | 0.04954000 |
| O | 3.12949100 | -0.37268400 | -1.34608300 |
| C | 1.84842900 | -0.72907800 | -1.60286900 |
| C | 1.14999600 | -1.56421700 | -0.82417200 |
| O | 2.64080700 | 0.45427000 | 0.77736700 |
| C | 2.32984800 | 2.66930600 | 1.51957800 |
| C | 2.52567700 | 1.76001500 | 0.31272000 |
| O | 1.38859200 | 1.80136600 | -0.53918000 |
| C | 1.05754200 | 3.09639300 | -1.01918800 |
| C | 0.71195700 | 4.00214000 | 0.16701300 |
| C | 1.93171600 | 4.06459000 | 1.06855400 |
| O | 3.54304900 | 2.69184400 | 2.23287600 |
| O | 1.69434300 | 4.82206600 | 2.23442400 |
| O | 0.41721500 | 5.32017600 | -0.23047800 |
| C | -0.06200200 | 2.92765200 | -2.02963800 |
| O | -1.19711700 | 2.27126100 | -1.45869400 |
| C | 5.30056800 | -3.17874100 | 1.19854700 |
| O | 5.04375600 | -2.42567500 | -0.97913800 |
| O | 6.23659300 | -4.12008100 | 0.73369100 |
| C | -2.18217100 | 3.05725000 | -0.94855100 |
| C | -3.32973900 | 2.31902100 | -0.42085100 |
| C | -3.40409300 | 0.97556600 | -0.47390100 |
| C | -4.45466300 | 0.10383100 | 0.03347500 |
| O | -2.09003800 | 4.27287600 | -0.93169500 |
| C | -5.66378600 | 0.56614700 | 0.56441200 |
| C | -6.61493200 | -0.33067900 | 1.03818000 |
| C | -6.36500700 | -1.69786800 | 0.98929300 |
| C | -5.15144200 | -2.17513200 | 0.45815300 |
| C | -4.20682800 | -1.28341500 | -0.02003400 |
| O | -7.28781100 | -2.57071100 | 1.45039100 |
| O | -5.03546800 | -3.53259500 | 0.47163000 |
| C | -3.81542300 | -4.08200300 | -0.00821700 |
| C | -0.28920900 | -1.77260200 | -1.07591100 |
| O | -0.89562900 | -2.77561700 | -0.77699900 |

Zero-point correction= 0.562421 (Hartree/Particle)
Thermal correction to Energy= 0.598826
Thermal correction to Enthalpy= 0.599770
Thermal correction to Gibbs Free Energy= 0.493731
Sum of electronic and zero-point Energies= -2060.647747
Sum of electronic and thermal Energies= -2060.611342
Sum of electronic and thermal Enthalpies= -2060.610398
Sum of electronic and thermal Free Energies= -2060.716437

| | | | |
|---|---|---|---|
| O | -0.94633300 | -0.74009700 | -1.65923600 |
| H | 3.32985200 | -1.69814800 | 1.71906800 |
| H | 1.16043700 | -2.30551700 | 1.17557000 |
| H | 1.26563100 | -4.44292200 | -0.34886800 |
| H | 3.82205500 | -4.98622500 | -0.52486000 |
| H | 4.50878300 | -0.09882600 | 0.07865600 |
| H | 1.46084900 | -0.25344900 | -2.49889400 |
| H | 1.51823400 | 2.24430100 | 2.13001700 |
| H | 3.42478700 | 2.05760500 | -0.25349800 |
| H | 1.91452100 | 3.53878700 | -1.55715600 |
| H | -0.12314100 | 3.56042800 | 0.73115400 |
| H | 2.76547000 | 4.50757500 | 0.49640900 |
| H | 3.46289200 | 3.37485600 | 2.91765300 |
| H | 1.33642400 | 5.68035100 | 1.95517900 |
| H | -0.51504800 | 5.33655500 | -0.51518700 |
| H | 0.27242600 | 2.27266300 | -2.83887000 |
| H | -0.35146400 | 3.89633100 | -2.44356800 |
| H | 5.79378700 | -2.23965500 | 1.49848500 |
| H | 4.81366200 | -3.61338400 | 2.07597800 |
| H | 4.46697500 | -2.24169900 | -1.73639400 |
| H | 6.57132800 | -3.78786000 | -0.11468300 |
| H | -4.09109900 | 2.94983900 | 0.02576600 |
| H | -2.58233400 | 0.44522600 | -0.94320900 |
| H | -5.87237400 | 1.63101200 | 0.60289500 |
| H | -7.56043700 | 0.00757700 | 1.44937900 |
| H | -3.26618300 | -1.64065600 | -0.43352700 |
| H | -6.93843000 | -3.47092200 | 1.33475000 |
| H | -3.91258100 | -5.16188400 | 0.09699500 |
| H | -3.65726000 | -3.82023700 | -1.05947300 |
| H | -2.96696000 | -3.71889200 | 0.57970000 |
| H | -0.47357200 | 0.10221200 | -1.51805000 |

| **Name** | | | **10-FMT-P** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | -2.78418700 | 0.56122800 | -0.53206600 |
| C | -4.11214400 | -0.00116600 | -1.09802800 |
| C | -5.16963700 | 0.89948200 | -0.49936200 |
| C | -4.63985100 | 1.97579800 | 0.07600400 |
| C | -3.12749200 | 1.96487800 | 0.07483600 |
| C | -2.17279600 | -0.31823500 | 0.54534700 |
| O | -2.10527400 | -1.69633700 | 0.13456700 |
| C | -3.23988400 | -2.21539200 | -0.36421700 |
| C | -4.24623800 | -1.48616300 | -0.87479900 |
| O | -0.86060500 | 0.09499800 | 0.74353800 |
| C | 0.94250900 | 0.74777900 | 2.15796100 |
| C | -0.36998000 | -0.05072800 | 2.07652300 |
| O | -0.26891200 | -1.39109600 | 2.45282400 |
| C | 0.90356700 | -2.17239300 | 2.17516000 |
| C | 2.18630700 | -1.33770600 | 2.13242300 |
| C | 1.98707900 | -0.05363100 | 2.91041800 |
| O | 0.78397900 | 1.98364700 | 2.82358700 |
| O | 3.22520000 | 0.62330700 | 2.93434400 |
| O | 3.22672900 | -2.13671800 | 2.65748000 |
| C | 0.72121000 | -3.02325600 | 0.92638100 |
| O | 0.71783200 | -2.26363300 | -0.26722700 |

Zero-point correction= 0.563269 (Hartree/Particle)
Thermal correction to Energy= 0.600232
Thermal correction to Enthalpy= 0.601176
Thermal correction to Gibbs Free Energy= 0.493852
Sum of electronic and zero-point Energies= -2060.649212
Sum of electronic and thermal Energies= -2060.612249
Sum of electronic and thermal Enthalpies= -2060.611304
Sum of electronic and thermal Free Energies= -2060.718628

| | | | |
|---|---|---|---|
| C | -2.55403200 | 3.07133600 | -0.81718000 |
| O | -2.70848400 | 2.11215500 | 1.42239000 |
| O | -1.17662000 | 2.83438100 | -1.17139900 |
| C | -0.22505000 | 3.14523500 | -0.29142100 |
| C | 1.13655200 | 2.79756200 | -0.71296600 |
| C | 1.40508200 | 1.66148300 | -1.37948700 |
| O | -0.46856200 | 3.65544700 | 0.79828800 |
| C | 2.75477200 | 1.16651900 | -1.65714900 |
| C | 3.81266300 | 2.03861200 | -1.92902900 |
| C | 5.09477500 | 1.54667100 | -2.15778500 |
| C | 5.33078200 | 0.17993500 | -2.09344500 |
| C | 4.27259000 | -0.70503200 | -1.80876300 |
| C | 2.98914600 | -0.22164700 | -1.61005000 |
| O | 6.57515900 | -0.30414600 | -2.30628900 |
| H | -2.02982100 | 0.64132900 | -1.32103300 |
| H | -4.12498300 | 0.15163000 | -2.18808300 |
| H | -6.22863200 | 0.68720200 | -0.60139400 |
| H | -5.18288600 | 2.78405900 | 0.55633300 |
| H | -2.75026200 | -0.29366900 | 1.47693800 |
| H | -3.26444600 | -3.30054700 | -0.33392400 |
| H | 1.32047700 | 0.90497700 | 1.13990500 |
| H | -1.10672900 | 0.38686200 | 2.75906200 |
| H | 0.99100100 | -2.84313300 | 3.03788300 |
| H | 2.42192500 | -1.05626800 | 1.09368500 |
| H | 1.64566000 | -0.27043100 | 3.93453500 |
| H | 0.47176800 | 2.66420600 | 2.20038800 |
| H | 3.05637200 | 1.52457500 | 3.25329100 |
| H | 4.00048500 | -1.55902100 | 2.76220600 |
| H | -0.20386900 | -3.60612200 | 1.02034300 |
| H | 1.56523700 | -3.71932300 | 0.86088000 |
| H | -0.12806900 | -1.78674500 | -0.29908600 |
| H | -3.07469200 | 3.07824200 | -1.77650600 |
| H | -2.64602800 | 4.05069100 | -0.33715200 |
| H | -1.95394500 | 2.72445100 | 1.47116800 |
| H | 1.92248000 | 3.40418900 | -0.27147800 |
| H | 0.57264200 | 1.01641600 | -1.66168300 |
| H | 3.62789200 | 3.10708700 | -1.99330800 |
| H | 5.92475200 | 2.20707200 | -2.38681600 |
| H | 2.17336000 | -0.90220000 | -1.37450100 |
| H | 6.54590600 | -1.27034100 | -2.19984600 |
| C | -5.40215500 | -2.24309200 | -1.38781800 |
| O | -5.59005000 | -3.43283200 | -1.26577900 |
| O | -6.27468200 | -1.44600200 | -2.05020000 |
| H | -6.99453200 | -2.01935500 | -2.36641000 |
| O | 4.64822800 | -2.01483800 | -1.76368800 |
| C | 3.70785300 | -2.94301800 | -1.24074500 |
| H | 2.80514200 | -2.98376800 | -1.85799500 |
| H | 4.20917100 | -3.91040500 | -1.24598600 |
| H | 3.43447500 | -2.66866400 | -0.21537400 |

| **Name** | | | **6-FMT-C5-H-OOH-P** | |
|---|---|---|---|---|
| Cartesian Coordinates | | | Energy | |
| C | 3.14031100 | -1.53118100 | 0.27097900 | Zero-point correction= 0.572861 (Hartree/Particle) |
| C | 1.80964400 | -2.09040500 | -0.25030200 | Thermal correction to Energy= 0.613782 |
| C | 2.10719700 | -3.48729200 | -0.65776200 | Thermal correction to Enthalpy= 0.614726 |

| | | | |
|---|---|---|---|
| C | 3.41762400 | -3.76120800 | -0.56959400 |
| C | 4.22606500 | -2.55448700 | -0.15038100 |
| C | 3.36724700 | -0.10521100 | -0.19813800 |
| O | 3.03773000 | 0.05965500 | -1.58806500 |
| C | 1.76611000 | -0.28192600 | -1.88602900 |
| C | 1.09046900 | -1.24097600 | -1.22918700 |
| O | 2.53222300 | 0.69021100 | 0.59441100 |
| C | 2.17473800 | 2.82836700 | 1.51192300 |
| C | 2.37881100 | 2.02522200 | 0.23373700 |
| O | 1.23112900 | 2.09503700 | -0.60207300 |
| C | 0.83083700 | 3.40946000 | -0.96107500 |
| C | 0.47320300 | 4.19399100 | 0.30532100 |
| C | 1.71033200 | 4.23732600 | 1.18374900 |
| O | 3.40537800 | 2.84418400 | 2.19515000 |
| O | 1.46865700 | 4.88792300 | 2.41127900 |
| O | 0.10898800 | 5.52517000 | 0.02647900 |
| C | -0.30495600 | 3.27310600 | -1.95884300 |
| O | -1.39160600 | 2.51252600 | -1.42358700 |
| C | 5.21359700 | -2.84121800 | 0.97643900 |
| O | 5.05187100 | -2.08993900 | -1.22157500 |
| O | 6.18971400 | -3.77186500 | 0.57286200 |
| C | -2.39667900 | 3.20185200 | -0.81888800 |
| C | -3.48456000 | 2.36454100 | -0.31396500 |
| C | -3.49413600 | 1.02746800 | -0.47207100 |
| C | -4.47161300 | 0.06225200 | 0.01035800 |
| O | -2.36387200 | 4.41514500 | -0.70538900 |
| C | -5.67867700 | 0.41325600 | 0.62456400 |
| C | -6.55181600 | -0.56995400 | 1.07651900 |
| C | -6.22361100 | -1.91295700 | 0.92516800 |
| C | -5.01130700 | -2.27836900 | 0.30937000 |
| C | -4.14705700 | -1.30032300 | -0.15083800 |
| O | -7.06898300 | -2.86963300 | 1.36792000 |
| O | -4.81202200 | -3.62371200 | 0.22852500 |
| C | -3.57593400 | -4.06132800 | -0.32050200 |
| C | -0.33113200 | -1.49873000 | -1.53978400 |
| O | -0.87115300 | -2.57064900 | -1.40011900 |
| O | -1.03871700 | -0.43626900 | -1.99049300 |
| H | 3.10149700 | -1.49731700 | 1.36799800 |
| H | 1.32613800 | -4.15982100 | -0.99893000 |
| H | 3.89919100 | -4.70244500 | -0.81706300 |
| H | 4.41090700 | 0.21612500 | -0.13800300 |
| H | 1.36508900 | 0.28771100 | -2.71922000 |
| H | 1.39759700 | 2.32136200 | 2.10388500 |
| H | 3.26262200 | 2.39159300 | -0.31579900 |
| H | 1.65283400 | 3.93681800 | -1.47657700 |
| H | -0.32677900 | 3.66735900 | 0.84680800 |
| H | 2.51159400 | 4.76012300 | 0.63286600 |
| H | 3.30850400 | 3.44286400 | 2.95259900 |
| H | 1.06411900 | 5.74724600 | 2.20975300 |
| H | -0.83067600 | 5.52154200 | -0.23286800 |
| H | 0.03925200 | 2.70946200 | -2.83045600 |
| H | -0.65183200 | 4.25824600 | -2.27903700 |
| H | 5.67253900 | -1.89147400 | 1.29439700 |
| H | 4.68294800 | -3.27286600 | 1.82925000 |
| H | 4.51181400 | -1.96153400 | -2.01691400 |

Thermal correction to Gibbs Free Energy= 0.496221
Sum of electronic and zero-point Energies= -2211.461610
Sum of electronic and thermal Energies= -2211.420689
Sum of electronic and thermal Enthalpies= -2211.419745
Sum of electronic and thermal Free Energies= -2211.538250

| | | | |
|---|---|---|---|
| H | 6.59159600 | -3.42731000 | -0.24041100 |
| H | -4.25563800 | 2.91606800 | 0.21356400 |
| H | -2.67009100 | 0.58087500 | -1.01769600 |
| H | -5.94628200 | 1.45847400 | 0.74640200 |
| H | -7.49430400 | -0.31861400 | 1.55189900 |
| H | -3.21115000 | -1.57149300 | -0.63396800 |
| H | -6.66929100 | -3.73668300 | 1.18273000 |
| H | -3.59986000 | -5.14968400 | -0.27817100 |
| H | -3.46970600 | -3.72860300 | -1.35785900 |
| H | -2.73381400 | -3.67860900 | 0.26526700 |
| H | -0.62033000 | 0.40743300 | -1.73153700 |
| O | 1.72566000 | -3.19391000 | 2.48232500 |
| H | 1.53293200 | -4.12654400 | 2.27912800 |
| O | 0.65451200 | -2.51224800 | 1.93882500 |
| H | 1.06428700 | -2.22096800 | 0.81157100 |

| **Name** | | | **6-FMT-O24-H-OOH-P** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 3.16544700 | -2.24018100 | 0.59218700 |
| C | 1.70564400 | -2.49399100 | 0.11900700 |
| C | 1.75794700 | -3.92441400 | -0.38384700 |
| C | 2.99364800 | -4.42348800 | -0.40017500 |
| C | 4.02335300 | -3.44048300 | 0.09765800 |
| C | 3.67878900 | -0.89414500 | 0.11901400 |
| O | 3.47503800 | -0.71863600 | -1.29156400 |
| C | 2.17744500 | -0.82375100 | -1.66121300 |
| C | 1.28153700 | -1.55790200 | -0.98963200 |
| O | 2.96097800 | 0.07040700 | 0.83945400 |
| C | 2.99510600 | 2.25881100 | 1.71011100 |
| C | 3.11341000 | 1.39853700 | 0.45813400 |
| O | 2.06546800 | 1.69326800 | -0.45836000 |
| C | 2.00336400 | 3.05276700 | -0.86407700 |
| C | 1.73772700 | 3.93613800 | 0.35932900 |
| C | 2.88206400 | 3.72683500 | 1.33469300 |
| O | 4.13976500 | 2.02011600 | 2.49287700 |
| O | 2.69757700 | 4.44411800 | 2.53449300 |
| O | 1.70810600 | 5.30597000 | 0.03545600 |
| C | 0.94939700 | 3.14972900 | -1.95139200 |
| O | -0.32153500 | 2.66646000 | -1.50188600 |
| C | 4.90077800 | -3.99969900 | 1.21742500 |
| O | 4.96896500 | -3.09614500 | -0.91713400 |
| O | 5.69057700 | -5.07054700 | 0.76261700 |
| C | -1.19024600 | 3.57299900 | -0.99163500 |
| C | -2.48553800 | 3.00651500 | -0.59496900 |
| C | -2.78393400 | 1.70627400 | -0.77209200 |
| C | -4.00528300 | 1.01021700 | -0.39013200 |
| O | -0.90372300 | 4.74978700 | -0.86762400 |
| C | -5.14349500 | 1.66528400 | 0.12757200 |
| C | -6.25717700 | 0.93985000 | 0.48350500 |
| C | -6.29891700 | -0.46797600 | 0.32044600 |
| C | -5.12909400 | -1.12661500 | -0.18327600 |
| C | -4.00928500 | -0.38634400 | -0.54086000 |
| O | -7.39447900 | -1.12852600 | 0.56608500 |
| O | -5.21100300 | -2.47421100 | -0.26080000 |
| C | -4.15646100 | -3.16495000 | -0.93085100 |

Zero-point correction= 0.573682 (Hartree/Particle)
Thermal correction to Energy= 0.611460
Thermal correction to Enthalpy= 0.612404
Thermal correction to Gibbs Free Energy= 0.502610
Sum of electronic and zero-point Energies= -2211.470734
Sum of electronic and thermal Energies= -2211.432957
Sum of electronic and thermal Enthalpies= -2211.432012
Sum of electronic and thermal Free Energies= -2211.541806

| | | | |
|---|---|---|---|
| C | -0.14661000 | -1.47839400 | -1.34824000 |
| O | -0.95055300 | -2.36280600 | -1.16034800 |
| O | -0.55594600 | -0.30727200 | -1.89684000 |
| H | 3.18639400 | -2.21488000 | 1.68721900 |
| H | 0.99779100 | -2.39882100 | 0.94976900 |
| H | 0.85553600 | -4.43389300 | -0.70700300 |
| H | 3.28315200 | -5.41598400 | -0.73154400 |
| H | 4.75769700 | -0.76903200 | 0.24527100 |
| H | 1.95359700 | -0.23972500 | -2.54911200 |
| H | 2.08011300 | 1.95294300 | 2.24052500 |
| H | 4.08901400 | 1.55969700 | -0.03108700 |
| H | 2.96116700 | 3.36480600 | -1.31644000 |
| H | 0.80054500 | 3.62035500 | 0.84157600 |
| H | 3.81928700 | 4.04523700 | 0.84602700 |
| H | 4.13054700 | 2.65951000 | 3.22290700 |
| H | 2.52833100 | 5.37050900 | 2.29849600 |
| H | 0.81420600 | 5.51112500 | -0.29293600 |
| H | 1.22293300 | 2.49954400 | -2.78666100 |
| H | 0.85951400 | 4.17897100 | -2.30637200 |
| H | 5.52513200 | -3.18296900 | 1.61525200 |
| H | 4.27096300 | -4.38289700 | 2.02511900 |
| H | 4.50058200 | -2.78715400 | -1.70768400 |
| H | 6.15541700 | -4.76046400 | -0.03100000 |
| H | -3.15656900 | 3.72534800 | -0.13657700 |
| H | -2.03868000 | 1.07240000 | -1.24069000 |
| H | -5.14460400 | 2.74493000 | 0.24078400 |
| H | -7.15044500 | 1.41502500 | 0.87555300 |
| H | -3.12119600 | -0.87717600 | -0.93255500 |
| H | -4.46420500 | -4.20928400 | -0.95644900 |
| H | -4.03896300 | -2.78304200 | -1.94965700 |
| H | -3.20767800 | -3.05897300 | -0.39693100 |
| H | 0.05451100 | 0.41802800 | -1.66425000 |
| O | -5.57296200 | -2.22435500 | 2.49946900 |
| H | -5.13786500 | -2.69753500 | 1.76069500 |
| O | -6.88531900 | -2.56562700 | 2.36075000 |
| H | -7.23155200 | -1.95232700 | 1.37447900 |

| **Name** | | | **10-FMT-C5-H-OOH-P** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 2.61888400 | -0.37426900 | 0.02942400 |
| C | 3.96990800 | 0.13506300 | -0.48220600 |
| C | 5.00122600 | -0.52731500 | 0.34363700 |
| C | 4.46469600 | -1.49550600 | 1.09913200 |
| C | 2.95589800 | -1.55993100 | 0.98918400 |
| C | 1.84281700 | 0.71343500 | 0.74559600 |
| O | 1.75148100 | 1.90068300 | -0.07660300 |
| C | 2.87519700 | 2.32209500 | -0.66987100 |
| C | 3.98951500 | 1.57198800 | -0.82153400 |
| O | 0.54064500 | 0.27697400 | 0.94124600 |
| C | -1.37261900 | -0.06671500 | 2.32202000 |
| C | -0.08526700 | 0.75192000 | 2.13554700 |
| O | -0.26378000 | 2.13530900 | 2.11351400 |
| C | -1.43656600 | 2.74189800 | 1.54655300 |
| C | -2.69088700 | 1.87152600 | 1.67705200 |
| C | -2.49608500 | 0.84594600 | 2.77461900 |

Zero-point correction= 0.573945 (Hartree/Particle)
Thermal correction to Energy= 0.612712
Thermal correction to Enthalpy= 0.613656
Thermal correction to Gibbs Free Energy= 0.502351
Sum of electronic and zero-point Energies= -2211.470638
Sum of electronic and thermal Energies= -2211.431871
Sum of electronic and thermal Enthalpies= -2211.430927
Sum of electronic and thermal Free Energies= -2211.542231

| | | | |
|---|---|---|---|
| O | -1.22984100 | -1.08380200 | 3.29098900 |
| O | -3.70658200 | 0.13335700 | 2.90673300 |
| O | -3.77824200 | 2.73722000 | 1.93161600 |
| C | -1.18801500 | 3.19368200 | 0.11464400 |
| O | -1.07394900 | 2.11573700 | -0.79457900 |
| C | 2.50037500 | -2.87986800 | 0.35837800 |
| O | 2.43608200 | -1.37605300 | 2.29585200 |
| O | 1.14410000 | -2.81519400 | -0.12697700 |
| C | 0.14363400 | -2.95225000 | 0.73933000 |
| C | -1.19622600 | -2.82723600 | 0.15530300 |
| C | -1.46495500 | -1.95590800 | -0.83216100 |
| O | 0.32154200 | -3.13953900 | 1.94073200 |
| C | -2.81171800 | -1.65727200 | -1.32338500 |
| C | -3.80175400 | -2.64151100 | -1.39137500 |
| C | -5.08393400 | -2.32651700 | -1.83314700 |
| C | -5.38965700 | -1.01978800 | -2.18912800 |
| C | -4.40076200 | -0.01997800 | -2.11284900 |
| C | -3.11590300 | -0.33501600 | -1.70093000 |
| O | -6.63508700 | -0.70556800 | -2.61220600 |
| H | 1.99141700 | -0.70353700 | -0.80671100 |
| H | 4.08288100 | -0.45635400 | -1.58716100 |
| H | 6.05444200 | -0.27554700 | 0.28235100 |
| H | 4.99834600 | -2.14891900 | 1.78233100 |
| H | 2.31600900 | 1.01560700 | 1.68733600 |
| H | 2.80996900 | 3.34340400 | -1.03273800 |
| H | -1.66253800 | -0.49332500 | 1.35311900 |
| H | 0.59503200 | 0.55911100 | 2.97248000 |
| H | -1.60274200 | 3.63144300 | 2.16478100 |
| H | -2.86685800 | 1.31699000 | 0.74128400 |
| H | -2.23396200 | 1.34094100 | 3.72264900 |
| H | -0.80961700 | -1.87129900 | 2.89951800 |
| H | -3.52311100 | -0.65090000 | 3.44898000 |
| H | -4.54513100 | 2.17606300 | 2.13201000 |
| H | -0.29061800 | 3.82473600 | 0.08651500 |
| H | -2.04579000 | 3.79446400 | -0.20838700 |
| H | -0.22234600 | 1.68155900 | -0.62126000 |
| H | 3.09455700 | -3.07956700 | -0.53512600 |
| H | 2.59431100 | -3.70668300 | 1.06964700 |
| H | 1.71315500 | -2.00952700 | 2.45283300 |
| H | -1.98474800 | -3.33245700 | 0.70643100 |
| H | -0.64347900 | -1.36983800 | -1.24500000 |
| H | -3.56107800 | -3.66750100 | -1.12812500 |
| H | -5.86026500 | -3.08080900 | -1.90940300 |
| H | -2.35530600 | 0.43880600 | -1.62407500 |
| H | -6.65997600 | 0.24857800 | -2.79801000 |
| C | 5.14015800 | 2.21860000 | -1.47753800 |
| O | 5.21463700 | 3.38283700 | -1.79776000 |
| O | 6.15297500 | 1.34688300 | -1.70152700 |
| H | 6.85874600 | 1.84955500 | -2.14467400 |
| O | -4.83968900 | 1.21803400 | -2.47948500 |
| C | -3.97368600 | 2.31438700 | -2.22506100 |
| H | -3.04041000 | 2.22137300 | -2.78934300 |
| H | -4.51632000 | 3.20416200 | -2.54278000 |
| H | -3.74388500 | 2.37632700 | -1.15534600 |
| O | 4.80813800 | -2.35922800 | -2.10245900 |

| | | | | |
|---|---|---|---|---|
| H | 5.72364700 | -2.15099200 | -2.36225900 | |
| O | 4.07882500 | -1.30198000 | -2.58399800 | |
| **Name** | | | | **10-FMT-O24-H-OOH-P** |
| Cartesian Coordinates | | | | Energy |
| C | 3.06174600 | -0.03735000 | -0.86602500 | Zero-point correction= 0.575012 (Hartree/Particle) |
| C | 4.25279000 | 0.89308000 | -1.20521900 | Thermal correction to Energy= 0.613130 |
| C | 5.43998300 | -0.04294100 | -1.24958700 | Thermal correction to Enthalpy= 0.614074 |
| C | 5.06874700 | -1.32053800 | -1.23854300 | Thermal correction to Gibbs Free Energy= 0.503743 |
| C | 3.57636200 | -1.50302600 | -1.07529000 | Sum of electronic and zero-point Energies= -2211.471946 |
| C | 2.56645100 | 0.12282500 | 0.56071400 | Sum of electronic and thermal Energies= -2211.433829 |
| O | 2.34720200 | 1.50564300 | 0.89502400 | Sum of electronic and thermal Enthalpies= -2211.432885 |
| C | 3.36517700 | 2.34039100 | 0.61708000 | Sum of electronic and thermal Free Energies= -2211.543215 |
| C | 4.32867000 | 2.08357100 | -0.28282800 | |
| O | 1.33239500 | -0.50845000 | 0.65770500 | |
| C | -0.16844700 | -2.01632700 | 1.72996400 | |
| C | 1.03319300 | -1.07499200 | 1.93383900 | |
| O | 0.85880000 | -0.09550200 | 2.91253100 | |
| C | -0.40693400 | 0.54678400 | 3.12765200 | |
| C | -1.59592800 | -0.32929000 | 2.73037000 | |
| C | -1.20023400 | -1.78894100 | 2.81740500 | |
| O | 0.20271600 | -3.37903800 | 1.74917800 | |
| O | -2.36145700 | -2.55594000 | 2.58194600 | |
| O | -2.66843000 | 0.00015200 | 3.58822200 | |
| C | -0.45064800 | 1.92027800 | 2.47307900 | |
| O | -0.51679100 | 1.86117700 | 1.06046400 | |
| C | 2.93730500 | -2.10557100 | -2.33136900 | |
| O | 3.38472700 | -2.33699400 | 0.05644100 | |
| O | 1.51124200 | -1.88661800 | -2.38449800 | |
| C | 0.70979200 | -2.68023900 | -1.67939100 | |
| C | -0.71777700 | -2.33029000 | -1.76595800 | |
| C | -1.13450200 | -1.05394500 | -1.72955200 | |
| O | 1.11938600 | -3.61157700 | -0.99579700 | |
| C | -2.53868100 | -0.65495900 | -1.61160000 | |
| C | -3.56618100 | -1.40963000 | -2.21540600 | |
| C | -4.88203600 | -1.02914100 | -2.07291300 | |
| C | -5.23585800 | 0.08957700 | -1.27902600 | |
| C | -4.18131600 | 0.85116200 | -0.67693400 | |
| C | -2.85198300 | 0.48689100 | -0.86016800 | |
| O | -6.48790100 | 0.37418800 | -1.05950900 | |
| H | 2.20466200 | 0.18180500 | -1.51038100 | |
| H | 4.11029300 | 1.29523000 | -2.21992300 | |
| H | 6.45668600 | 0.32420500 | -1.34125000 | |
| H | 5.72554900 | -2.18376400 | -1.28596400 | |
| H | 3.28112300 | -0.27054700 | 1.29328000 | |
| H | 3.32848200 | 3.26570200 | 1.18397200 | |
| H | -0.64691000 | -1.76542600 | 0.77587600 | |
| H | 1.90119700 | -1.65825700 | 2.25998800 | |
| H | -0.46262900 | 0.68366900 | 4.21415000 | |
| H | -1.88192200 | -0.12794100 | 1.68540700 | |
| H | -0.77890000 | -2.01829400 | 3.80833400 | |
| H | 0.43811700 | -3.66306900 | 0.84841900 | |
| H | -2.08604200 | -3.48161200 | 2.48573600 | |
| H | -3.35336900 | -0.67707300 | 3.46007600 | |
| H | 0.42188100 | 2.50091500 | 2.79807500 | |

| | | | |
|---|---|---|---|
| H | -1.35579800 | 2.43429200 | 2.81619100 |
| H | 0.36594900 | 1.60486300 | 0.74507200 |
| H | 3.31227500 | -1.59420600 | -3.21959300 |
| H | 3.14512700 | -3.17776000 | -2.40283600 |
| H | 2.65746500 | -2.96096300 | -0.10886300 |
| H | -1.40402200 | -3.16561300 | -1.65556800 |
| H | -0.38844800 | -0.26034100 | -1.69117600 |
| H | -3.31043000 | -2.27233800 | -2.82377200 |
| H | -5.69262800 | -1.58009000 | -2.53852200 |
| H | -2.05331700 | 1.05610100 | -0.38846700 |
| C | 5.35160800 | 3.13172200 | -0.45628000 |
| O | 5.48370800 | 4.12100000 | 0.22823400 |
| O | 6.16273200 | 2.87603700 | -1.51017100 |
| H | 6.79467800 | 3.61408700 | -1.56501100 |
| O | -4.58108900 | 1.92776700 | 0.04091300 |
| C | -3.66693500 | 2.46379000 | 0.99905100 |
| H | -2.78421100 | 2.89421500 | 0.51647700 |
| H | -4.22315200 | 3.23637300 | 1.52879900 |
| H | -3.36076700 | 1.67991200 | 1.70068100 |
| O | -5.57214700 | 2.74670300 | -2.41413900 |
| H | -5.10547300 | 2.97852800 | -1.58431600 |
| O | -6.84839600 | 2.50185300 | -1.99977400 |
| H | -6.75522000 | 1.46683900 | -1.39743700 |

| **Name** | | | **6-FMT-ANION** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 1.97722000 | -2.40378000 | 0.67975600 |
| C | 0.43975400 | -2.50330400 | 0.78709600 |
| C | 0.23619800 | -4.00185100 | 0.92701600 |
| C | 1.33212400 | -4.69987000 | 0.62292100 |
| C | 2.47263900 | -3.79921300 | 0.21462200 |
| C | 2.48306200 | -1.25694100 | -0.17451900 |
| O | 1.79628300 | -1.11219700 | -1.41104000 |
| C | 0.45448400 | -1.35880900 | -1.42132300 |
| C | -0.23914300 | -1.97255000 | -0.45446700 |
| O | 2.36503200 | -0.05538600 | 0.56240900 |
| C | 3.40344500 | 1.88558200 | 1.48907100 |
| C | 3.45999100 | 0.82098700 | 0.38694700 |
| O | 3.52653900 | 1.32748600 | -0.92175100 |
| C | 2.79788500 | 2.49944900 | -1.31928500 |
| C | 2.54779800 | 3.46499800 | -0.15152800 |
| C | 3.62290500 | 3.26936200 | 0.90357400 |
| O | 4.38822800 | 1.54039900 | 2.44953800 |
| O | 3.48159500 | 4.20203700 | 1.96034500 |
| O | 2.57646600 | 4.80834300 | -0.59967100 |
| C | 1.56110000 | 2.15631900 | -2.14943300 |
| O | 0.36412300 | 1.93942200 | -1.37602100 |
| C | 3.81267200 | -4.14650300 | 0.85267000 |
| O | 2.71534200 | -3.88582900 | -1.19677200 |
| O | 4.28778100 | -5.41390400 | 0.42326100 |
| C | -0.39695200 | 3.01790500 | -1.13563900 |
| C | -1.68109300 | 2.75148300 | -0.48207600 |
| C | -2.26898700 | 1.54357600 | -0.42640700 |
| C | -3.58743000 | 1.29485500 | 0.16561100 |
| O | -0.04650700 | 4.15417500 | -1.43865200 |

Zero-point correction= 0.549925 (Hartree/Particle)
Thermal correction to Energy= 0.587225
Thermal correction to Enthalpy= 0.588169
Thermal correction to Gibbs Free Energy= 0.479781
Sum of electronic and zero-point Energies= -2060.224295
Sum of electronic and thermal Energies= -2060.186995
Sum of electronic and thermal Enthalpies= -2060.186051
Sum of electronic and thermal Free Energies= -2060.294440

| | | | |
|---|---|---|---|
| C | -4.16295200 | 2.16035600 | 1.10418200 |
| C | -5.43470300 | 1.90636700 | 1.61036400 |
| C | -6.14449000 | 0.79355200 | 1.17713700 |
| C | -5.57480500 | -0.08783900 | 0.24154600 |
| C | -4.30157500 | 0.15643200 | -0.25220300 |
| O | -7.39485300 | 0.55670700 | 1.67324000 |
| O | -6.37089100 | -1.14331600 | -0.10212900 |
| C | -5.84795800 | -2.06801400 | -1.05368900 |
| C | -1.72594400 | -2.15311000 | -0.61830500 |
| O | -2.37264500 | -2.46959600 | 0.42127500 |
| O | -2.23911300 | -1.98461800 | -1.76334500 |
| H | 2.38522800 | -2.24115600 | 1.68306000 |
| H | 0.06546800 | -1.97167800 | 1.66967300 |
| H | -0.71961200 | -4.42788600 | 1.21530600 |
| H | 1.41962000 | -5.78274500 | 0.60839900 |
| H | 3.52772800 | -1.41085800 | -0.45965500 |
| H | -0.00193400 | -1.00662800 | -2.34111700 |
| H | 2.40901100 | 1.86891400 | 1.95396100 |
| H | 4.38893200 | 0.25200200 | 0.50050300 |
| H | 3.48593600 | 3.00772700 | -2.00325100 |
| H | 1.58600900 | 3.26365300 | 0.33805800 |
| H | 4.62493800 | 3.34650600 | 0.45736900 |
| H | 4.26367600 | 2.11117200 | 3.22579700 |
| H | 3.52447400 | 5.09447700 | 1.57709400 |
| H | 1.71977400 | 4.97784500 | -1.03393100 |
| H | 1.73293200 | 1.22092400 | -2.68337400 |
| H | 1.37216100 | 2.95535500 | -2.86828900 |
| H | 4.54221400 | -3.36036900 | 0.61009100 |
| H | 3.70059100 | -4.19898900 | 1.93793200 |
| H | 1.86423500 | -3.85451700 | -1.66638800 |
| H | 4.31835800 | -5.39695900 | -0.54824000 |
| H | -2.17060300 | 3.64694800 | -0.11109700 |
| H | -1.77329400 | 0.68636500 | -0.88469100 |
| H | -3.61539500 | 3.02717200 | 1.46133400 |
| H | -5.88838900 | 2.56397400 | 2.34583700 |
| H | -3.84369100 | -0.52255900 | -0.96630400 |
| H | -7.74922400 | -0.25402200 | 1.26476000 |
| H | -6.62781600 | -2.81417600 | -1.20240600 |
| H | -5.63003800 | -1.56265900 | -2.00035700 |
| H | -4.94180700 | -2.54426400 | -0.66738600 |

| **Name** | | | **6-FMT-DIANION** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 0.05754400 | -2.45873000 | 0.50043200 |
| C | -0.80230900 | -1.63758100 | -0.49313900 |
| C | -1.96235100 | -2.57618400 | -0.76576500 |
| C | -1.76369200 | -3.80244800 | -0.27929100 |
| C | -0.42217600 | -3.93430000 | 0.39855600 |
| C | 1.54548800 | -2.28305000 | 0.28300100 |
| O | 1.92436800 | -2.44684800 | -1.07834700 |
| C | 1.18594400 | -1.72937500 | -1.97959800 |
| C | -0.05995500 | -1.29007800 | -1.76503400 |
| O | 1.88950400 | -0.98619200 | 0.72830600 |
| C | 3.65811400 | 0.19273100 | 1.82438800 |
| C | 3.26883500 | -0.68465400 | 0.62477400 |

Zero-point correction= 0.536409 (Hartree/Particle)
Thermal correction to Energy= 0.573325
Thermal correction to Enthalpy= 0.574270
Thermal correction to Gibbs Free Energy= 0.465875
Sum of electronic and zero-point Energies= -2059.778150
Sum of electronic and thermal Energies= -2059.741234
Sum of electronic and thermal Enthalpies= -2059.740290
Sum of electronic and thermal Free Energies= -2059.848685

| | | | |
|---|---|---|---|
| O | 3.58665900 | -0.14757600 | -0.63574200 |
| C | 3.57646700 | 1.25997900 | -0.91514800 |
| C | 3.65015600 | 2.12328900 | 0.34703000 |
| C | 4.47754100 | 1.39468900 | 1.39147000 |
| O | 4.35628600 | -0.64338500 | 2.73377200 |
| O | 4.68698700 | 2.19716900 | 2.54036100 |
| O | 4.25445400 | 3.37077000 | 0.05645500 |
| C | 2.44715400 | 1.63151600 | -1.86966600 |
| O | 1.18304700 | 1.83944200 | -1.22075300 |
| C | -0.47608200 | -4.58153300 | 1.77754700 |
| O | 0.44975600 | -4.78613900 | -0.35736000 |
| O | -0.92287700 | -5.92806000 | 1.71416400 |
| C | 0.88389500 | 3.10101400 | -0.84390400 |
| C | -0.44726100 | 3.28591600 | -0.29807800 |
| C | -1.37662500 | 2.29828200 | -0.25634300 |
| C | -2.72106000 | 2.38003000 | 0.26095000 |
| O | 1.69787500 | 4.02098100 | -0.95478700 |
| C | -3.26216400 | 3.54164400 | 0.84094400 |
| C | -4.55655000 | 3.55565600 | 1.33054900 |
| C | -5.40714200 | 2.41353200 | 1.28071100 |
| C | -4.83502400 | 1.23726200 | 0.67443000 |
| C | -3.54520500 | 1.22687000 | 0.18894200 |
| O | -6.60947300 | 2.41312100 | 1.74442500 |
| O | -5.68359100 | 0.15401100 | 0.63201500 |
| C | -5.16089600 | -1.04132900 | 0.07322400 |
| C | -0.74150800 | -0.46485900 | -2.82707600 |
| O | -1.94359500 | -0.14078100 | -2.60993300 |
| O | -0.08386100 | -0.14276200 | -3.86009500 |
| H | -0.15682400 | -2.11376200 | 1.51776100 |
| H | -1.15914700 | -0.71594400 | -0.01902800 |
| H | -2.83575900 | -2.25636800 | -1.32580100 |
| H | -2.43879300 | -4.64771100 | -0.38156600 |
| H | 2.13900700 | -3.02806900 | 0.82171800 |
| H | 1.72852300 | -1.56215000 | -2.90408000 |
| H | 2.74166800 | 0.56856200 | 2.29708000 |
| H | 3.83945300 | -1.61799600 | 0.67827000 |
| H | 4.50817700 | 1.43264300 | -1.46686000 |
| H | 2.65255100 | 2.28949600 | 0.77722500 |
| H | 5.44115900 | 1.07636300 | 0.96715700 |
| H | 4.45568900 | -0.16196700 | 3.57172200 |
| H | 5.12870300 | 3.01474400 | 2.25489200 |
| H | 3.56943600 | 3.91953400 | -0.37143900 |
| H | 2.28282100 | 0.81143800 | -2.57221100 |
| H | 2.71874000 | 2.53188100 | -2.42438500 |
| H | 0.52123500 | -4.52774400 | 2.23736000 |
| H | -1.18462600 | -4.04166400 | 2.40982100 |
| H | 0.44869400 | -4.49604900 | -1.28548000 |
| H | -0.32935500 | -6.40401000 | 1.10941000 |
| H | -0.64213800 | 4.29105200 | 0.06235100 |
| H | -1.09328400 | 1.32914100 | -0.66472500 |
| H | -2.66061800 | 4.44445000 | 0.91249800 |
| H | -4.96409500 | 4.45811100 | 1.78015800 |
| H | -3.13481000 | 0.33049100 | -0.26733200 |
| H | -5.96240200 | -1.77875300 | 0.12797900 |
| H | -4.86936800 | -0.89135700 | -0.97325300 |

| | | | | |
|---|---|---|---|---|
| H | -4.29581000 | -1.39408700 | 0.64748000 | |
| **Name** | | | | **10-FMT-ANION** |
| Cartesian Coordinates | | | | Energy |
| C | -2.64612900 | 0.61269300 | 0.56378700 | Zero-point correction= 0.549381 (Hartree/Particle) |
| C | -3.83301300 | 1.50135000 | 0.11158000 | Thermal correction to Energy= 0.586344 |
| C | -4.97134400 | 1.06336900 | 1.00306400 | Thermal correction to Enthalpy= 0.587288 |
| C | -4.55668500 | 0.28818700 | 2.00294900 | Thermal correction to Gibbs Free Energy= 0.478773 |
| C | -3.08195300 | -0.03077500 | 1.92459900 | Sum of electronic and zero-point Energies= -2060.232817 |
| C | -2.30936400 | -0.46355300 | -0.45344700 | Sum of electronic and thermal Energies= -2060.195853 |
| O | -2.17700700 | 0.07097300 | -1.77207400 | Sum of electronic and thermal Enthalpies= -2060.194909 |
| C | -3.22984500 | 0.82746600 | -2.19180900 | Sum of electronic and thermal Free Energies= -2060.303424 |
| C | -4.07860000 | 1.46404700 | -1.37444600 | |
| O | -1.05989000 | -0.99167800 | -0.10580300 | |
| C | 0.43782800 | -2.79552200 | 0.26184000 | |
| C | -0.78199100 | -2.31700600 | -0.53530500 | |
| O | -0.60036700 | -2.40566800 | -1.92617500 | |
| C | 0.69354100 | -2.11910600 | -2.48743600 | |
| C | 1.83131100 | -2.85844100 | -1.75753500 | |
| C | 1.28945100 | -3.69920900 | -0.61429100 | |
| O | 0.04688900 | -3.51283400 | 1.41765600 | |
| O | 2.39863200 | -4.20820500 | 0.10758100 | |
| O | 2.51571200 | -3.65139600 | -2.71963200 | |
| C | 0.95065600 | -0.62598900 | -2.64438500 | |
| O | 1.19108900 | 0.06393200 | -1.42554700 | |
| C | -2.31791200 | 0.60358600 | 3.09429500 | |
| O | -2.97992000 | -1.45598600 | 1.95554500 | |
| O | -0.90210800 | 0.73642700 | 2.83135100 | |
| C | -0.11759300 | -0.33582000 | 2.89671200 | |
| C | 1.26087700 | -0.12886900 | 2.45602500 | |
| C | 1.64320400 | 0.95599500 | 1.75686700 | |
| O | -0.53038500 | -1.43528000 | 3.27543100 | |
| C | 2.95639700 | 1.16286400 | 1.14935900 | |
| C | 3.89941700 | 0.13555400 | 1.01768300 | |
| C | 5.12559800 | 0.38076900 | 0.40682100 | |
| C | 5.41799100 | 1.64892500 | -0.08062500 | |
| C | 4.47422300 | 2.68633400 | 0.03247000 | |
| C | 3.25079600 | 2.44082500 | 0.63694600 | |
| O | 6.62213000 | 1.87923400 | -0.67867400 | |
| H | -1.73965100 | 1.21508000 | 0.67813500 | |
| H | -3.60052900 | 2.54606900 | 0.36475600 | |
| H | -5.99015700 | 1.40837100 | 0.85488800 | |
| H | -5.16806300 | -0.11836800 | 2.80386500 | |
| H | -3.07029900 | -1.25244200 | -0.49622000 | |
| H | -3.28411600 | 0.88122000 | -3.27411600 | |
| H | 1.04411100 | -1.92351900 | 0.54715500 | |
| H | -1.64968800 | -2.94804200 | -0.31702800 | |
| H | 0.62896400 | -2.53714300 | -3.49659600 | |
| H | 2.53234500 | -2.13017800 | -1.32471500 | |
| H | 0.68321400 | -4.52745000 | -1.00865500 | |
| H | -0.07828100 | -2.87956400 | 2.15117800 | |
| H | 2.05361500 | -4.69965800 | 0.87261400 | |
| H | 3.32101800 | -3.99960700 | -2.30229600 | |
| H | 0.11244200 | -0.17459100 | -3.18795600 | |
| H | 1.85614500 | -0.50900700 | -3.24829700 | |

| | | | |
|---|---|---|---|
| H | 0.38577300 | 0.00895200 | -0.87540600 |
| H | -2.64865900 | 1.63383200 | 3.23055400 |
| H | -2.47142800 | 0.03801000 | 4.01746400 |
| H | -2.12486100 | -1.71059200 | 2.34786300 |
| H | 1.92040400 | -0.96920200 | 2.65283600 |
| H | 0.92096700 | 1.75686600 | 1.60188500 |
| H | 3.67858700 | -0.86686400 | 1.37302200 |
| H | 5.86397100 | -0.40720600 | 0.29245900 |
| H | 2.51044200 | 3.23017800 | 0.72268100 |
| H | 6.66350400 | 2.80988600 | -0.96613000 |
| C | -5.16635800 | 2.31809000 | -1.97177400 |
| O | -5.45713500 | 2.15808800 | -3.19317300 |
| O | -5.71672200 | 3.15890800 | -1.20359300 |
| O | 4.87716400 | 3.87880300 | -0.49481900 |
| C | 3.95906900 | 4.96691200 | -0.42332800 |
| H | 3.72619700 | 5.20462300 | 0.61940300 |
| H | 4.46172300 | 5.81162400 | -0.89270500 |
| H | 3.04025300 | 4.73012700 | -0.96893000 |

| **Name** | | | **10-FMT-DIANION** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy |
| C | 2.59840900 | -0.61333700 | 0.55749400 |
| C | 3.78278200 | -1.50084000 | 0.09594100 |
| C | 4.92252300 | -1.07550600 | 0.99201700 |
| C | 4.50952200 | -0.31024000 | 2.00020900 |
| C | 3.03486300 | 0.01014000 | 1.92766400 |
| C | 2.26933200 | 0.47761900 | -0.44681700 |
| O | 2.13797700 | -0.03822000 | -1.77343900 |
| C | 3.18637200 | -0.79642700 | -2.20033200 |
| C | 4.02994300 | -1.44802000 | -1.38935500 |
| O | 1.02227000 | 1.00900300 | -0.09751300 |
| C | -0.46193600 | 2.81800200 | 0.29439700 |
| C | 0.75726000 | 2.34330100 | -0.50503000 |
| O | 0.58102100 | 2.45640800 | -1.89510400 |
| C | -0.71706800 | 2.19890800 | -2.46074300 |
| C | -1.84006200 | 2.96144000 | -1.73111400 |
| C | -1.28692900 | 3.76222500 | -0.56422100 |
| O | -0.07177100 | 3.49134000 | 1.47626200 |
| O | -2.38814700 | 4.27968100 | 0.16401900 |
| O | -2.48724400 | 3.79403300 | -2.68570800 |
| C | -1.00663600 | 0.71213700 | -2.62410900 |
| O | -1.27248900 | 0.02257200 | -1.41028900 |
| C | 2.27075900 | -0.64126900 | 3.08945300 |
| O | 2.93098200 | 1.43452800 | 1.97963000 |
| O | 0.85911600 | -0.78066900 | 2.82750000 |
| C | 0.06626100 | 0.29694500 | 2.88174800 |
| C | -1.28985300 | 0.09897800 | 2.42590700 |
| C | -1.70184500 | -1.03277700 | 1.79359400 |
| O | 0.49288100 | 1.39336400 | 3.27837800 |
| C | -2.98016200 | -1.25783800 | 1.17269900 |
| C | -3.96007900 | -0.25484500 | 1.04479400 |
| C | -5.15332400 | -0.50596400 | 0.39346600 |
| C | -5.45990500 | -1.77599400 | -0.17757500 |
| C | -4.44063000 | -2.78875000 | -0.03657400 |
| C | -3.24939200 | -2.53173200 | 0.60573000 |

Zero-point correction= 0.536929 (Hartree/Particle)
Thermal correction to Energy= 0.573145
Thermal correction to Enthalpy= 0.574089
Thermal correction to Gibbs Free Energy= 0.467920
Sum of electronic and zero-point Energies= -2059.782037
Sum of electronic and thermal Energies= -2059.745821
Sum of electronic and thermal Enthalpies= -2059.744877
Sum of electronic and thermal Free Energies= -2059.851046

| | | | |
|---|---|---|---|
| O | -6.56548600 | -2.02080000 | -0.78724100 |
| H | 1.68890900 | -1.21279600 | 0.66298200 |
| H | 3.54696800 | -2.54751700 | 0.33774900 |
| H | 5.94050300 | -1.42122900 | 0.83971900 |
| H | 5.12224900 | 0.08609900 | 2.80530800 |
| H | 3.03524100 | 1.26241100 | -0.47744800 |
| H | 3.24207500 | -0.83771600 | -3.28312400 |
| H | -1.08568400 | 1.94839500 | 0.54628700 |
| H | 1.62916600 | 2.96367800 | -0.27290400 |
| H | -0.64067600 | 2.61821000 | -3.46853300 |
| H | -2.56885000 | 2.24758900 | -1.32161300 |
| H | -0.65950500 | 4.58563600 | -0.93514100 |
| H | 0.04390600 | 2.82999200 | 2.18851900 |
| H | -2.03647300 | 4.72036600 | 0.95653500 |
| H | -3.29489000 | 4.14681600 | -2.27701500 |
| H | -0.17458800 | 0.24381500 | -3.16290200 |
| H | -1.90975900 | 0.61794000 | -3.23542900 |
| H | -0.46564600 | 0.04353600 | -0.86005400 |
| H | 2.61020700 | -1.67040800 | 3.21495300 |
| H | 2.42629300 | -0.08515300 | 4.01829200 |
| H | 2.07529100 | 1.67611900 | 2.38183800 |
| H | -1.92942800 | 0.96873900 | 2.54321000 |
| H | -0.99272200 | -1.85781500 | 1.72074900 |
| H | -3.77732400 | 0.73864800 | 1.44791100 |
| H | -5.90081700 | 0.27725300 | 0.29181400 |
| H | -2.48945400 | -3.30358700 | 0.69199700 |
| C | 5.11432500 | -2.30037200 | -1.99498600 |
| O | 5.40547600 | -2.13034800 | -3.21505400 |
| O | 5.66236500 | -3.14991100 | -1.23477400 |
| O | -4.77468600 | -3.99869900 | -0.59936300 |
| C | -3.81759200 | -5.04197600 | -0.49856000 |
| H | -3.60935300 | -5.28353000 | 0.54992100 |
| H | -4.26090500 | -5.90742700 | -0.99169400 |
| H | -2.88449700 | -4.76918600 | -1.00453000 |

# References


1. M. G. Evans and M. Polanyi, *Trans. Faraday Soc.*, 1935, **31**, 875-894.
2. H. Eyring, *J. Chem. Phys.*, 1935, **3**, 107-115.
3. D. G. Truhlar, W. L. Hase and J. T. Hynes, *J. Phys. Chem.*, 1983, **87**, 2664-2682.
4. T. Furuncuoglu, I. Ugur, I. Degirmenci and V. Aviyente, *Macromolecules*, 2010, **43**, 1823-1835.
5. E. Vélez, J. Quijano, R. Notario, E. Pabón, J. Murillo, J. Leal, E. Zapata and G. Alarcón, *J. Phys. Org. Chem.*, 2009, **22**, 971-977.
6. E. Pollak and P. Pechukas, *J. Am. Chem. Soc.*, 1978, **100**, 2984-2991.
7. A. Fernández-Ramos, B. A. Ellingson, R. Meana-Pañeda, J. M. Marques and D. G. Truhlar, *Theor. Chem. Acc.*, 2007, **118**, 813-826.
8. C. Eckart, *Phy. Rev.*, 1930, **35**, 1303.
9. R. A. Marcus, *Annu. Rev. Phys. Chem.*, 1964, **15**, 155-196.
10. R. A. Marcus, *Rev. Mod. Phys.*, 1993, **65**, 599.
11. Y. Lu, A. Wang, P. Shi and H. Zhang, *PloS one*, 2017, **12**, e0169773.
12. Y. Lu, A. Wang, P. Shi, H. Zhang and Z. Li, *PloS one*, 2015, **10**, e0133259.
13. S. F. Nelsen, S. C. Blackstock and Y. Kim, *J. Am. Chem. Soc.*, 1987, **109**, 677-682.
14. S. F. Nelsen, M. N. Weaver, Y. Luo, J. R. Pladziewicz, L. K. Ausman, T. L. Jentzsch and J. J. O'Konek, *J. Phys. Chem. A*, 2006, **110**, 11665-11676.
15. A. Galano and J. R. Alvarez-Idaboy, *J. Comput. Chem.*, 2013, **34**, 2430-2445.
16. F. C. Collins and G. E. Kimball, *J. Colloid Sci.* , 1949, **4**, 425-437.
17. M. Von Smoluchowski, *Z. Phys. Chem*, 1917, **92**, 129-168.
18. D. G. Truhlar, *J. Chem. Educ.*, 1985, **62**, 104.
19. A. Einstein, *Ann. Phys.*, 1905, **17**, 549-560.
20. G. G. Stokes, *Mathematical and Physical Papers*, University Press, Cambridge, 1905.
21. A. Galano and J. Raúl Alvarez-Idaboy, *Int. J. Quantum Chem.*, 2019, **119**, e25665.
22. Q. V. Vo, T. V. Gon, M. V. Bay and A. Mechler, *J. Phys. Chem. B*, 2019, **123**, 10672-10679.
23. Q. V. Vo and A. Mechler, *J. Chem. Inf. Model.*, 2020, **60**, 316-321.
24. Y. Okuno, *Chem.: Eur. J.*, 1997, **3**, 212-218.
25. S. Benson, *The foundations of chemical kinetics:* , Malabar, Florida, 1982.
26. C. Iuga, J. R. Alvarez-Idaboy and A. Vivier-Bunge, *J. Phys. Chem. B*, 2011, **115**, 12234-12246.
27. J. R. Alvarez-Idaboy, L. Reyes and N. Mora-Diez, *Org. Biomol. Chem.*, 2007, **5**, 3682-3689.
28. T. H. Le, T. T. Tran and L. K. Huynh, *Chemom. Intell. Lab. Syst.*, 2018, **172**, 10-16.
29. E. Dzib, J. L. Cabellos, F. Ortíz-Chi, S. Pan, A. Galano and G. Merino, *Int. J. Quantum Chem.*, 2019, **119**, e25686.

30. E. Dzib, J. L. Cabellos, F. Ortiz-Chi, S. Pan, A. Galano and G. Merino, *Eyringpy 1.0.2*, 2018, Cinvestav, Mérida, Yucatán.