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*}

¹The University of Danang – University of Science and Education, Da Nang 550000, Vietnam. ²Quality assurance and Testing center 2, Da Nang 550000, Vietnam.

³Le Thanh Phuong High School, An My, Phu Yen 621640, Vietnam

⁴The University of Danang – University of Technology and Education, Danang 550000, Vietnam.

⁵Department 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 theoryS2
Table S2: The Cartesian coordinates and energies of FMT, ANION, DIANION, TSs in the studied media (G: gas
phase; P: pentyl ethanoate; H: water)S3
References

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

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

 ΔG^{\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 ΔG^{\sharp} for the SET pathway was computed following the equations (2,3).

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4} \left(1 + \frac{\Delta G_{SET}^{0}}{\lambda} \right)^{2}$$
(2)
$$\lambda \approx \Delta E_{SET} - \Delta G_{SET}^{0}$$
(3)

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{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 results¹⁵. 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}

$$k_{\rm app} = \frac{k_{\rm TST} \kappa_{\rm D}}{k_{\rm TST} + k_{\rm D}}$$
(4)
$$k_{\rm D} = 4\pi R_{AB} D_{AB} N_A$$
(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}

$$D_{A \text{ or } B} = \frac{k_{\text{B}}T}{6\pi\eta a_{A \text{ or } B}} \tag{6}$$

 η is the viscosity of the solvents (i.e. $\eta(H_2O) = 8.91 \times 10^{-4}$ Pa s, η (pentyl ethanoate) = 8.62×10^{-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
Cartesi	ian Coordinates	Energy
С	3.23396500 -1.79783900 0.632284	
С	1.81284900 -2.33312700 0.295832	
С	2.08366000 -3.76379500 -0.130152	200 Thermal correction to Enthalpy= 0.602090
С	3.38426900 -4.03953400 -0.223514	
С	4.25453400 -2.85987600 0.130680	000 Sum of electronic and zero-point Energies= -2060.607379
С	3.46281300 -0.41671000 0.049540	
0	3.12949100 -0.37268400 -1.34608	300 Sum of electronic and thermal Enthalpies= -2060.569656
С	1.84842900 -0.72907800 -1.602869	Sum of electronic and thermal Free Energies= -2060.677083
С	1.14999600 -1.56421700 -0.824172	
0	2.64080700 0.45427000 0.777367	
С	2.32984800 2.66930600 1.519578	
С	2.52567700 1.76001500 0.312720	
0	1.38859200 1.80136600 -0.53918	
С	1.05754200 3.09639300 -1.019188	
c	0.71195700 4.00214000 0.167013	
c	1.93171600 4.06459000 1.068554	
0	3.54304900 2.69184400 2.232876	
0	1.69434300 4.82206600 2.234424	
0	0.41721500 5.32017600 -0.230478	
C	-0.06200200 2.92765200 -2.029638	
0	-1.19711700 2.27126100 -1.45869	
c	5.30056800 -3.17874100 1.198547	
0	5.04375600 -2.42567500 -0.97913	
0	6.23659300 -4.12008100 0.73369	
c	-2.18217100 3.05725000 -0.94855	
c	-3.32973900 2.31902100 -0.42085	
c	-3.40409300 0.97556600 -0.473902	
C	-4.45466300 0.10383100 0.033475	
0	-2.09003800 4.27287600 -0.93169	
c	-5.66378600 0.56614700 0.564412	
C	-6.61493200 -0.33067900 1.038180	
C	-6.36500700 -1.69786800 0.989293	
C	-5.15144200 -2.17513200 0.458153	
c	-3.13144200 -2.17513200 0.458133	
0	-7.28781100 -2.57071100 1.45039	
	-5.03546800 -3.53259500 0.47163	
O C	-3.81542300 -4.08200300 -0.00821	
c		
0	-0.28920900 -1.77260200 -1.07591 -0.89562900 -2.77561700 -0.77699	
	-0.89562900 -2.77561700 -0.77699	
0	3.32985200 -1.69814800 1.71906	
H		
H	1.16043700 -2.30551700 1.17557(
H	1.26563100 -4.44292200 -0.34886	
Н	3.82205500 -4.98622500 -0.52486	
н	4.50878300 -0.09882600 0.078656	
Н	1.46084900 -0.25344900 -2.49889	
Н	1.51823400 2.24430100 2.130017	
Н	3.42478700 2.05760500 -0.253498	
Н	1.91452100 3.53878700 -1.557150	500

1		1
H	-0.12314100 3.56042800 0.73115400	
Н	2.76547000 4.50757500 0.49640900	
Н	3.46289200 3.37485600 2.91765300	
Н	1.33642400 5.68035100 1.95517900	
н	-0.51504800 5.33655500 -0.51518700	
Н	0.27242600 2.27266300 -2.83887000	
H	-0.35146400 3.89633100 -2.44356800	
Н	5.79378700 -2.23965500 1.49848500	
Н	4.81366200 -3.61338400 2.07597800	
Н	4.46697500 -2.24169900 -1.73639400	
Н	6.57132800 -3.78786000 -0.11468300	
Н	-4.09109900 2.94983900 0.02576600	
Н	-2.58233400 0.44522600 -0.94320900	
Н	-5.87237400 1.63101200 0.60289500	
Н	-7.56043700 0.00757700 1.44937900	
Н	-3.26618300 -1.64065600 -0.43352700	
H	-6.93843000 -3.47092200 1.33475000	
Н	-3.91258100 -5.16188400 0.09699500	
н	-3.65726000 -3.82023700 -1.05947300	
Н	-2.96696000 -3.71889200 0.57970000	
н	-0.47357200 0.10221200 -1.51805000	
Name		10-FMT-G
Cartesi	ian Coordinates	Energy
С	-2.78418700 0.56122800 -0.53206600	Zero-point correction= 0.565120 (Hartree/Particle)
С	-4.11214400 -0.00116600 -1.09802800	Thermal correction to Energy= 0.601579
С	-5.16963700 0.89948200 -0.49936200	Thermal correction to Enthalpy= 0.602523
С	-4.63985100 1.97579800 0.07600400	Thermal correction to Gibbs Free Energy= 0.497076
С	-3.12749200 1.96487800 0.07483600	Sum of electronic and zero-point Energies= -2060.611523
С	-2.17279600 -0.31823500 0.54534700	Sum of electronic and thermal Energies= -2060.575063
0	-2.10527400 -1.69633700 0.13456700	Sum of electronic and thermal Enthalpies= -2060.574119
С	-3.23988400 -2.21539200 -0.36421700	Sum of electronic and thermal Free Energies= -2060.679566
С	-4.24623800 -1.48616300 -0.87479900	
0	-0.86060500 0.09499800 0.74353800	
С	0.94250900 0.74777900 2.15796100	
С	-0.36998000 -0.05072800 2.07652300	
0	-0.26891200 -1.39109600 2.45282400	
С	0.90356700 -2.17239300 2.17516000	
С	2.18630700 -1.33770600 2.13242300	
С	1.98707900 -0.05363100 2.91041800	
0	0.78397900 1.98364700 2.82358700	
0	3.22520000 0.62330700 2.93434400	
0	3.22672900 -2.13671800 2.65748000	
C	0.72121000 -3.02325600 0.92638100	
0	0.71783200 -2.26363300 -0.26722700	
C	-2.55403200 3.07133600 -0.81718000	
0	-2.70848400 2.11215500 1.42239000	
0	-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	
0	-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	
	3.03477300 1.34007100 -2.13778300	

C 5.33078200 0.17993500 -2.09344500	
C 4.27259000 -0.70503200 -1.80876300	
C 2.98914600 -0.22164700 -1.61005000	
0 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	
Н -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	
Н 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 -2.0502000	
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 2.80514200 -2.38378800 -1.83799500 H 4.20917100 -3.91040500 -1.24598600	
H 3.43447500 -2.66866400 -0.21537400	
Name	6-FMT-C5-H-OOH-G
Cartesian Coordinates	
	Energy
	Zero-point correction= 0.575080 (Hartree/Particle) Thermal correction to Energy= 0.615289
C 1.80964400 -2.09040500 -0.25030200 C 2.10719700 -3.48729200 -0.65776200	Thermal correction to Energy= 0.615289 Thermal correction to Enthalpy= 0.616234
C 3.41762400 -3.76120800 -0.56959400	Thermal correction to Gibbs Free Energy= 0.500323
C 4.22606500 -2.55448700 -0.15038100	Sum of electronic and zero-point Energies= -2211.414574
C 3.36724700 -0.10521100 -0.19813800	Sum of electronic and thermal Energies= -2211.374364
O 3.03773000 0.05965500 -1.58806500	Sum of electronic and thermal Enthalpies= -2211.373420
C 1.76611000 -0.28192600 -1.88602900	Sum of electronic and thermal Free Energies= -2211.489331
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
С	1.71033200 4.23732600	1.18374900
0	3.40537800 2.84418400	2.19515000
0	1.46865700 4.88792300	2.41127900
0	0.10898800 5.52517000	0.02647900
c		-1.95884300
0		-1.42358700
c	5.21359700 -2.84121800	
0	5.05187100 -2.08993900	
1		
0	6.18971400 -3.77186500	
C		-0.81888800
C		-0.31396500
C		-0.47207100
C	-4.47161300 0.06225200	
0		-0.70538900
C	-5.67867700 0.41325600	0.62456400
C	-6.55181600 -0.56995400	1.07651900
C	-6.22361100 -1.91295700	0.92516800
С	-5.01130700 -2.27836900	
С	-4.14705700 -1.30032300	
0	-7.06898300 -2.86963300	
0	-4.81202200 -3.62371200	
c	-3.57593400 -4.06132800	
c	-0.33113200 -1.49873000	
0	-0.87115300 -2.57064900	
0	-1.03871700 -0.43626900	
H	3.10149700 -1.49731700	
H	1.32613800 -4.15982100	
<u>H</u>	3.89919100 -4.70244500	
H		-0.13800300
H		-2.71922000
Н	1.39759700 2.32136200	2.10388500
н	3.26262200 2.39159300	-0.31579900
н	1.65283400 3.93681800	-1.47657700
н	-0.32677900 3.66735900	0.84680800
н	2.51159400 4.76012300	0.63286600
н	3.30850400 3.44286400	2.95259900
H	1.06411900 5.74724600	2.20975300
н	-0.83067600 5.52154200	
H H		-2.83045600
H	-0.65183200 4.25824600	
1		
H		
<u>H</u>	4.68294800 -3.27286600	
H	4.51181400 -1.96153400	
Н	6.59159600 -3.42731000	
н	-4.25563800 2.91606800	
н	-2.67009100 0.58087500	-1.01769600
н	-5.94628200 1.45847400	0.74640200
н	-7.49430400 -0.31861400	1.55189900
н	-3.21115000 -1.57149300	
H	-6.66929100 -3.73668300	
н	-3.59986000 -5.14968400	
H	-3.46970600 -3.72860300	
H		
	-2.73381400 -3.67860900	0.26526700

Н	-0.62033000 0.40743300 -1.73153700	
0	1.72566000 -3.19391000 2.48232500	
H	1.53293200 -4.12654400 2.27912800	
0	0.65451200 -2.51224800 1.93882500	
Н	1.06428700 -2.22096800 0.81157100	
Name	1.00428700 -2.22050800 0.01157100	6-FMT-024-H-OOH-G
	an 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
0	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
С	1.28153700 -1.55790200 -0.98963200	
0	2.96097800 0.07040700 0.83945400	
C	2.99510600 2.25881100 1.71011100	
С	3.11341000 1.39853700 0.45813400	
0	2.06546800 1.69326800 -0.45836000	
С	2.00336400 3.05276700 -0.86407700	
С	1.73772700 3.93613800 0.35932900	
C	2.88206400 3.72683500 1.33469300	
0	4.13976500 2.02011600 2.49287700	
0	2.69757700 4.44411800 2.53449300	
0	1.70810600 5.30597000 0.03545600	
C	0.94939700 3.14972900 -1.95139200	
0	-0.32153500 2.66646000 -1.50188600	
C	4.90077800 -3.99969900 1.21742500	
0	4.96896500 -3.09614500 -0.91713400	
0	5.69057700 -5.07054700 0.76261700	
C	-1.19024600 3.57299900 -0.99163500	
C C	-2.48553800 3.00651500 -0.59496900 -2.78393400 1.70627400 -0.77209200	
c	-2.78393400 1.70627400 -0.77209200 -4.00528300 1.01021700 -0.39013200	
0	-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	
0	-7.39447900 -1.12852600 0.56608500	
0	-5.21100300 -2.47421100 -0.26080000	
С	-4.15646100 -3.16495000 -0.93085100	
С	-0.14661000 -1.47839400 -1.34824000	
0	-0.95055300 -2.36280600 -1.16034800	
0	-0.55594600 -0.30727200 -1.89684000	
Н	3.18639400 -2.21488000 1.68721900	
н	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	

Н		
1 11	4.08901400 1.55969700 -0.03108700	
Н	2.96116700 3.36480600 -1.31644000	
H	0.80054500 3.62035500 0.84157600	
Н	3.81928700 4.04523700 0.84602700	
H	4.13054700 2.65951000 3.22290700	
Н	2.52833100 5.37050900 2.29849600	
H	0.81420600 5.51112500 -0.29293600	
H	1.22293300 2.49954400 -2.78666100	
Н	0.85951400 4.17897100 -2.30637200	
Н	5.52513200 -3.18296900 1.61525200	
Н	4.27096300 -4.38289700 2.02511900	
H	4.50058200 -2.78715400 -1.70768400	
Н	6.15541700 -4.76046400 -0.03100000	
Н	-3.15656900 3.72534800 -0.13657700	
Н	-2.03868000 1.07240000 -1.24069000	
Н	-5.14460400 2.74493000 0.24078400	
H	-7.15044500 1.41502500 0.87555300	
Н	-3.12119600 -0.87717600 -0.93255500	
Н	-4.46420500 -4.20928400 -0.95644900	
H	-4.03896300 -2.78304200 -1.94965700	
Н	-3.20767800 -3.05897300 -0.39693100	
H	0.05451100 0.41802800 -1.66425000	
0	-5.57296200 -2.22435500 2.49946900	
Н	-5.13786500 -2.69753500 1.76069500	
0	-6.88531900 -2.56562700 2.36075000	
Н	-7.23155200 -1.95232700 1.37447900	
Name		10-FMT-C5-H-OOH-G
C. 1. (1998) MIL - 10, C. (1997)		
Cartesia	n Coordinates	Energy
Cartesia C	2.61888400 -0.37426900 0.02942400	Zero-point correction= 0.576179 (Hartree/Particle)
Cartesia C C	2.61888400 -0.37426900 0.02942400 3.96990800 0.13506300 -0.48220600	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040
Cartesian C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.34363700	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984
Cartesia C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.09913200	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502
Cartesian C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.98918400	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619
Cartesian C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.74559600	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759
Cartesian C C C C C C C C C O	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.07660300	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.66987100	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759
Cartesian C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.82153400	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.263780002.135309002.11351400-1.436566002.741898001.54655300	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.67705200-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.706582000.133357002.90673300	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.706582000.133357002.90673300-3.778242002.737220001.93161600	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.706582000.133357002.90673300-3.778242002.737220001.93161600-1.188015003.193682000.11464400	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.706582000.133357002.90673300-3.778242002.737220001.93161600-1.188015003.193682000.11464400-1.073949002.11573700-0.79457900	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.706582000.133357002.90673300-3.778242002.737220001.93161600-1.188015003.193682000.11464400-1.073949002.11573700-0.794579002.50037500-2.879868000.35837800	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.67705200-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.778242002.737220001.93161600-1.188015003.193682000.11464400-1.073949002.11573700-0.794579002.50037500-2.879868000.358378002.43608200-1.376053002.29585200	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.54655300-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.776582000.133357002.90673300-3.778242002.737220001.93161600-1.188015003.193682000.11464400-1.073949002.11573700-0.794579002.50037500-2.879868000.358378002.43608200-1.376053002.295852001.14410000-2.81519400-0.12697700	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815
Cartesian C C C C C C C C C C C C C C C C C C C	2.61888400-0.374269000.029424003.969908000.13506300-0.482206005.00122600-0.527315000.343637004.46469600-1.495506001.099132002.95589800-1.559931000.989184001.842817000.713435000.745596001.751481001.90068300-0.076603002.875197002.32209500-0.669871003.989515001.57198800-0.821534000.540645000.276974000.94124600-1.37261900-0.066715002.32202000-0.085267000.751920002.13554700-0.263780002.135309002.11351400-1.436566002.741898001.67705200-2.690887001.871526001.67705200-2.496085000.845946002.77461900-1.22984100-1.083802003.29098900-3.778242002.737220001.93161600-1.188015003.193682000.11464400-1.073949002.11573700-0.794579002.50037500-2.879868000.358378002.43608200-1.376053002.29585200	Zero-point correction=0.576179 (Hartree/Particle)Thermal correction to Energy=0.616040Thermal correction to Enthalpy=0.616984Thermal correction to Gibbs Free Energy=0.502502Sum of electronic and zero-point Energies=-2211.427619Sum of electronic and thermal Energies=-2211.387759Sum of electronic and thermal Enthalpies=-2211.386815

C	-1.46495500 -1.95590800 -0.83216100	
0	0.32154200 -3.13953900 1.94073200	
С	-2.81171800 -1.65727200 -1.32338500	
С	-3.80175400 -2.64151100 -1.39137500	
с	-5.08393400 -2.32651700 -1.83314700	
С	-5.38965700 -1.01978800 -2.18912800	
C	-4.40076200 -0.01997800 -2.11284900	
c	-3.11590300 -0.33501600 -1.70093000	
0	-6.63508700 -0.70556800 -2.61220600	
H H	1.99141700 -0.70353700 -0.80671100	
H	4.08288100 -0.45635400 -1.58716100	
H	6.05444200 -0.27554700 0.28235100	
Н		
Н	2.31600900 1.01560700 1.68733600	
Н	2.80996900 3.34340400 -1.03273800	
Н	-1.66253800 -0.49332500 1.35311900	
H	0.59503200 0.55911100 2.97248000	
Н	-1.60274200 3.63144300 2.16478100	
H	-2.86685800 1.31699000 0.74128400	
Н	-2.23396200 1.34094100 3.72264900	
Н	-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	
Н	-2.35530600 0.43880600 -1.62407500	
Н	-6.65997600 0.24857800 -2.79801000	
С	5.14015800 2.21860000 -1.47753800	
0	5.21463700 3.38283700 -1.79776000	
0	6.15297500 1.34688300 -1.70152700	
н	6.85874600 1.84955500 -2.14467400	
0	-4.83968900 1.21803400 -2.47948500	
с	-3.97368600 2.31438700 -2.22506100	
н	-3.04041000 2.22137300 -2.78934300	
н	-4.51632000 3.20416200 -2.54278000	
Н	-3.74388500 2.37632700 -1.15534600	
0	4.80813800 -2.35922800 -2.10245900	
н	5.72364700 -2.15099200 -2.36225900	
0	4.07882500 -1.30198000 -2.58399800	
Name		10-FMT-024-H-OOH-G
	n Coordinates	Energy
C	3.06174600 -0.03735000 -0.86602500	Zero-point correction= 0.576618 (Hartree/Particle)
c	4.25279000 0.89308000 -1.20521900	Thermal correction to Energy= 0.615889
c	5.43998300 -0.04294100 -1.24958700	Thermal correction to Enthalpy= 0.616834
c	5.06874700 -1.32053800 -1.23854300	Thermal correction to Gibbs Free Energy= 0.504160
c	3.57636200 -1.50302600 -1.07529000	Sum of electronic and zero-point Energies= -2211.424833
	3.37030200 -1.30302000 -1.07323000	Jum of electronic and zero-point Lifergies2211,424055

	С	2.56645100	0.12282500	0.56071400	Sum of electronic and thermal Energies=	-2211.385562
	0	2.34720200	1.50564300	0.89502400	Sum of electronic and thermal Enthalpies=	-2211.384618
	С	3.36517700	2.34039100	0.61708000	Sum of electronic and thermal Free Energies=	-2211.497292
	С	4.32867000	2.08357100	-0.28282800		
	0	1.33239500	-0.50845000	0.65770500		
	С	-0.16844700	-2.01632700	1.72996400		
	С		-1.07499200	1.93383900		
	0		-0.09550200	2.91253100		
	С	-0.40693400		3.12765200		
	С	-1.59592800		2.73037000		
	С		-1.78894100	2.81740500		
	0		-3.37903800	1.74917800		
	0		-2.55594000	2.58194600		
	0	-2.66843000		3.58822200		
	С	-0.45064800	1.92027800	2.47307900		
	0	-0.51679100		1.06046400		
	С			-2.33136900		
	0		-2.33699400	0.05644100		
	0		-1.88661800			
	С		-2.68023900			
	С		-2.33029000			
	С		-1.05394500			
	0		-3.61157700			
	С		-0.65495900			
	С		-1.40963000			
	С		-1.02914100			
	С	-5.23585800				
	С	-4.18131600				
	С	-2.85198300				
	0	-6.48790100		-1.05950900		
	Н	2.20466200				
	н	4.11029300		-2.21992300		
	Н	6.45668600				
	Н		-2.18376400			
	Н		-0.27054700	1.29328000		
	Н	3.32848200		1.18397200		
	Н		-1.76542600	0.77587600		
	Н		-1.65825700	2.25998800		
	Н	-0.46262900		4.21415000		
	Н		-0.12794100	1.68540700		
	Н		-2.01829400	3.80833400		
	Н		-3.66306900			
	Н		-3.48161200	2.48573600		
	Н		-0.67707300	3.46007600		
	Н		2.50091500	2.79807500		
	Н		2.43429200	2.81619100		
	Н	0.36594900		0.74507200		
	Н		-1.59420600			
	Н		-3.17776000			
	Н		-2.96096300			
	Н		-3.16561300			
	Н		-0.26034100			
	Н		-2.27233800			
	Н		-1.58009000			
L	Н	-2.05331/00	1.05610100	-0.38846/00		

C	5.35160800 3.13172200 -0.45628000	
0	5.48370800 4.12100000 0.22823400	
0	6.16273200 2.87603700 -1.51017100	
н	6.79467800 3.61408700 -1.56501100	
0	-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	
Н	-3.36076700 1.67991200 1.70068100	
0	-5.57214700 2.74670300 -2.41413900	
H	-5.10547300 2.97852800 -1.58431600	
0	-6.84839600 2.50185300 -1.99977400	
Н	-6.75522000 1.46683900 -1.39743700	
Name		6-FMT-P
Cartesia	n Coordinates	Energy
С	3.23396500 -1.79783900 0.63228400	Zero-point correction= 0.562421 (Hartree/Particle)
С	1.81284900 -2.33312700 0.29583200	Thermal correction to Energy= 0.598826
С	2.08366000 -3.76379500 -0.13015200	Thermal correction to Enthalpy= 0.599770
С	3.38426900 -4.03953400 -0.22351400	Thermal correction to Gibbs Free Energy= 0.493731
С	4.25453400 -2.85987600 0.13068000	Sum of electronic and zero-point Energies= -2060.647747
С	3.46281300 -0.41671000 0.04954000	Sum of electronic and thermal Energies= -2060.611342
0	3.12949100 -0.37268400 -1.34608300	Sum of electronic and thermal Enthalpies= -2060.610398
С	1.84842900 -0.72907800 -1.60286900	Sum of electronic and thermal Free Energies= -2060.716437
С	1.14999600 -1.56421700 -0.82417200	
0	2.64080700 0.45427000 0.77736700	
С	2.32984800 2.66930600 1.51957800	
С	2.52567700 1.76001500 0.31272000	
0	1.38859200 1.80136600 -0.53918000	
С	1.05754200 3.09639300 -1.01918800	
С	0.71195700 4.00214000 0.16701300	
С	1.93171600 4.06459000 1.06855400	
0	3.54304900 2.69184400 2.23287600	
0	1.69434300 4.82206600 2.23442400	
0	0.41721500 5.32017600 -0.23047800	
С	-0.06200200 2.92765200 -2.02963800	
0	-1.19711700 2.27126100 -1.45869400	
С	5.30056800 -3.17874100 1.19854700	
0	5.04375600 -2.42567500 -0.97913800	
0	6.23659300 -4.12008100 0.73369100	
С	-2.18217100 3.05725000 -0.94855100	
С	-3.32973900 2.31902100 -0.42085100	
С	-3.40409300 0.97556600 -0.47390100	
С	-4.45466300 0.10383100 0.03347500	
0	-2.09003800 4.27287600 -0.93169500	
С	-5.66378600 0.56614700 0.56441200	
С	-6.61493200 -0.33067900 1.03818000	
С	-6.36500700 -1.69786800 0.98929300	
С	-5.15144200 -2.17513200 0.45815300	
С	-4.20682800 -1.28341500 -0.02003400	
0	-7.28781100 -2.57071100 1.45039100	
0	-5.03546800 -3.53259500 0.47163000	
С	-3.81542300 -4.08200300 -0.00821700	
С	-0.28920900 -1.77260200 -1.07591100	
0	-0.89562900 -2.77561700 -0.77699900	

0 -0.9463330 -0.74009700 -1.65923600 H 1.15043700 -2.30551700 1.1755700 H 1.862205500 -4.9822200 -0.3488600 H 3.82205500 -0.5248600 H 1.66943700 -0.5748600 H 1.6924300 -2.4988400 H 1.6924300 -2.3180100 H 1.6924300 -2.3189200 H 1.91452100 3.5687600 H -0.0574500 -0.3254800 H -0.12742600 -2.571500 H -0.3724500 -2.2786500 H -0.3724500 -2.2385500 H -0.7724500 -2.2385500 H -4.6697500 -2.2488900 H -4.6697500 -2.2488900 H -4.6697500 -2.238500 H -4.6975700 -1.7659400 H -4.5323400 0.0257600 H -5.571500 -1.2489200 H -3.65726000 -3.1483200 H -4.03757200 0.32025700 H </th <th></th> <th></th> <th></th>			
H 1.15643700 2.3051700 1.17557000 H 1.3663100 4.4922020 0.3488400 H 3.8627500 -0.5248600 0.0786500 H 1.4604400 0.25344900 2.3488400 H 1.46042700 2.057500 0.2534800 H 1.46042700 2.0575500 0.3537670 H 0.1213100 3.5602800 0.3115400 H 0.1234500 2.348500 1.9551300 H 0.32745600 2.2365500 1.9848500 H 0.37745600 2.2365500 1.9848500 H 5.6933100 2.4435800 H 4.81366200 3.783400 H 0.57132800 3.783400 H 4.81366200 3.6334400 J 0.44352600 -1.4483300 H -3.6573200 3.2023700 H -3.6572500 3.2322300 H -3.657200 3.2322300 H -4.63843000 -3.6326020 H -3.6572500 0.5324500 H -3.6572500 <td>0</td> <td>-0.94633300 -0.74009700 -1.65923600</td> <td></td>	0	-0.94633300 -0.74009700 -1.65923600	
H 1.25653100 -4.44292200 -0.3488600 H 3.822050 -4.96872500 -0.25844900 -2.49889400 H 1.46084900 -0.25344900 -2.49899400 H 1.5182400 2.24491010 2.1301700 H 3.42478700 0.5077500 -0.4549800 H -0.12314100 3.56042800 0.73115400 H -0.757500 0.49649000 -1.716500 H -0.51504800 5.33655500 -0.51518700 H -0.51504800 5.33655500 -1.73639400 H -0.3514600 3.8652000 -1.73639400 H -4.69109900 2.94983900 0.02576600 H -3.587237400 1.63101200 0.60289500 H -3.561300 1.43937900 H -3.65726000 -3.1889200 0.55970000 H -3.8203700 1.05947300 H -3.65726000 -3.189200 0.5976000 H -3.4572600 0.43985200 1.9597000 H -3.65726000 -3.189200 0.5926600 -3.1	Н		
H 3.82205500 4.98622500 0.52348000 H 1.46084900 0.25344900 2.49899400 H 1.16084900 0.2534900 2.49899400 H 1.151822400 2.4442100 2.1301700 H 1.12427670 0.5075000 0.25349800 H 1.13622400 3.5378700 1.5571560 H 1.33642400 5.66035100 1.95517900 H 1.33642400 5.66035100 1.95517900 H 0.3254600 2.4358800 0.31538700 H 0.3254600 3.8653300 0.2435600 H 4.366200 3.6138400 2.07597800 H 4.43166200 0.43425000 0.02576600 H -5.87237400 1.63101200 0.60289500 H -5.643000 0.02577600 4.43877000 H -5.643200 0.1532060 0.53206600 H -5.633100 1.0547300 0.0227700 H -3.65726000 3.82023700 -105947300 H -5.6383000 -1.63934800 0.602320	H	1.16043700 -2.30551700 1.17557000	
H 4.5087300 -0.09882600 0.07865600 H 1.6084900 -0.25344900 2.13001700 H 3.42478700 2.05760500 -0.25349800 H 1.915120 3.56042800 0.73115400 H -0.755700 0.46464900 -0.7115500 H -0.755700 0.4546490 2.1765300 H -0.5150400 5.7057800 -4.8758700 H -0.5150400 5.23655500 -0.51518700 H -0.72746600 -2.7266300 -1.7453900 H -0.5150400 5.3665500 -0.51518700 H 4.57373700 -2.3965900 -1.7453900 H 4.57373700 -0.2376500 -1.44937900 H -5.6513300 -0.452200 -0.8285700 H -3.02581300 -1.6405500 -0.5977000 H -3.0264300 -1.5184200 0.0597700 H -3.02669000 -1.5189200 0.5797000 H -3.02669000 -1.5189200 0.5797000 H -3.02669000 -1.5189200 0.5797000 </td <td> Н</td> <td>1.26563100 -4.44292200 -0.34886800</td> <td></td>	Н	1.26563100 -4.44292200 -0.34886800	
H 1.46084900 2.23449000 2.49895400 H 1.5182400 2.2449100 2.1301700 H 3.42478700 2.03766500 -0.25349800 H 1.91452100 3.53878700 -155715600 H -0.25240800 3.7495600 2.1575300 H -2.76547000 4.5975750 0.49640900 H -3.365500 0.1515700 H 0.2724600 2.27266300 -2.8387000 H 0.35146400 3.8663100 -2.44356800 H -0.35146400 3.8663100 -2.44356800 H 4.4697500 -2.21469900 -1.7383400 H -4.697500 -2.4169900 -1.7483400 H -4.697500 -2.4149700 0.6028500 H -5.87237400 1.63101200 0.6028500 H -3.6518300 1.6405500 -2.4943700 H -3.6518300 0.69493200 0.5797000 H -3.851200 0.5512660 2.7727600 C -2.7481700 0.5512660 2.7727600 C <td>Н</td> <td>3.82205500 -4.98622500 -0.52486000</td> <td></td>	Н	3.82205500 -4.98622500 -0.52486000	
H 1.51823400 2.24430100 2.13001700 H 3.4478700 2.0576050 -0.25349800 H 1.91452100 3.53878700 -1.5571560 H -0.12314100 3.56042800 2.3115400 H 3.46289200 3.37485600 2.91765300 H -0.51504800 5.3365500 -0.51518700 H -0.3164000 3.8603100 -2.48356800 H -0.3134600 -2.48356800 H 4.3136200 -3.133400 -0.7579700 H -4.6697500 -2.44356800 H -4.8136200 -3.133400 0.02757600 H -4.6133400 0.02757600 H -5.7327800 0.0275600 H -5.613200 -5.43325700 H -3.6572600 -3.43325700 H -3.6572600 -3.2023700 H -3.6572600 -3.2024700 H -2.6663600 -1.5180500 Marce Energy Energy C -2.78418700 0.5612280 C -2.172796	Н	4.50878300 -0.09882600 0.07865600	
H 3.42478700 2.65765000 -0.25349800 H 1.91452100 3.56378700 -1.55715600 H -0.12314100 3.6042800 0.73115400 H 2.726547000 4.5075750 0.49640900 H 3.4528200 3.5378500 0.91765300 H 0.51504800 5.3655500 -0.51518700 H 0.3516400 3.99633100 -2.44356800 H 4.7532800 -3.1738400 0.7577300 H 4.46697500 2.24169900 1.73639400 H -4.6927800 2.34883900 0.02576600 H -5.87237400 1.63101200 0.60289500 H -5.6643000 -0.43352700 1.48937900 H -3.26613800 -1.64065600 -0.43352700 H -3.26613800 -1.64065600 -0.43352700 H -3.66732000 -1.2320201 -1.51805000 H -3.66742000 -5.6128400 0.53206600 C -2.78418700 0.56122800 -2.6901400 C -2.78418700 0.4984200 <t< td=""><td>Н</td><td>1.46084900 -0.25344900 -2.49889400</td><td></td></t<>	Н	1.46084900 -0.25344900 -2.49889400	
H 191452100 3.53878700 -1.55715600 H -0.12314100 3.56042800 0.73115400 H 2.7654700 4.50757500 0.48640900 H 3.3642400 5.8603100 1.55517900 H 0.35144600 3.89633100 -2.44356800 H -0.51504480 3.89633100 -2.44356800 H -0.35146400 3.89633100 -2.44356800 H -3.1384020 0.5775600 -1.73639400 H 4.46697500 -2.24169900 -0.73639400 H -4.5112800 -3.7878600 -0.11468300 H -4.5112800 -3.7878600 -0.143835700 H -4.528234400 0.60289500 H -3.2672600 -3.24052700 1.05947300 H -3.9125810 5.1618400 0.06089500 H -3.65726000 -3.1889200 0.57970000 H -3.9125810 -15050700 Lartesian Coordinates Energy C -2.78418700 0.5612800 -5320600 C -2.1654700	Н	1.51823400 2.24430100 2.13001700	
H -0.12314100 3.56042800 0.43115400 H 2.76547000 4.5075750 0.49640900 H 3.3425200 3.3748500 2.91765300 H 0.51504800 5.3865500 0.55115700 H 0.27242620 2.2766300 -2.4386700 H 0.27242600 2.2365500 -2.4386700 H 4.4667500 2.2416900 -1.7639400 H 4.4667500 2.2416900 -1.7639400 H -4.09109900 2.9498390 0.02576600 H -5.6723700 0.44322600 -0.4332700 H -5.6750300 0.0257700 -1.44937900 H -3.91258100 -5.6188400 0.0699500 H -3.65726000 -3.3128200 0.5320600 H -3.6572600 -5.188200 0.57970000 H -4.69385100 1.05947300 C -2.78413700 0.55122800 0.45936200 C -3.1258100 0.5797590400 2.1702100 H -3.6672600 0.314356700 2.1702100	Н		
H 2.76547000 4.50757500 0.49640900 H 3.3642400 5.60035100 1.95517900 H 0.51546400 3.89633100 -2.43556800 H -0.035146400 3.89633100 -2.43556800 H -0.035146400 3.89633100 -2.44356800 H -0.35146400 3.89633100 -2.44356800 H 4.31366200 -3.61338400 2.07597800 H 4.46697500 -2.24169900 -1.7639400 H -4.0510900 0.02576600 H -5.57237400 1.63101200 0.06289500 H -3.5626000 -3.7189200 0.13475000 H -3.266618300 -1.69347300 1.05947300 H -3.65726000 -3.7189200 0.57970000 H -3.6572600 -3.82023700 -1.9547300 H -3.6572600 -3.87023700 1.05947300 H -3.6572600 -3.71889200 0.57970000 H -3.6572600 -3.970802 -1.99694800 C -2.76418700 0.56122800 -0.593700	Н	1.91452100 3.53878700 -1.55715600	
H 3.4628200 3.37485600 2.91765300 H 1.33642400 5.68035100 1.95517900 H 0.27242600 2.27266300 -2.3887000 H 0.27347800 2.23965500 1.49848500 H 5.79378700 2.23965500 1.49848500 H 4.6667500 2.21469900 1.73639400 H 4.6667500 2.24169900 1.73639400 H -4.6019990 2.9493800 0.02576600 H -4.528233400 0.46325200 0.93420900 H -7.56043700 0.06795700 1.44937900 H -3.25618300 -1.6405500 -0.43352700 H -3.65726000 -3.82023700 -1.05947300 H -3.65726000 -3.82023700 -1.05947300 H -3.65726000 -3.71289200 0.57970000 H -3.6572600 -3.82023700 -1.05947300 H -3.6572600 -3.2108200 -0.5797000 C -2.78418700 0.0514650 -0.9980200 C -2.78418700 0.03145670	Н	-0.12314100 3.56042800 0.73115400	
H 1.33642400 5.68035100 1.95517900 H 0.27242600 2.27266300 -2.8388700 H 0.35146400 3.89633100 -2.44356800 H 5.79378700 2.23965500 1.949845500 H 4.81366200 3.61338400 2.07597800 H 4.81366200 3.61338400 2.07597800 H 4.46697500 2.24169900 1.73639400 H -6.587237400 0.44522600 0.94320900 H -2.56233700 0.00757700 1.44337900 H -3.6045800 -0.43352700 0.44352700 H -3.6045800 -0.43352700 0.51184800 H -3.6045800 -0.43352700 0.5118400 H -3.6045800 -0.51805000 1.9547300 H -3.6054800 -0.51805000 1.9547300 H -3.6375200 3.8202370 -0.5947300 H -0.6375200 0.5180800 -0.43952700 C -2.78418700 0.56122800 -0.5326600 C -3.6385510 1.9553700 0			
H -0.51504800 5.3365500 -0.5181700 H -0.35146400 3.8963100 -2.4355800 H 5.79378700 -2.2365500 1.49848500 H 4.81366200 -2.43156800 -1.73633400 H 4.46697500 -2.24169900 -1.73633400 H 4.46697500 -2.44169900 -2.73633400 H -6.9138200 -3.7878600 -0.11468300 H -5.57132800 -3.7878600 -0.41327900 H -5.5643700 0.00757700 1.44937900 H -3.26513300 -1.64065600 -0.4332700 H -3.6572600 -3.32232700 -1.05947300 H -3.6572600 -3.2189200 0.57970000 H -2.6565000 -3.7189200 0.57970000 H -2.6565000 -3.2180200 0.53206600 C -2.78418700 0.5612280 -0.59320800 C -4.1214400 -0.0116600 -1.09802800 C -3.12749200 1.96487800 0.76604201 C -3.12749200 1.96487800	Н	3.46289200 3.37485600 2.91765300	
H 0.2724600 2.2766300 -2.8387000 H 5.7937700 -2.23965500 1.49845500 H 4.8136200 -3.61338400 2.07597800 H 4.46697500 -2.24169900 -1.73639400 H 4.46997500 -2.24169900 -1.73639400 H -4.90109900 2.9483300 0.02576600 H -2.58233400 0.44522600 -0.94320900 H -3.5643300 1.64065600 0.43352700 H -3.56613300 -3.6405600 0.33475000 H -3.55726000 3.8023700 1.53475000 H -3.56726000 3.2023700 1.53475000 H -3.65726000 -3.71889200 0.57970000 H -3.65726000 -3.5325600 2.779700 C -2.78418700 0.56122800 -0.5320600 C -3.1698100 1.09802800 1.maral correction to Entergy= 0.600232 C -4.63985100 1.97579800 0.07604000 Sum of electronic and thermal Energies= -2060.612249 Sum of electronic and thermal Energies=	Н	1.33642400 5.68035100 1.95517900	
H -0.35146400 3.89633100 -2.43586200 H 5.79378700 -2.2365500 1.49848500 H 4.81366200 -3.61338400 0.07597800 H 4.46697500 -2.24169900 -1.73639400 H -4.09109900 2.9488300 0.022576600 H -4.0910900 0.044522600 -0.94320900 H -5.87237400 1.6405500 -0.3325700 H -5.65343000 -3.16405500 -1.3475000 H -3.6512800 -5.16188400 0.09699500 H -3.6572600 -3.32023700 -1.05947300 H -3.6572600 -3.31282200 0.57970000 H -3.6572600 -3.122200 0.512800 C -2.78418700 0.55122800 -0.53266600 C -2.78418700 0.5512800 0.53266000 C -3.12749200 1.95847800 0.7483600 C -3.12749200 1.95847800 0.7483600 C -3.12749200 1.9583700 0.34825700 C -3.12749200 1.9683700	Н		
H 5.79378700 -2.2365500 1.49848500 H 4.81366200 -3.61338400 2.07597800 H 4.46697500 -2.24169900 -1.73639400 H 6.57132800 -3.78786000 -0.11468300 H -5.8233400 0.4522600 -9.94329000 H -5.87337400 1.6301200 0.60289500 H -7.56043700 0.00757700 1.44937900 H -3.326613300 -3.47092200 1.34475000 H -6.33843000 -3.47092200 1.34937900 H -3.91258100 -5.16188400 0.09699500 H -3.65726000 -3.82023700 -1.05947300 H -3.65726000 -3.82023700 -1.05947300 H -0.4757200 0.1022120 -1.5190500 ID-FMT-P Cartesian Coordinates Energy C -2.78418700 0.56122800 -0.53206000 C -3.12749200 0.3842200 0.74834800 C -3.12749200 0.7483500 0.74834800 C -3.12749	Н	0.27242600 2.27266300 -2.83887000	
H 4.81366200 -3.61338400 2.07597800 H 4.46597500 -2.24169900 -1.73639400 H -4.09109900 2.94983900 0.02576600 H -4.09109900 2.94983900 0.02576600 H -2.58233400 0.40522600 -9.9320900 H -5.87237400 0.60289500 H -7.56043700 0.00757700 1.44937900 H -3.26518300 -1.64065600 -0.3325700 H -3.65726000 -3.47092200 0.53943000 H -3.65726000 -3.71889200 0.57970000 H -3.65726000 -1.51805000 Zero-point correction = 0.563269 (Hartree/Particle) C -2.78418700 0.56122800 -0.53206600 Zero-point correction to Energy= 0.600232 C -4.11214400 -0.0716600 1.05802800 Thermal correction to 5lbs Free Energye 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and thermal Enthalpies= -2060.649212 Sum of electronic and thermal Free Energies= -2060.611204 Sum of electronic and thermal Enthalpies= <td></td> <td>-0.35146400 3.89633100 -2.44356800</td> <td></td>		-0.35146400 3.89633100 -2.44356800	
H 4.46697500 -2.24169900 -1.73633400 H -6.5713280 -3.7878600 -0.11468300 H -4.09109900 0.24576600 -0.94320900 H -2.58233400 0.44522600 -0.94320900 H -5.8723740 1.6301020 0.6028500 H -7.56043700 0.00757700 1.44937900 H -3.26618300 -1.64065600 -0.43352700 H -3.31258100 0.516188400 0.09699500 H -3.65726000 -3.82023700 1.05947300 H -2.9669600 -3.71889200 0.57970000 H -0.47357200 0.10221200 -1.5180500 Name Energy 0.600232 C -2.76418700 0.55122800 -0.5320600 C -3.12749200 1.96487600 0.07483600 C -3.12749200 1.96487600 0.07483600 C -3.12749200 1.96487600 0.07483600 C -3.12749200 1.96487600 0.37483600 C -3.23988400 -2.21539200 0.3641700			
H 6.57132800 -3.78780000 -0.11468300 H -4.0910900 2.94983900 0.02576600 H -2.58233400 0.44522600 -0.94329000 H -5.87237400 1.63101200 0.60289500 H -5.6618300 -1.64065600 -0.43352700 H -6.93843000 -3.47092200 1.33475000 H -3.91258100 -5.1618400 0.0599500 H -3.9266696000 -3.71889200 0.57970000 H -0.47357200 0.10221200 -1.51805000 Name Energy C -2.78418700 0.56122800 -0.53260600 C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Energy= 0.600232 C -3.12749200 1.9487800 0.07480400 Sum of electronic and thermal Energies= -2060.649212 C -3.12749200 1.9487800 0.54534700 Sum of electronic and thermal Energies= -2060.649212 C -3.2398400 -2.1539200 0.3452700 Sum of electronic and thermal Energies= -2060.649212 C -3.2398400	Н		
H -4.09109900 2.94983900 0.02576600 H -2.58233400 0.44522600 -0.94320900 H -5.87237400 0.00757700 1.44937900 H -3.26618300 -1.44065600 -0.43352700 H -3.91258100 -5.16188400 0.09699500 H -3.91258100 -5.16188400 0.0599500 H -3.65726000 -3.7188200 0.57970000 H -2.96696000 -3.7188200 0.57970000 H -2.9669600 -1.51805000 Name C -2.78418700 0.56122800 -0.53206600 C -4.11214400 -0.0016600 -1.09802800 C -4.63985100 1.9579800 0.07600400 C -4.63985100 1.9579800 0.07604000 C -3.12749200 1.9643700 0.3453700 O -2.10527400 -0.3823500 0.543470 G -3.23988400 -2.21539200 0.34456700 C -3.23988400 -2.4523800 0.47453800 C </td <td>H</td> <td>4.46697500 -2.24169900 -1.73639400</td> <td></td>	H	4.46697500 -2.24169900 -1.73639400	
H -2.58233400 0.44522600 -0.94320900 H -5.87237400 1.63101200 0.00289500 H -7.56043700 0.00757700 1.44393700 H -3.26618300 -1.6406560 -0.43352700 H -3.65726000 -3.82023700 -1.05947300 H -3.65726000 -3.82023700 -1.58947300 H -2.96696000 -3.7188200 0.57970000 H -3.65726000 -3.82023700 -1.58947300 H -2.96696000 -3.7188200 0.57970000 H -3.65726000 -3.82023700 -1.5894700 C -2.78418700 0.5612800 -0.53206600 C -4.11214400 -0.0016600 -1.09802800 Thermal correction to Enregy= 0.600232 C -4.63985100 1.9579800 0.0760400 Thermal correction to Enthalpy= 0.601176 C -2.17279600 -3.12749200 0.3482300 0.494354700 Sum of electronic and thermal Enregies= -2060.612249 O -2.10527400 -1.6963700 0.74353800 C -3.23988400 -2.1579	Н		
H -5.87237400 1.63101200 0.60289500 H -7.56043700 0.00757700 1.44937900 H -6.93843000 -1.64065600 0.43352700 H -6.93843000 -3.47092200 1.33475000 H -6.93843000 -3.82023700 1.05947300 H -2.96569000 -3.71882920 0.57970000 H -0.47357200 0.10221200 -1.51805000 IO-FMT-P Cartesian Coordinates C -2.78418700 0.56122800 -0.53206600 C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Energy= 0.600232 C -5.16963700 0.89948200 -0.49936200 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07604000 Thermal correction to Gibbs Free Energy= -2060.649212 C -2.17279600 -3.1823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.32988400 -2.18630700 0.13456700 Sum of electronic and thermal Energies= -2060.612249 <tr< td=""><td>Н</td><td>-4.09109900 2.94983900 0.02576600</td><td></td></tr<>	Н	-4.09109900 2.94983900 0.02576600	
H -7.56043700 0.00757700 1.44937900 H -3.26518300 -1.64065600 -0.43352700 H -3.91258100 -5.16188400 0.09699500 H -3.91258100 -3.71889200 0.57970000 H -2.96566000 -3.71889200 0.57970000 H -2.05696000 -3.71889200 0.57970000 H -0.47357200 0.10221200 -1.51805000 Name Energy 0.0016600 -1.09802800 C -2.78418700 0.56122800 -0.53206600 C -4.63985100 1.97578800 0.0760400 C -3.12749200 1.96487800 0.07483600 C -3.12749200 1.96487800 0.07483600 C -3.12749200 1.96487800 0.07483600 C -3.10527400 -1.8963700 0.34325700 C -3.2398400 -2.21539200 -0.36421700 C -3.2398400 -2.217576100 0.7435800 C -0.36998000 0.7477900 2.15796100 C -0.36981000 -1.33170600	H	-2.58233400 0.44522600 -0.94320900	
H -3.26618300 -1.64065600 -0.43352700 H -6.93843000 -3.4709200 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 Io-FMT-P Cartesian Coordinates Energy C -2.78418700 0.56122800 -0.53206600 C -4.112214400 -0.00116600 -1.09802800 C -3.12749200 1.96487800 0.07600400 C -3.12749200 1.96487800 0.07483600 C -2.10527400 -1.31823500 0.54524700 C -3.2398400 -2.21539200 0.3454700 C -3.2398400 -2.1539200 0.345421700 C -4.42623800 1.48616300 -0.87479900 O -0.8690500 0.94735300 1.3455700 C -3.2398400 -2.1752900 0.37453800 C -3.23988400 <td>H</td> <td>-5.87237400 1.63101200 0.60289500</td> <td></td>	H	-5.87237400 1.63101200 0.60289500	
H -6.93843000 -3.47092200 1.33475000 H -3.91258100 -5.16188400 0.09699500 H -3.65726000 -3.71882020 0.57970000 H -0.47357200 0.10221200 -1.51805000 Name C -2.78418700 0.56122800 -0.53206600 C -2.78418700 0.56122800 -0.53206600 C -4.11214400 -0.0116600 -1.09802800 C -5.16963700 0.89948200 -0.49936200 C -4.32985100 1.97579800 0.07600400 C -3.12749200 1.96487800 0.7483600 C -2.17279600 -0.31823500 0.54534700 Sum of electronic and zero-point Energies= -2060.612249 Sum of electronic and thermal Energies= -2060.611304 C -3.23988400 -2.21539200 0.36421700 C -0.3660500 0.09499800 0.74353800 C -0.36998000 0.74353800 Sum of electronic and thermal Energies= -2060.611304 Sum of electronic and thermal Fine Energies -2060.61224	Н	-7.56043700 0.00757700 1.44937900	
H -3.91258100 -5.16188400 0.09699500 H -3.65726000 -3.82023700 -1.05947300 H -2.96696000 -3.71889200 0.5770000 H -0.47357200 0.1022120 -1.5180500 ID-FMT-P Cartesian Coordinates Energy C -2.78418700 0.56122800 0.53206600 Zero-point correction to Energy= 0.600232 C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Entraly= 0.60176 C -4.63985100 1.97579800 0.0760400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.6953700 0.13456700 Sum of electronic and thermal Energies= -2060.612249 Sum of electronic and thermal Enthalpies -2060.612249 Sum of electronic and thermal Free Energies= -2060.718628 C -4.24623800 -0.87479900 0.74533800 C -32988400 2.17596100 C -0.86060500 0.0949800 <td< td=""><td>Н</td><td>-3.26618300 -1.64065600 -0.43352700</td><td></td></td<>	Н	-3.26618300 -1.64065600 -0.43352700	
H -3.65726000 -3.82023700 -1.05947300 H -2.96696000 -3.71889200 0.57970000 H -0.4735720 0.10221200 -1.51805000 10-FMT-P Cartesian Coordinates Energy C -2.78418700 0.56122800 -0.53206600 C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Energy= 0.600232 C -4.63985100 1.9757800 0.07483600 Thermal correction to Enthalpy= 0.601176 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.10527400 -1.6963700 0.3456700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.6963700 0.34356700 Sum of electronic and thermal Energies= -2060.718628 C -3.2398400 -2.1753900 0.74353800 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.0572800 2.17516000 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000	H	-6.93843000 -3.47092200 1.33475000	
H -2.96696000 -3.71889200 0.57970000 H -0.47357200 0.10221200 -1.51805000 Name Io-FMT-P Cartesian Coordinates Energy C -2.78418700 0.56122800 -0.53206600 C -2.78418700 0.56122800 -0.5320600 C -4.11214400 -0.00116600 1.09802800 C -5.16963700 0.89948200 -0.49936200 C -4.63985100 1.97579800 0.07604000 C -3.12749200 1.96487800 0.07483600 C -2.10527400 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -0.36421700 C -4.24623800 -0.47353800 C -4.24623800 -0.47353800 C -4.24623800 -0.74353800 C -0.36998000 0.74753800 C -0.36998000 0.74753800 C -0.36998000 0.74753800 C -0.36998000 0.05052300 O <t< td=""><td>H</td><td>-3.91258100 -5.16188400 0.09699500</td><td></td></t<>	H	-3.91258100 -5.16188400 0.09699500	
H -0.47357200 0.10221200 -1.51805000 Name 10-FMT-P C -2.78418700 0.56122800 -0.503269 (Hartree/Particle) C -2.78418700 0.56122800 -0.53206600 Zero-point correction to Energy= 0.600232 C -4.11214400 -0.00116600 -0.9903200 Thermal correction to Energy= 0.60176 C -4.63985100 1.97579800 0.0760400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.10527400 -0.4963700 0.13456700 Sum of electronic and thermal Energies= -2060.611304 C -3.2398400 -2.21539200 -0.36421700 Sum of electronic and thermal Enthalpies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.745280200 2.15796100 Sum of electronic and thermal Free Energies=	H	-3.65726000 -3.82023700 -1.05947300	
Name 10-FMT-P Cartesian Coordinates Energy C -2.78418700 0.56122800 -0.53206600 Zero-point correction= 0.563269 (Hartree/Particle) C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Energy= 0.600232 C -5.16963700 0.89948200 -0.49936200 Thermal correction to Enthalpy= 0.601176 C -4.63985100 1.97579800 0.07600400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.17279600 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Energies= -2060.718628 C -0.36998000 -0.7477900 2.15796100 C -0.3699800 2.07652300 O <		-2.96696000 -3.71889200 0.57970000	
Cartesian Coordinates Energy C -2.78418700 0.56122800 -0.53206600 Zero-point correction= 0.563269 (Hartree/Particle) C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Energy= 0.600232 C -5.16963700 0.89948200 -0.49936200 Thermal correction to Enthalpy= 0.601176 C -4.63985100 1.97579800 0.07600400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611204 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Energies= -2060.718628 C -4.24623800 -1.48616300 0.74353800 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.05072800 2.07552300 O -0.26891200 -1.39109600 2.45282400 C 1.98707900	Н	-0.47357200 0.10221200 -1.51805000	
C -2.78418700 0.56122800 -0.53206600 Zero-point correction= 0.563269 (Hartree/Particle) C -4.11214400 -0.00116600 -1.09802800 Thermal correction = 0.563269 (Hartree/Particle) C -5.16963700 0.89948200 -0.49936200 Thermal correction to Energy= 0.600232 C -3.12749200 1.96487800 0.07600400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Enthalpies= -2060.718628 C -4.24623800 1.48616300 -0.74553800 C -0.36998000 0.74353800 C 0.90356700 -2.17239300 2.15796100 C 2.18630700 2.13242300 C 1.98707900 1.93109600 2.45282400 2.138434400 2.91041800			10-FMT-P
C -4.11214400 -0.00116600 -1.09802800 Thermal correction to Energy= 0.600232 C -5.16963700 0.89948200 -0.49936200 Thermal correction to Enthalpy= 0.601176 C -4.63985100 1.97579800 0.07600400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.17279600 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Free Energies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36699500 0.74777900 2.15796100 C -0.66991200 -1.39109600 C 1.9870700 -0.372300 2.17516000 C -1.38770600 2.13242300 C 1.98707900 0.62330700 2			
C -5.16963700 0.89948200 -0.49936200 Thermal correction to Enthalpy= 0.601176 C -4.63985100 1.97579800 0.07600400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.17279600 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Free Energies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 C -0.86060500 0.09499800 0.74353800 C -0.60176 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.777900 2.15796100 C Sum of electronic and thermal Free Energies= -2060.718628 C 0.90356700 -2.17239300 2.17516000 C 1.38707900 2.13242300 </td <td></td> <td></td> <td></td>			
C -4.63985100 1.97579800 0.07600400 Thermal correction to Gibbs Free Energy= 0.493852 C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.17279600 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Energies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 C -0.86060500 0.09499800 0.74353800 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.05072800 2.07652300 Sum of electronic and thermal Free Energies= -2060.718628 C 0.90356700 2.17239300 2.17516000 C 2.18630700 1.33770600 2.13242300 C 1.98707900 0.05363100 2.91041800 O 3.22520000 0.62330700 2.93434400			
C -3.12749200 1.96487800 0.07483600 Sum of electronic and zero-point Energies= -2060.649212 C -2.17279600 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Energies= -2060.611204 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Energies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 C -0.86060500 0.09499800 0.74353800 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.05072800 2.07652300 Sum of electronic and thermal Free Energies= -2060.718628 O -0.26891200 -1.39109600 2.45282400 C -1.33770600 2.13242300 C 1.98707900 -0.05363100 2.91041800 -2.18630700 2.83258700 O 3.22520000 0.62330700 2.93434400 -3.22572000 -2.13671800 2.65748000 C 0.72121000 -3.02325600 </td <td></td> <td></td> <td></td>			
C -2.17279600 -0.31823500 0.54534700 Sum of electronic and thermal Energies= -2060.612249 O -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Enthalpies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Enthalpies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 C -0.86060500 0.09499800 0.74353800 Sum of electronic and thermal Free Energies= -2060.718628 C -0.94250900 0.74777900 2.15796100 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.05072800 2.07652300 Sum of electronic and thermal Free Energies= -2060.718628 C -0.36998000 -0.05072800 2.15796100 Energies= -2060.718628 C -0.36998000 -0.05072800 2.15796100 Energies= -2060.718628 C 0.90356700 -2.17239300 2.17516000 Energies= -2060.718628 C 1.98707900 -0.05363100 2.91041800			
0 -2.10527400 -1.69633700 0.13456700 Sum of electronic and thermal Enthalpies= -2060.611304 C -3.23988400 -2.21539200 -0.36421700 Sum of electronic and thermal Free Energies= -2060.718628 C -4.24623800 -1.48616300 -0.87479900 Sum of electronic and thermal Free Energies= -2060.718628 0 -0.86060500 0.09499800 0.74353800 Sum of electronic and thermal Free Energies= -2060.718628 C 0.94250900 0.74777900 2.15796100 Sum of electronic and thermal Free Energies= -2060.718628 C 0.94250900 0.74777900 2.15796100 Sum of electronic and thermal Free Energies= -2060.718628 C 0.94250900 0.74777900 2.15796100 Sum of electronic and thermal Free Energies= -2060.718628 O -0.26891200 -1.39109600 2.45282400 Sum of electronic and thermal Free Energies= -2060.718628 C 0.90356700 -2.17239300 2.17516000 Sum of electronic and thermal Free Energies= -2060.718628 C 1.98707900 -0.05363100 2.91041800 Sum of electronic and thermal Free Energies= -2060.718628			
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			
C-4.24623800-1.48616300-0.87479900O-0.860605000.094998000.74353800C0.942509000.747779002.15796100C-0.36998000-0.050728002.07652300O-0.26891200-1.391096002.45282400C0.90356700-2.172393002.17516000C2.18630700-1.337706002.13242300C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
O-0.860605000.094998000.74353800C0.942509000.747779002.15796100C-0.36998000-0.050728002.07652300O-0.26891200-1.391096002.45282400C0.90356700-2.172393002.17516000C2.18630700-1.337706002.13242300C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			Sum of electronic and thermal Free Energies= -2060.718628
C0.942509000.747779002.15796100C-0.36998000-0.050728002.07652300O-0.26891200-1.391096002.45282400C0.90356700-2.172393002.17516000C2.18630700-1.337706002.13242300C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
C-0.36998000-0.050728002.07652300O-0.26891200-1.391096002.45282400C0.90356700-2.172393002.17516000C2.18630700-1.337706002.13242300C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
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			
C0.90356700-2.172393002.17516000C2.18630700-1.337706002.13242300C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
C2.18630700-1.337706002.13242300C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
C1.98707900-0.053631002.91041800O0.783979001.983647002.82358700O3.225200000.623307002.93434400O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
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 3.22520000 0.62330700 2.93434400 O 3.22672900 -2.13671800 2.65748000 C 0.72121000 -3.02325600 0.92638100			
O3.22672900-2.136718002.65748000C0.72121000-3.023256000.92638100			
C 0.72121000 -3.02325600 0.92638100			
O 0.71783200 -2.26363300 -0.26722700			
	0	0.71783200 -2.26363300 -0.26722700	

С	-2.55403200 3.07133600 -0.81718000	
0	-2.70848400 2.11215500 1.42239000	
0	-1.17662000 2.83438100 -1.17139900	
C	-0.22505000 3.14523500 -0.29142100	
С	1.13655200 2.79756200 -0.71296600	
С	1.40508200 1.66148300 -1.37948700	
0	-0.46856200 3.65544700 0.79828800	
C	2.75477200 1.16651900 -1.65714900	
С	3.81266300 2.03861200 -1.92902900	
С	5.09477500 1.54667100 -2.15778500	
С	5.33078200 0.17993500 -2.09344500	
С	4.27259000 -0.70503200 -1.80876300	
С	2.98914600 -0.22164700 -1.61005000	
0	6.57515900 -0.30414600 -2.30628900	
Н	-2.02982100 0.64132900 -1.32103300	
н	-4.12498300 0.15163000 -2.18808300	
Н	-6.22863200 0.68720200 -0.60139400	
н	-5.18288600 2.78405900 0.55633300	
н	-2.75026200 -0.29366900 1.47693800	
Н	-3.26444600 -3.30054700 -0.33392400	
Н	1.32047700 0.90497700 1.13990500	
Н	-1.10672900 0.38686200 2.75906200	
н	0.99100100 -2.84313300 3.03788300	
Н	2.42192500 -1.05626800 1.09368500	
H	1.64566000 -0.27043100 3.93453500	
Н	0.47176800 2.66420600 2.20038800	
Н	3.05637200 1.52457500 3.25329100	
Н	4.00048500 -1.55902100 2.76220600	
H	-0.20386900 -3.60612200 1.02034300	
H	1.56523700 -3.71932300 0.86088000	
Н	-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	
н	3.62789200 3.10708700 -1.99330800	
H H	5.92475200 2.20707200 -2.38681600	
н.	2.17336000 -0.90220000 -1.37450100	
н	6.54590600 -1.27034100 -2.19984600	
c	-5.40215500 -2.24309200 -1.38781800	
0	-5.59005000 -3.43283200 -1.26577900	
0	-6.27468200 -1.44600200 -2.05020000	
H	-6.99453200 -2.01935500 -2.36641000	
0	4.64822800 -2.01483800 -1.76368800	
C	3.70785300 -2.94301800 -1.24074500	
H	2.80514200 -2.98376800 -1.85799500	
Н	4.20917100 -3.91040500 -1.24598600	
H H	3.43447500 -2.66866400 -0.21537400	
Name		6-FMT-C5-H-OOH-P
	n Coordinates	Energy
C	3.14031100 -1.53118100 0.27097900	Zero-point correction= 0.572861 (Hartree/Particle)
C	1.80964400 -2.09040500 -0.25030200	
C	2.10719700 -3.48729200 -0.65776200	

С	3.41762400	-3.76120800	-0.56959400	The
C	4.22606500	-2.55448700	-0.15038100	Sum
C	3.36724700	-0.10521100	-0.19813800	Sum
0	3.03773000	0.05965500	-1.58806500	Sun
C	1.76611000	-0.28192600	-1.88602900	Sun
C	1.09046900	-1.24097600	-1.22918700	
0	2.53222300	0.69021100	0.59441100	
C	2.17473800	2.82836700	1.51192300	
С	2.37881100	2.02522200	0.23373700	
0	1.23112900	2.09503700	-0.60207300	
С	0.83083700	3.40946000	-0.96107500	
С	0.47320300	4.19399100	0.30532100	
С	1.71033200	4.23732600	1.18374900	
0	3.40537800	2.84418400	2.19515000	
0	1.46865700	4.88792300	2.41127900	
0	0.10898800	5.52517000	0.02647900	
С	-0.30495600	3.27310600	-1.95884300	
0	-1.39160600	2.51252600	-1.42358700	
С	5.21359700	-2.84121800	0.97643900	
0		-2.08993900		
0	6.18971400	-3.77186500	0.57286200	
С	-2.39667900	3.20185200	-0.81888800	
С	-3.48456000	2.36454100	-0.31396500	
С	-3.49413600	1.02746800	-0.47207100	
с	-4.47161300	0.06225200	0.01035800	
0			-0.70538900	
С	-5.67867700	0.41325600	0.62456400	
С		-0.56995400	1.07651900	
С		-1.91295700	0.92516800	
С		-2.27836900	0.30937000	
С		-1.30032300	-0.15083800	
0	-7.06898300	-2.86963300	1.36792000	
0		-3.62371200		
С		-4.06132800		
С		-1.49873000	-1.53978400	
0		-2.57064900		
0	-1.03871700			
н	3.10149700	-1.49731700	1.36799800	
н	1.32613800	-4.15982100	-0.99893000	
н	3.89919100	-4.70244500	-0.81706300	
н	4.41090700	0.21612500	-0.13800300	
н	1.36508900	0.28771100	-2.71922000	
н	1.39759700	2.32136200	2.10388500	
н	3.26262200	2.39159300	-0.31579900	
H	1.65283400	3.93681800	-1.47657700	
н	-0.32677900	3.66735900	0.84680800	
H	2.51159400	4.76012300	0.63286600	
н	3.30850400	3.44286400	2.95259900	
H	1.06411900	5.74724600	2.20975300	
H	-0.83067600	5.52154200	-0.23286800	
н	0.03925200	2.70946200	-2.83045600	
н	-0.65183200	4.25824600	-2.27903700	
н	5.67253900	-1.89147400	1.29439700	
н	4.68294800	-3.27286600	1.82925000	
н	4.51181400	-1.96153400	-2.01691400	
		1.00100.00	1.01001.00	1

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 Energi	es= -2211.538250

-		
H	6.59159600 -3.42731000 -0.24041100	
Н	-4.25563800 2.91606800 0.21356400	
Н	-2.67009100 0.58087500 -1.01769600	
Н	-5.94628200 1.45847400 0.74640200	
Н	-7.49430400 -0.31861400 1.55189900	
Н	-3.21115000 -1.57149300 -0.63396800	
H	-6.66929100 -3.73668300 1.18273000	
H	-3.59986000 -5.14968400 -0.27817100	
Н	-3.46970600 -3.72860300 -1.35785900	
Н	-2.73381400 -3.67860900 0.26526700	
Н	-0.62033000 0.40743300 -1.73153700	
0	1.72566000 -3.19391000 2.48232500	
H	1.53293200 -4.12654400 2.27912800	
0	0.65451200 -2.51224800 1.93882500	
Н	1.06428700 -2.22096800 0.81157100	
Nam	e	6-FMT-O24-H-OOH-P
Carte	esian Coordinates	Energy
С	3.16544700 -2.24018100 0.59218700	Zero-point correction= 0.573682 (Hartree/Particle)
С	1.70564400 -2.49399100 0.11900700	Thermal correction to Energy= 0.611460
С	1.75794700 -3.92441400 -0.38384700	Thermal correction to Enthalpy= 0.612404
C	2.99364800 -4.42348800 -0.40017500	Thermal correction to Gibbs Free Energy= 0.502610
С	4.02335300 -3.44048300 0.09765800	Sum of electronic and zero-point Energies= -2211.470734
С	3.67878900 -0.89414500 0.11901400	Sum of electronic and thermal Energies= -2211.432957
0	3.47503800 -0.71863600 -1.29156400	Sum of electronic and thermal Enthalpies= -2211.432012
С	2.17744500 -0.82375100 -1.66121300	Sum of electronic and thermal Free Energies= -2211.541806
С	1.28153700 -1.55790200 -0.98963200	
0	2.96097800 0.07040700 0.83945400	
С	2.99510600 2.25881100 1.71011100	
С	3.11341000 1.39853700 0.45813400	
0	2.06546800 1.69326800 -0.45836000	
С	2.00336400 3.05276700 -0.86407700	
C	1.73772700 3.93613800 0.35932900	
С	2.88206400 3.72683500 1.33469300	
0	4.13976500 2.02011600 2.49287700	
0	2.69757700 4.44411800 2.53449300	
0	1.70810600 5.30597000 0.03545600	
C	0.94939700 3.14972900 -1.95139200	
0	-0.32153500 2.66646000 -1.50188600	
C	4.90077800 -3.99969900 1.21742500	
0	4.96896500 -3.09614500 -0.91713400	
0	5.69057700 -5.07054700 0.76261700	
С	-1.19024600 3.57299900 -0.99163500	
C	-2.48553800 3.00651500 -0.59496900	
С	-2.78393400 1.70627400 -0.77209200	
С	-4.00528300 1.01021700 -0.39013200	
0	-0.90372300 4.74978700 -0.86762400	
С	-5.14349500 1.66528400 0.12757200	
С	-6.25717700 0.93985000 0.48350500	
C	-6.29891700 -0.46797600 0.32044600	
С	-5.12909400 -1.12661500 -0.18327600	
С	-4.00928500 -0.38634400 -0.54086000	
0	-7.39447900 -1.12852600 0.56608500	
0	-5.21100300 -2.47421100 -0.26080000	
С	-4.15646100 -3.16495000 -0.93085100	
-		

C	-0.14661000 -1.47839400 -1.34824000	
0	-0.95055300 -2.36280600 -1.16034800	
0	-0.55594600 -0.30727200 -1.89684000	
н	3.18639400 -2.21488000 1.68721900	
Н	0.99779100 -2.39882100 0.94976900	
н	0.85553600 -4.43389300 -0.70700300	
H	3.28315200 -5.41598400 -0.73154400	
H	4.75769700 -0.76903200 0.24527100	
н	1.95359700 -0.23972500 -2.54911200	
Н	2.08011300 1.95294300 2.24052500	
Н	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	
Н	-5.14460400 2.74493000 0.24078400	
H	-7.15044500 1.41502500 0.87555300	
Н	-3.12119600 -0.87717600 -0.93255500	
H	-4.46420500 -4.20928400 -0.95644900	
H	-4.03896300 -2.78304200 -1.94965700	
Н	-3.20767800 -3.05897300 -0.39693100	
Н	0.05451100 0.41802800 -1.66425000	
0	-5.57296200 -2.22435500 2.49946900	
H	-5.13786500 -2.69753500 1.76069500	
0	-6.88531900 -2.56562700 2.36075000	
Н	-7.23155200 -1.95232700 1.37447900	
Nam	e	10-FMT-C5-H-OOH-P
Carte	esian Coordinates	Energy
C	2.61888400 -0.37426900 0.02942400	Zero-point correction= 0.573945 (Hartree/Particle)
C	3.96990800 0.13506300 -0.48220600	Thermal correction to Energy= 0.612712
C	5.00122600 -0.52731500 0.34363700	Thermal correction to Enthalpy= 0.613656
C	4.46469600 -1.49550600 1.09913200	Thermal correction to Gibbs Free Energy= 0.502351
С	2.95589800 -1.55993100 0.98918400	Sum of electronic and zero-point Energies= -2211.470638
С	1.84281700 0.71343500 0.74559600	Sum of electronic and thermal Energies= -2211.431871
0	1.75148100 1.90068300 -0.07660300	Sum of electronic and thermal Enthalpies= -2211.430927
С	2.87519700 2.32209500 -0.66987100	Sum of electronic and thermal Free Energies= -2211.542231
С	3.98951500 1.57198800 -0.82153400	
0	0.54064500 0.27697400 0.94124600	
С	-1.37261900 -0.06671500 2.32202000	
С	-0.08526700 0.75192000 2.13554700	
0	-0.26378000 2.13530900 2.11351400	
С	-1.43656600 2.74189800 1.54655300	
С	-2.69088700 1.87152600 1.67705200	
С	-2.49608500 0.84594600 2.77461900	
		1

0	-1.22984100	-1.08380200	3.29098900	
0	-3.70658200	0.13335700	2.90673300	
0	-3.77824200	2.73722000	1.93161600	
С	-1.18801500	3.19368200	0.11464400	
0	-1.07394900	2.11573700	-0.79457900	
С	2.50037500	-2.87986800	0.35837800	
0	2.43608200	-1.37605300	2.29585200	
0	1.14410000	-2.81519400	-0.12697700	
С	0.14363400	-2.95225000	0.73933000	
С	-1.19622600	-2.82723600	0.15530300	
С	-1.46495500	-1.95590800	-0.83216100	
0	0.32154200	-3.13953900	1.94073200	
С	-2.81171800	-1.65727200	-1.32338500	
С	-3.80175400	-2.64151100	-1.39137500	
С	-5.08393400	-2.32651700	-1.83314700	
С	-5.38965700	-1.01978800	-2.18912800	
С	-4.40076200	-0.01997800	-2.11284900	
С	-3.11590300	-0.33501600	-1.70093000	
0	-6.63508700	-0.70556800	-2.61220600	
Н	1.99141700	-0.70353700	-0.80671100	
Н	4.08288100	-0.45635400	-1.58716100	
Н	6.05444200	-0.27554700	0.28235100	
Н	4.99834600	-2.14891900	1.78233100	
Н	2.31600900	1.01560700	1.68733600	
Н	2.80996900	3.34340400	-1.03273800	
Н	-1.66253800	-0.49332500	1.35311900	
Н	0.59503200	0.55911100	2.97248000	
Н	-1.60274200	3.63144300	2.16478100	
Н	-2.86685800	1.31699000	0.74128400	
Н	-2.23396200	1.34094100	3.72264900	
Н	-0.80961700	-1.87129900	2.89951800	
Н	-3.52311100	-0.65090000	3.44898000	
Н	-4.54513100	2.17606300	2.13201000	
Н	-0.29061800	3.82473600	0.08651500	
Н	-2.04579000	3.79446400	-0.20838700	
Н	-0.22234600	1.68155900	-0.62126000	
Н	3.09455700	-3.07956700	-0.53512600	
Н	2.59431100	-3.70668300	1.06964700	
Н	1.71315500	-2.00952700	2.45283300	
Н	-1.98474800	-3.33245700	0.70643100	
Н	-0.64347900	-1.36983800	-1.24500000	
Н	-3.56107800	-3.66750100	-1.12812500	
Н	-5.86026500	-3.08080900	-1.90940300	
Н	-2.35530600	0.43880600	-1.62407500	
Н	-6.65997600	0.24857800	-2.79801000	
С	5.14015800	2.21860000	-1.47753800	
0	5.21463700	3.38283700	-1.79776000	
0	6.15297500	1.34688300	-1.70152700	
Н	6.85874600	1.84955500	-2.14467400	
0	-4.83968900	1.21803400	-2.47948500	
С	-3.97368600	2.31438700	-2.22506100	
Н	-3.04041000	2.22137300	-2.78934300	
Н	-4.51632000	3.20416200	-2.54278000	
Н	-3.74388500	2.37632700	-1.15534600	
0	4.80813800	-2.35922800	-2.10245900	

Н	5.72364700 -2.15099200 -2.36225900	
0	4.07882500 -1.30198000 -2.58399800	
Name		10-FMT-024-H-OOH-P
	Coordinates	Energy
С	3.06174600 -0.03735000 -0.86602500	Zero-point correction= 0.575012 (Hartree/Particle)
С	4.25279000 0.89308000 -1.20521900	Thermal correction to Energy= 0.613130
С	5.43998300 -0.04294100 -1.24958700	Thermal correction to Enthalpy= 0.614074
С	5.06874700 -1.32053800 -1.23854300	Thermal correction to Gibbs Free Energy= 0.503743
С	3.57636200 -1.50302600 -1.07529000	Sum of electronic and zero-point Energies= -2211.471946
С	2.56645100 0.12282500 0.56071400	Sum of electronic and thermal Energies= -2211.433829
0	2.34720200 1.50564300 0.89502400	Sum of electronic and thermal Enthalpies= -2211.432885
С	3.36517700 2.34039100 0.61708000	Sum of electronic and thermal Free Energies= -2211.543215
С	4.32867000 2.08357100 -0.28282800	
0	1.33239500 -0.50845000 0.65770500	
С	-0.16844700 -2.01632700 1.72996400	
С	1.03319300 -1.07499200 1.93383900	
0	0.85880000 -0.09550200 2.91253100	
С	-0.40693400 0.54678400 3.12765200	
С	-1.59592800 -0.32929000 2.73037000	
С	-1.20023400 -1.78894100 2.81740500	
0	0.20271600 -3.37903800 1.74917800	
0	-2.36145700 -2.55594000 2.58194600	
0	-2.66843000 0.00015200 3.58822200	
С	-0.45064800 1.92027800 2.47307900	
0	-0.51679100 1.86117700 1.06046400	
С	2.93730500 -2.10557100 -2.33136900	
0	3.38472700 -2.33699400 0.05644100	
0	1.51124200 -1.88661800 -2.38449800	
С	0.70979200 -2.68023900 -1.67939100	
С	-0.71777700 -2.33029000 -1.76595800	
С	-1.13450200 -1.05394500 -1.72955200	
0	1.11938600 -3.61157700 -0.99579700	
С	-2.53868100 -0.65495900 -1.61160000	
С	-3.56618100 -1.40963000 -2.21540600	
С	-4.88203600 -1.02914100 -2.07291300	
С	-5.23585800 0.08957700 -1.27902600	
С	-4.18131600 0.85116200 -0.67693400	
С	-2.85198300 0.48689100 -0.86016800	
0	-6.48790100 0.37418800 -1.05950900	
Н	2.20466200 0.18180500 -1.51038100	
Н	4.11029300 1.29523000 -2.21992300	
Н	6.45668600 0.32420500 -1.34125000	
Н	5.72554900 -2.18376400 -1.28596400	
Н	3.28112300 -0.27054700 1.29328000	
н	3.32848200 3.26570200 1.18397200	
Н	-0.64691000 -1.76542600 0.77587600	
Н	1.90119700 -1.65825700 2.25998800	
Н	-0.46262900 0.68366900 4.21415000	
н	-1.88192200 -0.12794100 1.68540700	
н	-0.77890000 -2.01829400 3.80833400	
н	0.43811700 -3.66306900 0.84841900	
н	-2.08604200 -3.48161200 2.48573600	
Н	-3.35336900 -0.67707300 3.46007600	
Н	0.42188100 2.50091500 2.79807500	

Н	-1.35579800 2.43429200 2.81619100	
Н	0.36594900 1.60486300 0.74507200	
Н	3.31227500 -1.59420600 -3.21959300	
н	3.14512700 -3.17776000 -2.40283600	
Н	2.65746500 -2.96096300 -0.10886300	
н	-1.40402200 -3.16561300 -1.65556800	
Н	-0.38844800 -0.26034100 -1.69117600	
н	-3.31043000 -2.27233800 -2.82377200	
н	-5.69262800 -1.58009000 -2.53852200	
н	-2.05331700 1.05610100 -0.38846700	
с	5.35160800 3.13172200 -0.45628000	
0	5.48370800 4.12100000 0.22823400	
0	6.16273200 2.87603700 -1.51017100	
н	6.79467800 3.61408700 -1.56501100	
0	-4.58108900 1.92776700 0.04091300	
с	-3.66693500 2.46379000 0.99905100	
Н	-2.78421100 2.89421500 0.51647700	
H	-4.22315200 3.23637300 1.52879900	
н	-3.36076700 1.67991200 1.70068100	
0	-5.57214700 2.74670300 -2.41413900	
H	-5.10547300 2.97852800 -1.58431600	
0	-6.84839600 2.50185300 -1.99977400	
H	-6.75522000 1.46683900 -1.39743700	
Name	0.75522000 1.40005500 1.55745700	6-FMT-ANION
100.000.000.000.000.000.000	an Coordinates	Energy
C	1.97722000 -2.40378000 0.67975600	Zero-point correction= 0.549925 (Hartree/Particle)
c	0.43975400 -2.50330400 0.78709600	Thermal correction to Energy= 0.587225
c	0.23619800 -4.00185100 0.92701600	Thermal correction to Enthalpy= 0.588169
c	1.33212400 -4.69987000 0.62292100	Thermal correction to Gibbs Free Energy= 0.479781
c	2.47263900 -3.79921300 0.21462200	Sum of electronic and zero-point Energies= -2060.224295
c	2.47203900 -3.79921300 0.21402200	Sum of electronic and thermal Energies= -2060.224235
0	1.79628300 -1.11219700 -1.41104000	Sum of electronic and thermal Entergies2060.186955
c	0.45448400 -1.35880900 -1.42132300	Sum of electronic and thermal Enthalpies – -2060.180031
c	-0.23914300 -1.97255000 -0.45446700	Sum of electronic and thermal free Energies2060.294440
0	2.36503200 -0.05538600 0.56240900	
C	3.40344500 1.88558200 1.48907100	
C	3.45999100 0.82098700 0.38694700	
0	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	
0	4.38822800 1.54039900 2.44953800	
0	3.48159500 4.20203700 1.96034500	
0	2.57646600 4.80834300 -0.59967100	
C	1.56110000 2.15631900 -2.14943300	
0	0.36412300 1.93942200 -1.37602100	
C	3.81267200 -4.14650300 0.85267000	
0	2.71534200 -3.88582900 -1.19677200	
0	4.28778100 -5.41390400 0.42326100	
C	-0.39695200 3.01790500 -1.13563900	
C	-1.68109300 2.75148300 -0.48207600	
	2 2000200 4 54257000 0 42040700	
C	-2.26898700 1.54357600 -0.42640700	
C C	-2.26898700 1.54357600 -0.42640700 -3.58743000 1.29485500 0.16561100	

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	
0	-7.39485300 0.55670700 1.67324000	
0	-6.37089100 -1.14331600 -0.10212900	
С	-5.84795800 -2.06801400 -1.05368900	
С	-1.72594400 -2.15311000 -0.61830500	
0	-2.37264500 -2.46959600 0.42127500	
0	-2.23911300 -1.98461800 -1.76334500	
н	2.38522800 -2.24115600 1.68306000	
н	0.06546800 -1.97167800 1.66967300	
н	-0.71961200 -4.42788600 1.21530600	
н	1.41962000 -5.78274500 0.60839900	
н	3.52772800 -1.41085800 -0.45965500	
н	-0.00193400 -1.00662800 -2.34111700	
H	2.40901100 1.86891400 1.95396100	
н	4.38893200 0.25200200 0.50050300	
н	3.48593600 3.00772700 -2.00325100	
н	1.58600900 3.26365300 0.33805800	
н	4.62493800 3.34650600 0.45736900	
н	4.26367600 2.11117200 3.22579700	
H	3.52447400 5.09447700 1.57709400	
H	1.71977400 4.97784500 -1.03393100	
н	1.73293200 1.22092400 -2.68337400	
н.	1.37216100 2.95535500 -2.86828900	
н	4.54221400 -3.36036900 0.61009100	
н.	3.70059100 -4.19898900 1.93793200	
н.	1.86423500 -3.85451700 -1.66638800	
н	4.31835800 -5.39695900 -0.54824000	
н.	-2.17060300 3.64694800 -0.11109700	
н.	-1.77329400 0.68636500 -0.88469100	
н	-3.61539500 3.02717200 1.46133400	
Н	-5.88838900 2.56397400 2.34583700	
H 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	
	-4.94180700 -2.54426400 -0.66738600	
Name	7.34100700 -2.34420400 -0.00738000	6-FMT-DIANION
	n Coordinates	Energy
Cartesia	0.05754400 -2.45873000 0.50043200	Zero-point correction= 0.536409 (Hartree/Particle)
c	-0.80230900 -1.63758100 -0.49313900	Thermal correction to Energy= 0.573325
c	-1.96235100 -2.57618400 -0.76576500	Thermal correction to Enthalpy= 0.57325
c	-1.76369200 -3.80244800 -0.76378300	Thermal correction to Gibbs Free Energy= 0.465875
c	-0.42217600 -3.93430000 0.39855600	Sum of electronic and zero-point Energies= -2059.778150
c c	1.54548800 -2.28305000 0.28300100	Sum of electronic and thermal Energies= -2059.778150
0	1.92436800 -2.244684800 -1.07834700	Sum of electronic and thermal Energies= -2059.741234 Sum of electronic and thermal Enthalpies= -2059.740290
C	1.18594400 -1.72937500 -1.97959800	Sum of electronic and thermal Free Energies= -2059.848685
C	-0.05995500 -1.29007800 -1.76503400	
0	1.88950400 -0.98619200 0.72830600	
C	3.65811400 0.19273100 1.82438800	
С	3.26883500 -0.68465400 0.62477400	

ſ	0	3.58665900	-0.14757600	-0.63574200	
	С	3.57646700	1.25997900	-0.91514800	
	С	3.65015600	2.12328900	0.34703000	
	С	4.47754100	1.39468900	1.39147000	
	0	4.35628600	-0.64338500	2.73377200	
	0	4.68698700	2.19716900	2.54036100	
	0	4.25445400	3.37077000	0.05645500	
	С	2.44715400	1.63151600		
	0	1.18304700	1.83944200		
	С	-0.47608200		1.77754700	
	0		-4.78613900		
	0		-5.92806000	1.71416400	
	C	0.88389500	3.10101400		
	С	-0.44726100	3.28591600		
	C	-1.37662500	2.29828200		
	C	-2.72106000	2.38003000	0.26095000	
	õ	1.69787500	4.02098100		
	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	
	0	-6.60947300	2.41312100	1.74442500	
	0	-5.68359100	0.15401100	0.63201500	
	c		-1.04132900	0.07322400	
	C		-0.46485900		
	0		-0.46485900		
	0		-0.14078100		
	н		-0.14276200	1.51776100	
	H H		-0.71594400 -2.25636800		
			-2.25636800		
	H		-4.64771100		
	Н Ц			0.82171800	
	Н	2.74166800	-1.56215000	-2.90408000 2.29708000	
	Н		0.56856200		
	Н		-1.61799600	0.67827000	
	Н	4.50817700		-1.46686000	
	Н	2.65255100	2.28949600	0.77722500	
	Н	5.44115900	1.07636300	0.96715700	
	Н	4.45568900	-0.16196700	3.57172200	
	Н	5.12870300	3.01474400	2.25489200	
	Н	3.56943600	3.91953400	-0.37143900	
	Н	2.28282100		-2.57221100	
	н	2.71874000		-2.42438500	
	н	0.52123500	-4.52774400	2.23736000	
	н	-1.18462600	-4.04166400	2.40982100	
	Н	0.44869400	-4.49604900	-1.28548000	
	Н	-0.32935500	-6.40401000	1.10941000	
	Н	-0.64213800	4.29105200	0.06235100	
	Н	-1.09328400	1.32914100	-0.66472500	
	Н	-2.66061800	4.44445000	0.91249800	
	Н	-4.96409500	4.45811100	1.78015800	
	Н	-3.13481000	0.33049100	-0.26733200	
	Н	-5.96240200	-1.77875300	0.12797900	
	Н	-4.86936800	-0.89135700	-0.97325300	
					694

Н	-4.29581000 -1.39408700 0.64748000	
Name		10-FMT-ANION
Cartesian	Coordinates	Energy
С	-2.64612900 0.61269300 0.56378700	Zero-point correction= 0.549381 (Hartree/Particle)
С	-3.83301300 1.50135000 0.11158000	Thermal correction to Energy= 0.586344
С	-4.97134400 1.06336900 1.00306400	Thermal correction to Enthalpy= 0.587288
С	-4.55668500 0.28818700 2.00294900	Thermal correction to Gibbs Free Energy= 0.478773
С	-3.08195300 -0.03077500 1.92459900	Sum of electronic and zero-point Energies= -2060.232817
С	-2.30936400 -0.46355300 -0.45344700	Sum of electronic and thermal Energies= -2060.195853
0	-2.17700700 0.07097300 -1.77207400	Sum of electronic and thermal Enthalpies= -2060.194909
С	-3.22984500 0.82746600 -2.19180900	Sum of electronic and thermal Free Energies= -2060.303424
С	-4.07860000 1.46404700 -1.37444600	
0	-1.05989000 -0.99167800 -0.10580300	
С	0.43782800 -2.79552200 0.26184000	
С	-0.78199100 -2.31700600 -0.53530500	
0	-0.60036700 -2.40566800 -1.92617500	
С	0.69354100 -2.11910600 -2.48743600	
С	1.83131100 -2.85844100 -1.75753500	
С	1.28945100 -3.69920900 -0.61429100	
0	0.04688900 -3.51283400 1.41765600	
0	2.39863200 -4.20820500 0.10758100	
0	2.51571200 -3.65139600 -2.71963200	
С	0.95065600 -0.62598900 -2.64438500	
0	1.19108900 0.06393200 -1.42554700	
С	-2.31791200 0.60358600 3.09429500	
0	-2.97992000 -1.45598600 1.95554500	
0	-0.90210800 0.73642700 2.83135100	
С	-0.11759300 -0.33582000 2.89671200	
С	1.26087700 -0.12886900 2.45602500	
С	1.64320400 0.95599500 1.75686700	
0	-0.53038500 -1.43528000 3.27543100	
С	2.95639700 1.16286400 1.14935900	
С	3.89941700 0.13555400 1.01768300	
С	5.12559800 0.38076900 0.40682100	
С	5.41799100 1.64892500 -0.08062500	
С	4.47422300 2.68633400 0.03247000	
С	3.25079600 2.44082500 0.63694600	
0	6.62213000 1.87923400 -0.67867400	
Н	-1.73965100 1.21508000 0.67813500	
Н	-3.60052900 2.54606900 0.36475600	
Н	-5.99015700 1.40837100 0.85488800	
Н	-5.16806300 -0.11836800 2.80386500	
Н	-3.07029900 -1.25244200 -0.49622000	
Н	-3.28411600 0.88122000 -3.27411600	
Н	1.04411100 -1.92351900 0.54715500	
Н	-1.64968800 -2.94804200 -0.31702800	
H	0.62896400 -2.53714300 -3.49659600	
н	2.53234500 -2.13017800 -1.32471500	
Н	0.68321400 -4.52745000 -1.00865500	
н	-0.07828100 -2.87956400 2.15117800	
н	2.05361500 -4.69965800 0.87261400	
н	3.32101800 -3.99960700 -2.30229600	
Н	0.11244200 -0.17459100 -3.18795600	
Н	1.85614500 -0.50900700 -3.24829700	

Н	0.38577300 0.00895200 -0.87540600	
Н	-2.64865900 1.63383200 3.23055400	
H	-2.47142800 0.03801000 4.01746400	
Н	-2.12486100 -1.71059200 2.34786300	
H	1.92040400 -0.96920200 2.65283600	
Н	0.92096700 1.75686600 1.60188500	
Н	3.67858700 -0.86686400 1.37302200	
Н	5.86397100 -0.40720600 0.29245900	
Н	2.51044200 3.23017800 0.72268100	
Н	6.66350400 2.80988600 -0.96613000	
С	-5.16635800 2.31809000 -1.97177400	
0	-5.45713500 2.15808800 -3.19317300	
0	-5.71672200 3.15890800 -1.20359300	
0	4.87716400 3.87880300 -0.49481900	
С	3.95906900 4.96691200 -0.42332800	
н	3.72619700 5.20462300 0.61940300	
Н	4.46172300 5.81162400 -0.89270500	
Н	3.04025300 4.73012700 -0.96893000	
Name		10-FMT-DIANION
Cartesiar	Coordinates	Energy
С	2.59840900 -0.61333700 0.55749400	Zero-point correction= 0.536929 (Hartree/Particle)
С	3.78278200 -1.50084000 0.09594100	Thermal correction to Energy= 0.573145
с	4.92252300 -1.07550600 0.99201700	Thermal correction to Enthalpy= 0.574089
С	4.50952200 -0.31024000 2.00020900	Thermal correction to Gibbs Free Energy= 0.467920
С	3.03486300 0.01014000 1.92766400	Sum of electronic and zero-point Energies= -2059.782037
С	2.26933200 0.47761900 -0.44681700	Sum of electronic and thermal Energies= -2059.745821
0	2.13797700 -0.03822000 -1.77343900	Sum of electronic and thermal Enthalpies= -2059.744877
с	3.18637200 -0.79642700 -2.20033200	Sum of electronic and thermal Free Energies= -2059.851046
C	4.02994300 -1.44802000 -1.38935500	
0	1.02227000 1.00900300 -0.09751300	
с	-0.46193600 2.81800200 0.29439700	
С	0.75726000 2.34330100 -0.50503000	
0	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	
0	-0.07177100 3.49134000 1.47626200	
0	-2.38814700 4.27968100 0.16401900	
0	-2.48724400 3.79403300 -2.68570800	
c	-1.00663600 0.71213700 -2.62410900	
0	-1.27248900 0.02257200 -1.41028900	
c	2.27075900 -0.64126900 3.08945300	
0	2.93098200 1.43452800 1.97963000	
0	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	
0	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	
	-4.44063000 -2.78875000 -0.03657400	
C		
C	-3.24939200 -2.53173200 0.60573000	

Ē		
	0	-6.56548600 -2.02080000 -0.7872410
	Н	1.68890900 -1.21279600 0.66298200
	Н	3.54696800 -2.54751700 0.33774900
	Н	5.94050300 -1.42122900 0.83971900
	Н	5.12224900 0.08609900 2.80530800
	Н	3.03524100 1.26241100 -0.47744800
	Н	3.24207500 -0.83771600 -3.28312400
	Н	-1.08568400 1.94839500 0.54628700
	Н	1.62916600 2.96367800 -0.27290400
	Н	-0.64067600 2.61821000 -3.46853300
	Н	-2.56885000 2.24758900 -1.3216130
	Н	-0.65950500 4.58563600 -0.93514100
	Н	0.04390600 2.82999200 2.18851900
	Н	-2.03647300 4.72036600 0.95653500
	Н	-3.29489000 4.14681600 -2.2770150
	Н	-0.17458800 0.24381500 -3.16290200
	Н	-1.90975900 0.61794000 -3.23542900
	н	-0.46564600 0.04353600 -0.86005400
	Н	2.61020700 -1.67040800 3.21495300
	н	2.42629300 -0.08515300 4.01829200
	н	2.07529100 1.67611900 2.38183800
	Н	-1.92942800 0.96873900 2.54321000
	н	-0.99272200 -1.85781500 1.72074900
	Н	-3.77732400 0.73864800 1.44791100
	н	-5.90081700 0.27725300 0.29181400
	н	-2.48945400 -3.30358700 0.69199700
	С	5.11432500 -2.30037200 -1.99498600
	0	5.40547600 -2.13034800 -3.2150540
	0	5.66236500 -3.14991100 -1.2347740
	0	-4.77468600 -3.99869900 -0.5993630
	С	-3.81759200 -5.04197600 -0.49856000
	н	-3.60935300 -5.28353000 0.54992100
	Н	-4.26090500 -5.90742700 -0.9916940
	н	-2.88449700 -4.76918600 -1.0045300
Ŀ		

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. luga, 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.