Electronic Supplementary Information

for

Cooperativity and Serial Ligand Catalysis in an Allylic Amination Reaction by Pd(II)-bis-sulfoxide and Brønsted Acid

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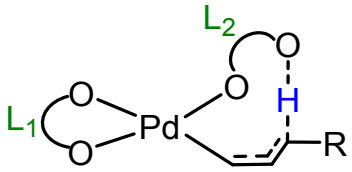
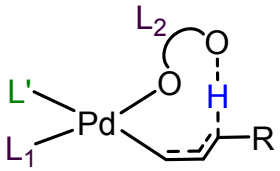
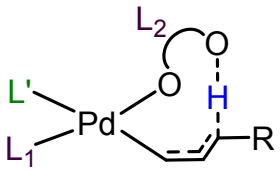
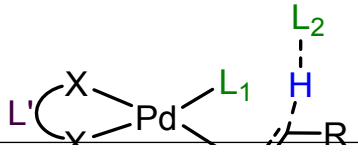
1. The mode of coordination and equations used for calculating the Gibbs free energy and barrier for C–H activation

Table S1. Different Coordination Modes and the Corresponding Equations Used for Calculating the Gibbs free Energies for the C–H Activation.[i] Here, the Substrate Homoallylic Boc-protected Amine is Represented as S

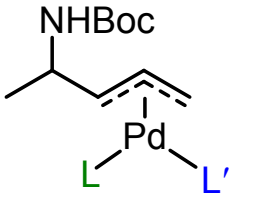
entry	mode of coordination	mode	ligands involved	equation
1		**a**	L_1=AcO^- L_2=AcO^-	$Pd(OAc)_2$ + S
		b	L_1=$DBPO^-$ L_2=AcO^-	$Pd(OAc)_2$ + S + DBPOH – AcOH
		c	L_1=AcO^- L_2=$DBPO^-$	$Pd(OAc)_2$ + S + DBPOH – AcOH
		d	L_1=$DBPO^-$ L_2=$DBPO^-$	$Pd(OAc)_2$ + S + 2DBPOH – 2AcOH
2		**e**	L′=BS L_1=AcO^- L_2=AcO^-	$Pd(OAc)_2$ + S + BS
		f	L′=BS L_1=AcO^- L_2=$DBPO^-$	$Pd(OAc)_2$ + S + BS + DBPOH – AcOH
		g	L′=BS L_1=$DBPO^-$ L_2=AcO^-	$Pd(OAc)_2$ + S + BS + DBPOH – AcOH
		h	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	$Pd(OAc)_2$ + S + BS + 2DBPOH – 2AcOH
3		**i**	L′=BQ L_1=AcO^- L_2=AcO^-	$Pd(OAc)_2$ + S + BQ
		j	L′=BQ L_1=AcO^- L_2=$DBPO^-$	$Pd(OAc)_2$ + S + BQ + DBPOH – AcOH
		k	L′=BQ L_1=$DBPO^-$ L_2=AcO^-	$Pd(OAc)_2$ + S + BQ + DBPOH – AcOH
		l	L′=BQ L_1=$DBPO^-$ L_2=$DBPO^-$	$Pd(OAc)_2$ + S + BQ + 2DBPOH – 2AcOH
4		**m**	L′=BS L_1=AcO^- L_2=AcO^-	$Pd(OAc)_2$ + S + BS
			L′=BS	$Pd(OAc)_2$ + S + BS +

		n	L_1=AcO^- L_2= $DBPO^-$	DBPOH – AcOH
		o	L′=BS L_1=$DBPO^-$ L_2= AcO^-	$Pd(OAc)_2$ + S + BS + DBPOH – AcOH
		p	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	$Pd(OAc)_2$ + S + BQ + 2DBPOH – 2AcOH
		q	L′=BQ L_1=AcO^- L_2=AcO^-	$Pd(OAc)_2$ + S + BQ
		r	L′=BQ L_1=AcO^- L_2= $DBPO^-$	$Pd(OAc)_2$ + S + BQ + DBPOH – AcOH
		s	L′=BQ L_1= $DBPO^-$ L_2= AcO^-	$Pd(OAc)_2$ + S + BQ + DBPOH – AcOH
		t	L′=BQ L_1=$DBPO^-$ L_2=$DBPO^-$	$Pd(OAc)_2$ + S + BQ + 2DBPOH – 2AcOH

[i] Energy of $Pd(OAc)_2$ is taken as one third energy of $[Pd_3(OAc)_6]$ trimer with a triangular disposition of Pd centers.

2. The mode of coordination and equations used for calculating the Gibbs free energy and barrier for C–O bond formation

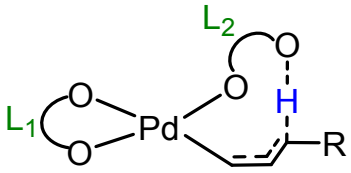
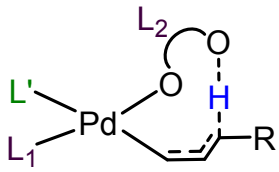
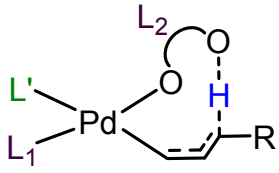
Table S2. Different Coordination Modes and the Corresponding Equations Used for Calculating the Gibbs free Energies for the C–O bond formation.[i] Here, the Substrate Homoallylic Boc-protected Amine is Represented as S

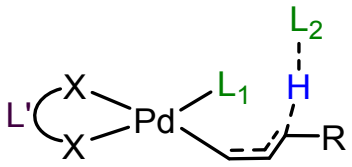
mode of coordination		ligand involved	equation used
 L-anionic, L'-neutral	**u**	L=AcO^- L′=BS	$Pd(OAc)_2$ + S + BS
	v	L=AcO^- L′=BQ	$Pd(OAc)_2$ + S + BQ – AcOH
	w	L=$DBPO^-$ L′=BS	$Pd(OAc)_2$ + S + BQ + DBPOH – 2 AcOH
	x	L=$DBPO^-$ L′=BQ	1 $Pd(OAc)_2$ + S + BS + DBPOH – AcOH

[i] Energy of $Pd(OAc)_2$ is taken as one third energy of $[Pd_3(OAc)_6]$ trimer with a triangular disposition of Pd centers.

3. Standard State corrected relative Gibbs free energies for the allylic C−H activation transition states

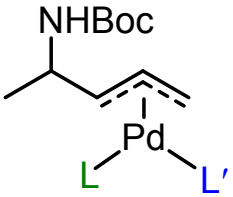
Table S3. Standard State Corrected Relative Gibbs Free Energies (in kcal/mol) for the Allylic C−H Activation Transition States with Respect to the Separated Reactants and the Elementary Step Barriers with Respect to the Corresponding Preceding Intermediates Obtained at the $SMD_{(1,4\text{-dioxane})}$/B3LYP-D3/6-31G**,SDD(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd) Level of Theory

entry	mode of coordination	mode	ligands involved	elementary step barrier	ΔG_{rel}
1		**a**	L_1=AcO^- L_2=AcO^-	20.0	33.9
		b	L_1=$DBPO^-$ L_2=AcO^-	22.2	30.9
		c	L_1=AcO^- L_2=$DBPO^-$	10.5	24.0
		d	L_1=$DBPO^-$ L_2=$DBPO^-$	16.1	19.8
2		**e**	L′=BS L_1=AcO^- L_2=AcO^-	20.4	31.1
		f	L′=BS L_1=AcO^- L_2=$DBPO^-$	10.5	24.5
		g	L′=BS L_1=$DBPO^-$ L_2=AcO^-	12.0	25.0
		h	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	11.1	17.6
3		**i**	L′=BQ L_1=AcO^- L_2=AcO^-	15.9	47.1
		j	L′=BQ L_1=AcO^- L_2=$DBPO^-$	14.3	40.5
		k	L′=BQ L_1=$DBPO^-$ L_2=AcO^-	29.7	36.7
			L′=BQ	18.5	37.2

		l	L_1=DBPO$^-$ L_2=DBPO$^-$		
4		**m**	L′=BS L_1=AcO$^-$ L_2=AcO$^-$	28.7	32.6
		n	L′=BS L_1=AcO$^-$ L_2= DBPO$^-$	4.5	24.1
		o	L′=BS L_1=DBPO$^-$ L_2= AcO$^-$	8.6	22.2
		p	L′=BS L_1=DBPO$^-$ L_2=DBPO$^-$	22.4	17.0
		q	L′=BQ L_1=AcO$^-$ L_2=AcO$^-$	37.3	49.4
		r	L′=BQ L_1=AcO$^-$ L_2= DBPO$^-$	24.5	39.7
		s	L′=BQ L_1= DBPO$^-$ L_2= AcO$^-$	32.1	43.7
		t	L′=BQ L_1=DBPO$^-$ L_2=DBPO$^-$	26.0	34.1

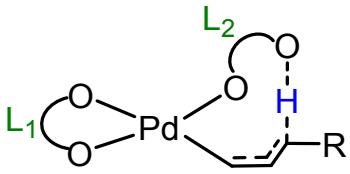
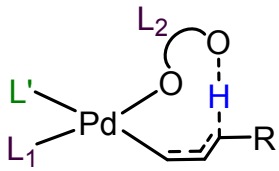
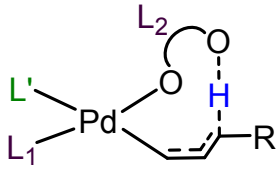
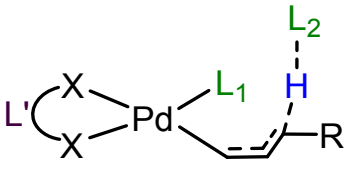
4. Standard State corrected relative Gibbs free energies for the C–O bond formation transition states

Table S4. Standard State Corrected Relative Gibbs Free Energies (in kcal/mol) for the Allylic C–O Bond Formation Transition States with Respect to the Separated Reactants and the Elementary Step Barriers with Respect to the Corresponding Preceding Intermediates Obtained at the SMD$_{(1,4\text{-dioxane})}$/B3LYP-D3/6-31G**,SDD(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd) Level of Theory

ligands involved		ligand involved	elementary step barrier	ΔG_{rel}
 L-anionic, L'-neutral	**u**	L=AcO$^-$ L′=BS	37.7	42.9
	v	L=AcO$^-$ L′=BQ	1.5	28.6
	w	L=DBPO$^-$ L′=BS	34.9	28.6
	x	L=DBPO$^-$ L′=BQ	1.9	19.0

5. The Gibbs free energies and enthalpies of transition states for the C–H activation

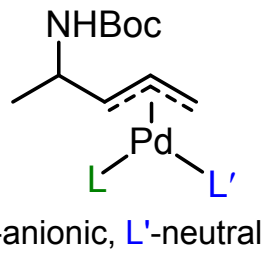
Table S5. The Gibbs Free Energies and Enthalpies (in a.u.) of Transition States for the C–H Activation

entry	mode of coordination	mode	ligands involved	free energy	enthalpy
1		**a**	L_1=AcO$^-$ L_2=AcO$^-$	-1182.398774	-1182.311507
		b	L_1=DBPO$^-$ L_2=AcO$^-$	-1911.806068	-1911.691727
		c	L_1=AcO$^-$ L_2=DBPO$^-$	-1911.817121	-1911.698222
		d	L_1=DBPO$^-$ L_2=DBPO$^-$	-2641.226266	-2641.082232
2		**e**	L′=BS L_1=AcO$^-$ L_2=AcO$^-$	-2670.894074	-2670.76571
		f	L′=BS L_1=AcO$^-$ L_2=DBPO$^-$	-3400.30709	-3400.155591
		g	L′=BS L_1=DBPO$^-$ L_2=AcO$^-$	-3400.306311	-3400.152535
		h	L′=BS L_1=DBPO$^-$ L_2=DBPO$^-$	-4129.720723	-4129.544843
3		**i**	L′=BQ L_1=AcO$^-$ L_2=AcO$^-$	-1563.786506	-1563.687044
		j	L′=BQ L_1=AcO$^-$ L_2=DBPO$^-$	-2293.199414	-2293.072655
		k	L′=BQ L_1=DBPO$^-$ L_2=AcO$^-$	-2293.20556	-2293.073512
		l	L′=BQ L_1=DBPO$^-$ L_2=DBPO$^-$	-3022.607177	-3022.453416
4		**m**	L′=BS L_1=AcO$^-$ L_2=AcO$^-$	-2670.891647	-2670.765101
		n	L′=BS L_1=AcO$^-$ L_2= DBPO$^-$	-3400.307797	-3398.928259
		o	L′=BS L_1=DBPO$^-$ L_2= AcO$^-$	-3400.310753	-3400.155181

		p	L′=BS L_1=DBPO$^-$ L_2=DBPO$^-$	-4129.72156	-4129.538797
		q	L′=BQ L_1=AcO$^-$ L_2=AcO$^-$	-1563.782718	-1563.681409
		r	L′=BQ L_1=AcO$^-$ L_2= DBPO$^-$	-2293.200811	-2293.068635
		s	L′=BQ L_1= DBPO$^-$ L_2= AcO$^-$	-2293.194371	-2293.068000
		t	L′=BQ L_1=DBPO$^-$ L_2=DBPO$^-$	-3022.612119	-3022.454721

6. The Gibbs free energies and enthalpies of transition states for the C–O bond formation

Table S6. The Gibbs Free Energies and Enthalpies (in a.u.) of Transition States for the C–O Bond Formation

ligands involved		ligand involved	free energy	enthalpy
 L-anionic, L'-neutral	**u**	L=AcO$^-$ L′=BS	-2670.875204	-2670.745124
	v	L=AcO$^-$ L′=BQ	-1334.758009	-1334.666493
	w	L=DBPO$^-$ L′=BS	-3400.300606	-3400.143065
	x	L=DBPO$^-$ L′=BQ	-2064.175751	-2064.056842

7. Relative Gibbs free energy of intermediates

Table S7. Relative Gibbs Free Energies (in kcal/mol) of Key Intermediates with Various Ligand Combinations

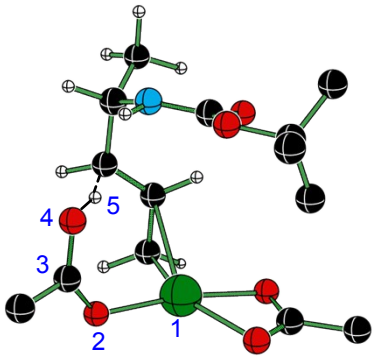
Intermediate	ligands involved	ΔGrel	
		L1	L2
2'	L_1=AcO$^-$ L_2=AcO$^-$	17.1	14.6
	L_1=DBPO$^-$ L_2=AcO$^-$	13.4	9.3

	L_1=AcO^- L_2=$DBPO^-$	8.5	14.1
	L_1=$DBPO^-$ L_2=$DBPO^-$	0.8	4.4
	L′=BS L_1=AcO^- L_2=AcO^-	13.2	13.4
	L′=BS L_1=AcO^- L_2=$DBPO^-$	12.5	16.7
	L′=BS L_1=$DBPO^-$ L_2=AcO^-	13.6	15.6
	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	3.3	9.1
	L′=BQ L_1=AcO^- L_2=AcO^-	30.9	33.0
	L′=BQ L_1=AcO^- L_2=$DBPO^-$	24.0	28.8
	L′=BQ L_1=$DBPO^-$ L_2=AcO^-	-9.3	9.6
	L′=BQ L_1=$DBPO^-$ L_2=$DBPO^-$	14.3	21.4
	L′=BS L_1=AcO^- L_2=AcO^-	3.4	6.6
	L′=BS L_1=AcO^- L_2= $DBPO^-$	21.5	22.2
	L′=BS L_1=$DBPO^-$ L_2= AcO^-	16.8	16.3
	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	-11.3	-2.6
	L′=BQ L_1=AcO^- L_2=AcO^-	12.9	14.8
	L′=BQ L_1=AcO^- L_2= $DBPO^-$	9.7	15.5
	L′=BQ L_1= $DBPO^-$ L_2= AcO^-	10.8	14.3

	L′=BQ L_1=DBPO$^-$ L_2=DBPO$^-$	3.5	10.7
4	L_1=AcO$^-$ L′=AcOH	21.4	22.8
	L_1=AcO$^-$ L′=BS	1.3	1.5
	L_1=AcO$^-$ L′=BQ	21.8	22.1
	L_1=AcO$^-$ L′=DBPOH	8.9	12.5
	L_1= DBPO$^-$ L′=AcOH	9.5	13.5
	L_1= DBPO$^-$ L′=BS	0.6	0.8
	L_1= DBPO$^-$ L′=BQ	12.4	16.1
	L_1= DBPO$^-$ L′=DBPOH	8.7	13.1
	L=DBPO$^-$ L′=BS L_2=AcOH	-8.0	-3.6
	L_1=AcO$^-$ L′=BS L_2=AcOH	5.2	7.9

M1= B3LYP-D3/6-31G**,LANL2DZ(Pd) ; M2 = $SMD_{(1,4\text{-dioxane})}$/B3LYP-D3/6-31G**,SDD(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd)

8. Wiberg Bond Indices of Selected Bonds in the C–H Activation Transition States in Moes a



a

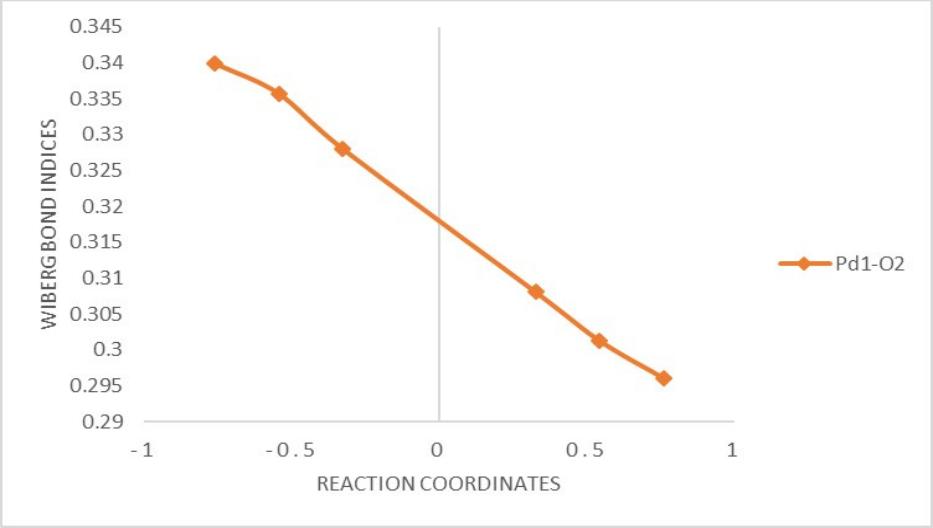
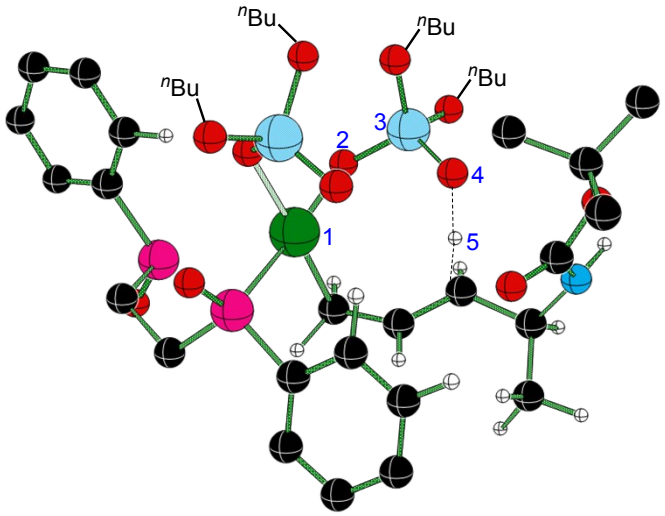


Fig. S1. Plot of Wiberg bond indices of selected bonds, Pd1–O2 for the C–H activation transition state **[2′-4]** in mode **a**. The X-axis corresponds to the reaction coordinate and the Y-axis is the Wiberg Bond Indices at specified points. It can be noticed from the Wiberg bond indices that the bond Pd1-O2 exhibits a progressive decrease indicating that the bond gets weaker as the reaction proceeds.

9. Wiberg bond indices of selected bonds in the C–H activation transition state [2′-4] in mode h



h

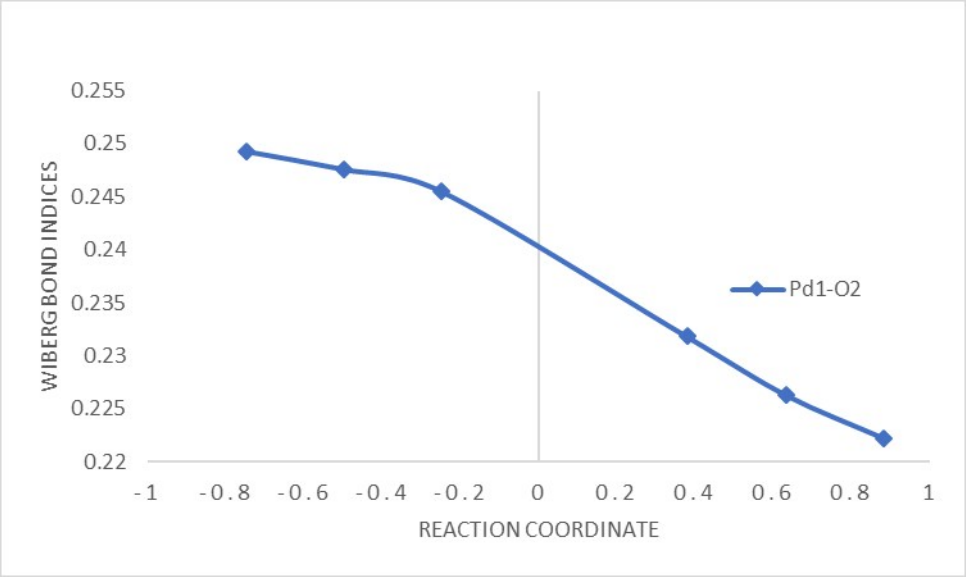


Fig. S2. Plot of Wiberg bond indices of selected bonds, Pd1–O2 for the C–H Activation transition state **[2′-4]** in mode **h**. The X-axis corresponds to the reaction coordinate and the Y-axis is the Wiberg Bond Indices at specified points. It can be noticed from the Wiberg bond indices that the Pd1-O2 bond order exhibits a progressive decrease, indicating that the bond gets weaker as the reaction proceeds.

10. Energetic span calculations

Table S8. The Calculation of Energetic Span (δE in kcal/mol) using Different Combinations of TDI and TDTS (highlighted one corresponds to the most preferred pathway)

TDI		TDTS^{i}		δE
2'	14.6	**TS[2′-4]$_a$**	34.6	20
		TS[4′-6]$_v$	29.3	28.1
	9.3	**TS[2′-4]$_b$**	31.6	22.3
		TS[4′-6]$_x$	19.7	28.2
	14.1	**TS[2′-4]$_c$**	24.5	10.4
		TS[4′-6]$_v$	29.3	28.6

	4.4	**TS[2′-4]$_{d}$**	20.5	16.1
		TS[4′-6]$_{x}$	19.7	33.14
	13.4	**TS[2′-4]$_{e}$**	33.8	20.4
		TS[4′-6]$_{u}$	45.7	64.8
	16.7	**TS[2′-4]$_{f}$**	27.2	10.5
		TS[4′-6]$_{u}$	45.7	61.5
	15.6	**TS[2′-4]$_{g}$**	27.7	11.4
		TS[4′-6]$_{w}$	31.3	35
	9.1	**TS[2′-4]$_{h}$**	20.2	11.1
		TS[4′-6]$_{w}$	31.3	41.5
	33	**TS[2′-4]$_{i}$**	49.7	16.7
		TS[4′-6]$_{v}$	29.3	9.73
	28.8	**TS[2′-4]$_{j}$**	43.2	14.4
		TS[4′-6]$_{v}$	29.3	13.93
	9.6	**TS[2′-4]$_{k}$**	39.4	29.8
		TS[4′-6]$_{x}$	19.7	27.9
	21.4	**TS[2′-4]$_{l}$**	39.9	18.5
		TS[4′-6]$_{x}$	19.7	16.14
	6.6	**TS[2′-4]$_{m}$**	35.3	28.7
		TS[4′-6]$_{u}$	45.7	71.6
	22.2	**TS[2′-4]$_{n}$**	26.7	4.5
		TS[4′-6]$_{u}$	45.7	56.0
	16.3	**TS[2′-4]$_{o}$**	24.9	8.6
		TS[4′-6]$_{w}$	31.3	34.3

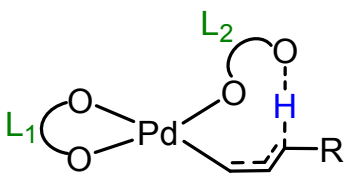
	-2.6	**TS[2′-4]$_{p}$**	19.7	22.3
		TS[4′-6]$_{w}$	31.3	53.2
	14.8	**TS[2′-4]$_{q}$**	52.1	37.3
		TS[4′-6]$_{v}$	29.3	27.9
	15.5	**TS[2′-4]$_{r}$**	42.3	26.8
		TS[4′-6]$_{v}$	29.3	27.23
	14.3	**TS[2′-4]$_{s}$**	46.4	32.1
		TS[4′-6]$_{x}$	19.7	23.2
	10.7	**TS[2′-4]$_{t}$**	36.8	26.1
		TS[4′-6]$_{x}$	19.7	26.8
4	22.8	**TS[2′-4]$_{a}$**	34.6	25.2
		TS[4′-6]$_{v}$	29.3	6.5
	1.5	**TS[2′-4]$_{m}$**	35.3	66.3
		TS[2′-4]$_{e}$	33.8	64.8
		TS[2′-4]$_{n}$	26.7	57.7
		TS[2′-4]$_{f}$	27.2	58.2
		TS[4′-6]$_{u}$	45.7	44.2
	22.1	**TS[2′-4]$_{q}$**	52.1	43.4
		TS[2′-4]$_{i}$	49.7	41.0
		TS[2′-4]$_{r}$	42.3	33.6
		TS[2′-4]$_{j}$	43.2	34.5
		TS[4′-6]$_{v}$	29.3	7.2
	12.5	**TS[2′-4]$_{c}$**	24.5	25.4
		TS[4′-6]$_{v}$	29.3	16.6

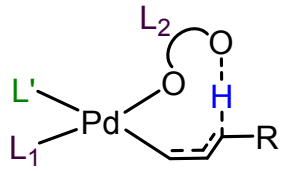
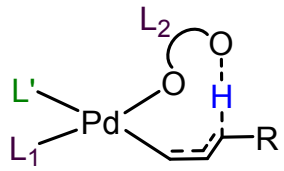
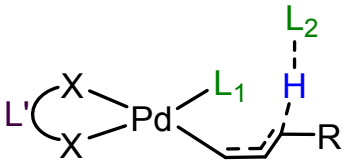
	13.5	**TS[2′-4]$_b$**	31.6	35.9
		TS[4′-6]$_x$	19.7	6.2
	16.1	**TS[2′-4]$_k$**	39.4	41.14
		TS[2′-4]$_s$	46.4	48.14
		TS[2′-4]$_l$	39.9	41.64
		TS[2′-4]$_t$	36.8	38.54
		TS[4′-6]$_x$	19.7	3.6
	13.1	**TS[2′-4]$_d$**	20.5	25.2
		TS[4′-6]$_x$	19.7	6.6
	-3.6	**TS[2′-4]$_g$**	27.7	50.6
		TS[2′-4]$_o$	24.9	47.8
		TS[2′-4]$_h$	20.2	43.1
		TS[4′-6]$_x$	19.7	23.3
		TS[4′-6]$_w$	31.3	34.9

[i] The suffixes on TDTS corresponds to the mode of ligands as given in Tables 1 and 2 in the main text.

11. Relative Gibbs free energies of the key intermediates with various ligand combinations with f-polarization function to Pd

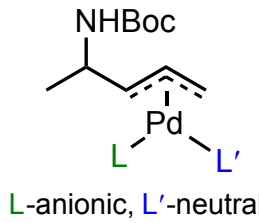
Table S9. Relative Gibbs Free Energies (in kcal/mol) of Key Intermediates with Various Ligand Combinations in C–H Activation Obtained through Incorporating f-polarization Function on Pd

entry	mode of coordination	mode	ligands	ΔG_{rel} M3
1		**a**	L_1=AcO$^-$ L_2=AcO$^-$	36.1
		b	L_1=DBPO$^-$ L_2=AcO$^-$	28.4
		c	L_1=AcO$^-$ L_2=DBPO$^-$	31.3
		d	L_1=DBPO$^-$ L_2=DBPO$^-$	22.9
2		**e**	L′=BS	38.6

			L_1=AcO^- L_2=AcO^-	
		f	L′=BS L_1=AcO^- L_2=$DBPO^-$	36.0
		g	L′=BS L_1=$DBPO^-$ L_2=AcO^-	35.6
		h	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	30.2
3		**i**	L′=BQ L_1=AcO^- L_2=AcO^-	36.0
		j	L′=BQ L_1=AcO^- L_2=$DBPO^-$	49.6
		k	L′=BQ L_1=$DBPO^-$ L_2=AcO^-	44.6
		l	L′=BQ L_1=$DBPO^-$ L_2=$DBPO^-$	47.9
4		**m**	L′=BS L_1=AcO^- L_2=AcO^-	41.3
		n	L′=BS L_1=AcO^- L_2=$DBPO^-$	32.6
		o	L′=BS L_1=$DBPO^-$ L_2= AcO^-	30.2
		p	L′=BS L_1=$DBPO^-$ L_2=$DBPO^-$	26.1
		q	L′=BQ L_1=AcO^- L_2=AcO^-	54.5
		r	L′=BQ L_1=AcO^- L_2=$DBPO^-$	46.3
		s	L′=BQ L_1=$DBPO^-$ L_2= AcO^-	50.6
		t	L′=BQ L_1=$DBPO^-$ L_2=$DBPO^-$	46.3

M3= $SMD_{(dioxane)}$/B3LYP-D3/6-31G**,SDD(f)(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd)

Table S10. Relative Gibbs Free Energies (in kcal/mol) of Key Transition States with Various Ligand Combinations in C–C Bond Formation Obtained through Incorporating f-polarization Function on Pd

mode of coordination	mode	ligand involved	ΔG_{rel}
			M3
	**u**	L=AcO^- L′=BS	51.8
	v	L=AcO^- L′=BQ	26.7
	w	L=$DBPO^-$ L′=BS	37.9
	x	L=$DBPO^-$ L′=BQ	19.8

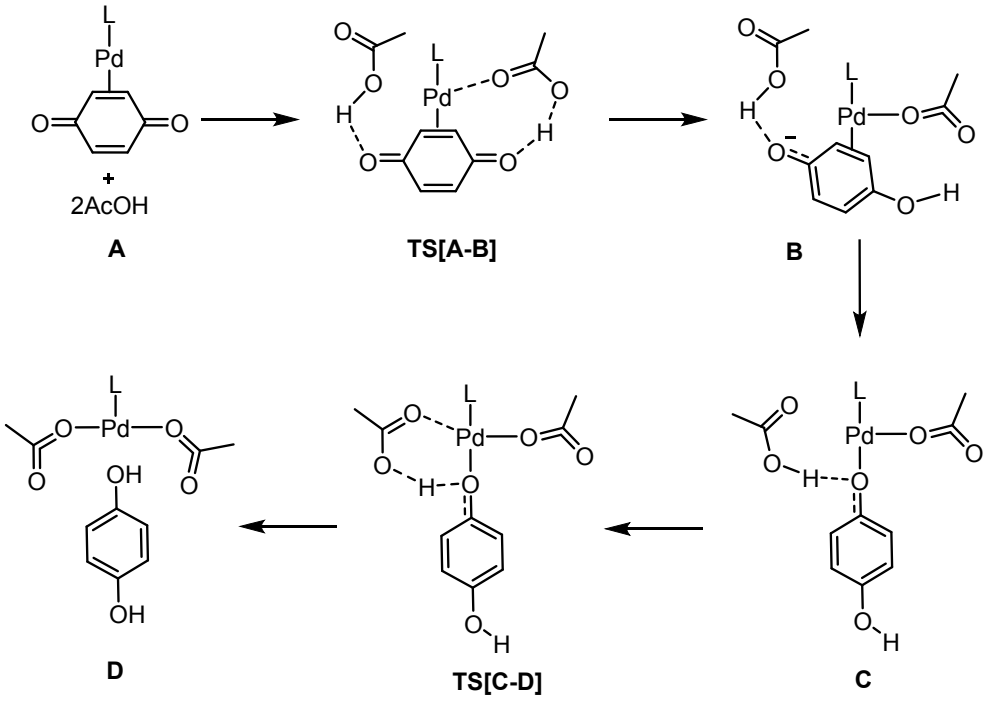
M3= $SMD_{(dioxane)}$/B3LYP-D3/6-31G**,SDD(f)(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd)

12. Energy span calculations in the condensed phase

Table S10. Energetic Span Calculations at the $SMD_{(dioxane)}$/B3LYP-D3/6-31G**,SDD(f)(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd)

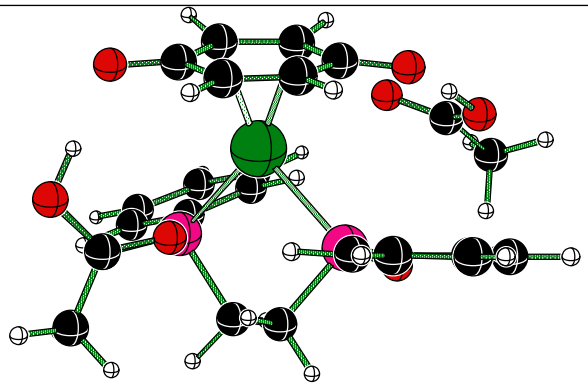
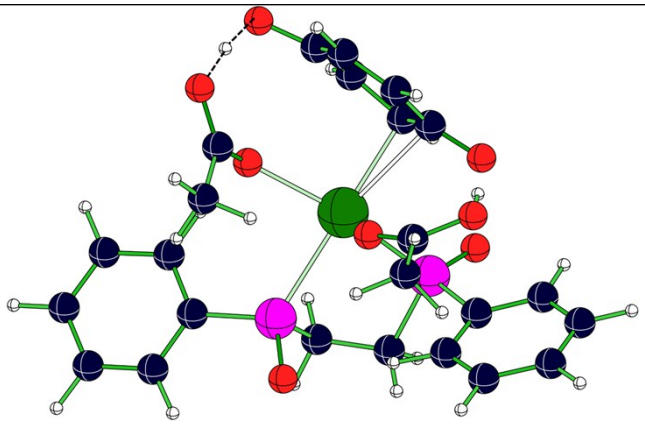
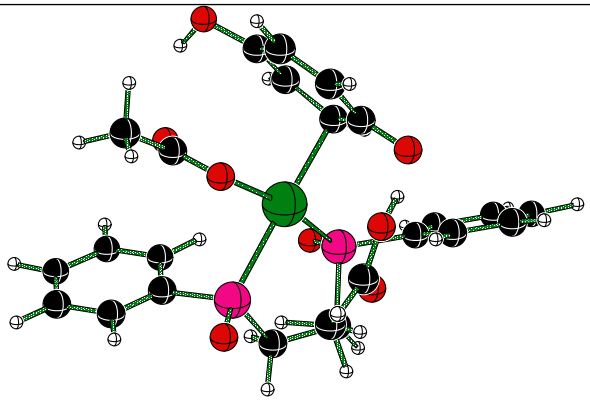
TDI		TDTS[a]		δE
4	-1.9	**TS[4′-6]$_x$**	19.5	21.4

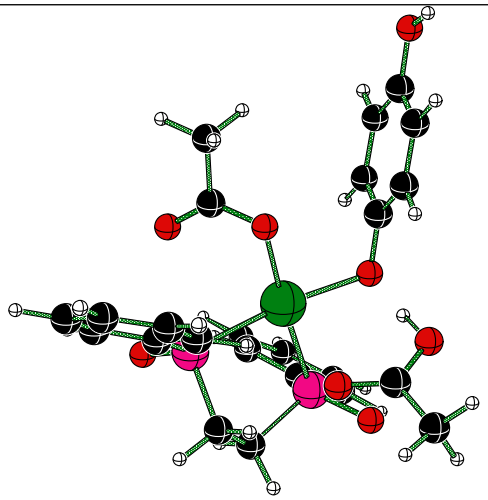
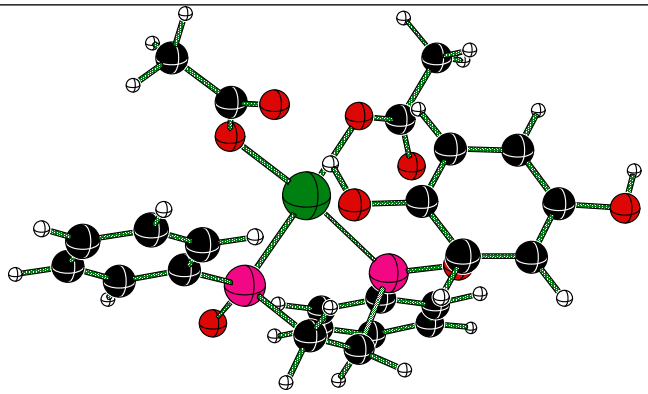
14. Geometries and relative free energies of Pd re-oxidation



Scheme S1. Re-oxidation of palladium in presence of benzoquinone. L=BS

Table S11. Geometries and Relative Free Energies of Pd Re-oxidation Obtained at the $SMD_{(1,4\text{-dioxane})}$/B3LYP-D3/6-31G**,SDD(Pd)//B3LYP-D3/6-31G**,LANL2DZ(Pd) Level of Theory

	Geometry	ΔΔG in kcal/mol
A		0.0
TS[A-B]		2.2
B		1.5

C		0.8
D		0.9

15. The optimized Cartesian coordinates of all the stationary points in the solvent phase (in the continuum dielectric of 1,4-dioxane) for the formation of oxazolidinone product (7) at the B3LYP-D3/6-31G level of theory**

Pd acetate-trimer

Number of imaginary frequencies : 0

Electronic energy : -1751.3931303
Zero-point correction= 0.314942 (Hartree/Particle)
Thermal correction to Energy= 0.349693
Thermal correction to Enthalpy= 0.350637
Thermal correction to Gibbs Free Energy= 0.241080
Sum of electronic and zero-point Energies= -1751.078188
Sum of electronic and thermal Energies= -1751.043438
Sum of electronic and thermal Enthalpies= -1751.042494
Sum of electronic and thermal Free Energies= -1751.152050

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Cartesian Coordinates

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46	1.608182	0.926492	-0.003179
8	2.311390	0.003526	-1.677911
8	2.658721	-0.338039	1.219417
6	2.244167	-1.352660	1.853482
8	1.170250	-1.998891	1.661926
46	-0.001156	-1.852020	0.000278
6	2.277184	-1.247726	-1.879374
8	1.601279	-2.113722	-1.250138
8	1.159449	1.986475	1.678020
8	1.022389	2.456010	-1.236614
6	-0.061779	2.596441	-1.874119
8	-1.156830	1.987543	-1.678615
46	-1.606916	0.928609	0.002868
6	0.065193	2.596833	1.873381
8	-1.019127	2.457743	1.235827
8	-2.311252	0.007053	1.677885
8	-2.659062	-0.334943	-1.219379
6	-2.278756	-1.244208	1.879706
6	-2.245909	-1.350394	-1.853003
8	-1.603912	-2.111263	1.250832
8	-1.172762	-1.997890	-1.661319
6	3.175371	-1.774192	-2.978615
1	4.095030	-2.150970	-2.518690
1	2.687607	-2.602068	-3.495582
1	3.433591	-0.974863	-3.673821
6	-0.064430	3.636149	-2.974535
1	-0.342988	4.599922	-2.535234
1	0.930826	3.726618	-3.411206
1	-0.804250	3.378024	-3.733452
6	0.069000	3.636712	2.973634
1	-0.925443	3.725878	3.412457
1	0.810838	3.379792	3.730968
1	0.344999	4.600836	2.533491
6	-3.178280	-1.768826	2.978731
1	-2.696494	-2.603543	3.490163
1	-3.427696	-0.970730	3.678605
1	-4.102732	-2.134581	2.519464
6	-3.156095	-1.871428	-2.944960
1	-3.921750	-2.502744	-2.481807
1	-3.654050	-1.039617	-3.445443
1	-2.589273	-2.474240	-3.655158
6	3.153544	-1.874057	2.945937
1	3.648981	-1.042116	3.448743
1	2.586838	-2.479297	3.654136
1	3.921412	-2.502708	2.482836

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3 (Nboc-amine)

Number of imaginary frequencies : 0
Electronic energy : = -597.7719941
Zero-point correction= 0.282886 (Hartree/Particle)
Thermal correction to Energy= 0.298380
Thermal correction to Enthalpy= 0.299325
Thermal correction to Gibbs Free Energy= 0.240170
Sum of electronic and zero-point Energies= -597.489108
Sum of electronic and thermal Energies= -597.473614
Sum of electronic and thermal Enthalpies= -597.472669
Sum of electronic and thermal Free Energies= -597.531824

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Cartesian Coordinates

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6	3.337524	2.420206	-0.168121
6	3.304153	1.275775	0.517622
6	3.335075	-0.095641	-0.098664
6	2.061995	-0.917677	0.187403
6	2.137478	-2.307136	-0.453181
7	0.904642	-0.170464	-0.309180
1	3.296758	3.386438	0.325937
1	3.217646	1.306974	1.604600
1	3.422927	2.429550	-1.252843
1	3.474298	-0.017893	-1.184818
1	1.049646	0.787219	-0.598614
1	1.956445	-1.042867	1.275005
1	2.258292	-2.220828	-1.538365
1	2.987496	-2.868221	-0.050076
1	1.220696	-2.860516	-0.243353
1	4.187530	-0.664898	0.293480
6	-0.361223	-0.492991	0.089946
8	-0.653915	-1.508688	0.704818
8	-1.222320	0.475809	-0.314219
6	-2.660604	0.355454	-0.053328
6	-3.219630	1.633840	-0.681702
1	-2.992582	1.665932	-1.751212
1	-4.305442	1.672296	-0.553226
1	-2.780473	2.517010	-0.208600
6	-3.220597	-0.885472	-0.756075
1	-2.973520	-0.856878	-1.821966
1	-2.808431	-1.796020	-0.321200
1	-4.310718	-0.903780	-0.656569
6	-2.922112	0.333184	1.456231
1	-2.513734	-0.571093	1.907378
1	-2.461635	1.205974	1.929929
1	-4.000172	0.370625	1.643187

AcOH

Number of imaginary frequencies : 0
Electronic energy : = -229.0904106
Zero-point correction= 0.061990 (Hartree/Particle)
Thermal correction to Energy= 0.066553
Thermal correction to Enthalpy= 0.067497
Thermal correction to Gibbs Free Energy= 0.034788
Sum of electronic and zero-point Energies= -229.028421
Sum of electronic and thermal Energies= -229.023858
Sum of electronic and thermal Enthalpies= -229.022913
Sum of electronic and thermal Free Energies= -229.055622

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Cartesian Coordinates

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6	0.093377	0.126042	-0.000076
8	0.776392	-1.047227	-0.000016
8	0.644969	1.203426	0.000011
6	-1.396064	-0.109530	0.000002
1	-1.679591	-0.693479	-0.880646
1	-1.679550	-0.691618	0.881891
1	-1.914878	0.848072	-0.000954
1	1.719252	-0.811637	0.000193

DBPOH

Number of imaginary frequencies : 0

Electronic energy : = -958.6809119
Zero-point correction= 0.277624 (Hartree/Particle)
Thermal correction to Energy= 0.294761
Thermal correction to Enthalpy= 0.295705
Thermal correction to Gibbs Free Energy= 0.229400
Sum of electronic and zero-point Energies= -958.403288
Sum of electronic and thermal Energies= -958.386151
Sum of electronic and thermal Enthalpies= -958.385207
Sum of electronic and thermal Free Energies= -958.451512

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Cartesian Coordinates

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8	0.044671	1.821703	1.524773
15	-0.014070	1.442688	0.093448
8	0.276304	2.653472	-0.935471
8	-1.403336	0.869880	-0.460004
6	-1.985106	-0.273165	0.217817
6	-3.405105	-0.446404	-0.292152
6	-4.107551	-1.648494	0.350882
6	-5.542427	-1.827980	-0.154488
8	1.006597	0.297752	-0.382077

6	2.377985	0.359559	0.083186
6	3.038509	-0.971737	-0.230668
6	4.508700	-1.006199	0.203949
6	5.180213	-2.347776	-0.105397
1	-1.969411	-0.095260	1.299535
1	-1.373229	-1.156877	-0.000515
1	-3.966724	0.473216	-0.087299
1	-3.376847	-0.564134	-1.382371
1	-3.529630	-2.560460	0.148704
1	-4.114539	-1.526339	1.442364
1	-6.026807	-2.689646	0.315737
1	-6.149452	-0.942085	0.063160
1	-5.561136	-1.983468	-1.239037
1	2.382533	0.567263	1.159048
1	2.886262	1.183837	-0.432962
1	2.477511	-1.768962	0.272740
1	2.958876	-1.160820	-1.308295
1	5.056604	-0.196759	-0.297093
1	4.576085	-0.800393	1.280693
1	5.154747	-2.562170	-1.179686
1	6.227659	-2.352714	0.212323
1	4.670254	-3.170412	0.408386
1	0.103099	3.496590	-0.493712

BS

Number of imaginary frequencies : 0
Electronic energy : = -1488.0909801
Zero-point correction= 0.247038 (Hartree/Particle)
Thermal correction to Energy= 0.263928
Thermal correction to Enthalpy= 0.264872
Thermal correction to Gibbs Free Energy= 0.199649
Sum of electronic and zero-point Energies= -1487.843942
Sum of electronic and thermal Energies= -1487.827053
Sum of electronic and thermal Enthalpies= -1487.826108
Sum of electronic and thermal Free Energies= -1487.891331

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Cartesian Coordinates

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6	-4.033579	-1.127836	0.403236
6	-3.235232	-0.156860	-0.183985
6	-3.700087	1.132720	-0.420924
6	-4.995185	1.460121	-0.035254
6	-5.807476	0.498863	0.562759
6	-5.330350	-0.790786	0.779191
16	-1.567983	-0.626719	-0.698560
8	-1.417404	-2.102628	-0.455874
6	-0.732492	0.180927	0.731054

6	0.732459	-0.180872	0.731070
16	1.567980	0.626698	-0.698573
8	1.417458	2.102612	-0.455921
6	3.235234	0.156830	-0.183999
6	4.033551	1.127832	0.403235
6	5.330317	0.790798	0.779213
6	5.807472	-0.498841	0.562786
6	4.995212	-1.460112	-0.035245
6	3.700115	-1.132735	-0.420942
1	0.877378	-1.266096	0.651778
1	1.231976	0.194688	1.632481
1	-0.877411	1.266146	0.651696
1	-1.232014	-0.194575	1.632489
1	3.059233	-1.870795	-0.903519
1	3.622881	2.126877	0.541361
1	5.375112	-2.464158	-0.208234
1	5.973113	1.537714	1.239331
1	6.822937	-0.756421	0.854529
1	-3.059184	1.870754	-0.903512
1	-3.622984	-2.126908	0.541382
1	-5.375075	2.464170	-0.208250
1	-5.973160	-1.537696	1.239294
1	-6.822935	0.756472	0.854498

BQ

Number of imaginary frequencies : 0
Electronic energy : = -381.4573678
Zero-point correction= 0.085257 (Hartree/Particle)
Thermal correction to Energy= 0.091492
Thermal correction to Enthalpy= 0.092436
Thermal correction to Gibbs Free Energy= 0.054737
Sum of electronic and zero-point Energies= -381.372110
Sum of electronic and thermal Energies= -381.365876
Sum of electronic and thermal Enthalpies= -381.364932
Sum of electronic and thermal Free Energies= -381.402630

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Cartesian Coordinates

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6	0.671488	-1.270084	0.000002
6	-0.671491	-1.270082	0.000011
6	-1.445430	0.000005	-0.000033
6	-0.671494	1.270079	0.000010
6	0.671491	1.270081	0.000002
6	1.445436	0.000005	-0.000083
1	1.260869	-2.182259	0.000033
1	-1.260875	-2.182255	0.000046
1	-1.260840	2.182277	0.000045

1	1.260833	2.182281	0.000034
8	-2.670305	-0.000004	0.000012
8	2.670307	-0.000005	0.000037

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2 [L1′=L2′=AcO¯, L=AcOH]

Number of imaginary frequencies : 0
Electronic energy : HF=-814.0396158
Zero-point correction= 0.167021 (Hartree/Particle)
Thermal correction to Energy= 0.183610
Thermal correction to Enthalpy= 0.184554
Thermal correction to Gibbs Free Energy= 0.119861
Sum of electronic and zero-point Energies= -813.872595
Sum of electronic and thermal Energies= -813.856006
Sum of electronic and thermal Enthalpies= -813.855061
Sum of electronic and thermal Free Energies= -813.919755

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Cartesian Coordinates

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46	0.475803	-0.140866	0.311617
8	2.234893	-1.104287	-0.195850
8	-0.795429	-1.666545	0.462791
8	-2.146324	-0.804171	-1.137443
8	2.176667	1.064372	0.077660
6	2.858585	0.013250	-0.185601
6	4.332580	0.077235	-0.437624
1	4.604288	1.060448	-0.825575
1	4.859249	-0.082537	0.509388
1	4.628122	-0.711545	-1.131958
6	-1.851953	-1.670508	-0.311420
6	-2.722918	-2.896975	-0.083386
1	-3.070082	-2.914091	0.953870
1	-3.575838	-2.875562	-0.762583
1	-2.135104	-3.804687	-0.246192
8	-1.056388	1.151541	0.889574
6	-1.664191	1.889839	0.111664
8	-2.741502	2.499818	0.600809
6	-1.271745	2.120810	-1.317808
1	-0.191799	2.278419	-1.370673
1	-1.509352	1.189919	-1.843968
1	-1.792913	2.967096	-1.772575
1	-3.160999	3.044679	-0.079420

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2 [L1′=L2′=AcO¯, L=DBPOH]

Number of imaginary frequencies : 0
Electronic energy : HF=-1543.6785772

Zero-point correction= 0.383276 (Hartree/Particle)
Thermal correction to Energy= 0.411289
Thermal correction to Enthalpy= 0.412233
Thermal correction to Gibbs Free Energy= 0.321652
Sum of electronic and zero-point Energies= -1543.295301
Sum of electronic and thermal Energies= -1543.267288
Sum of electronic and thermal Enthalpies= -1543.266344
Sum of electronic and thermal Free Energies= -1543.356925

Cartesian Coordinates

46	-0.520291	1.153178	-0.389298
8	-1.860860	2.692685	0.005838
8	1.230256	1.990503	0.149282
8	1.796242	0.624422	1.872811
8	-2.505670	0.812412	-0.898329
6	-2.812181	1.979467	-0.462166
6	-4.223953	2.471103	-0.505273
1	-4.540266	2.565130	-1.548658
1	-4.876107	1.736709	-0.024197
1	-4.305061	3.436918	-0.005626
6	1.962264	1.627994	1.141455
6	3.138801	2.548112	1.403450
1	2.773720	3.563328	1.580619
1	3.707921	2.196741	2.264091
1	3.779853	2.580616	0.518396
8	0.400461	-0.588291	-0.969973
8	1.817356	-2.620404	-0.260582
15	0.481974	-1.789718	-0.018332
8	-0.609181	-2.898948	-0.312806
8	0.371626	-1.368902	1.486512
6	3.081035	-2.073006	0.224519
1	3.742654	-2.939227	0.299552
1	2.931940	-1.662536	1.228890
6	3.645970	-1.018478	-0.718796
1	2.898269	-0.234220	-0.874848
1	3.829628	-1.475999	-1.698422
6	4.934435	-0.400023	-0.162959
1	4.715096	0.066073	0.806522
1	5.673615	-1.188440	0.033771
6	5.534789	0.640477	-1.113263
1	4.814713	1.438708	-1.327317
1	6.432670	1.100750	-0.688753
1	5.810968	0.185920	-2.071057
6	-1.966089	-2.511998	-0.692509
1	-1.912413	-1.725471	-1.451214
1	-2.383353	-3.414220	-1.145968
6	-2.787109	-2.060390	0.506803
1	-2.334179	-1.158986	0.932957
1	-2.748135	-2.835741	1.281126

6	-4.238717	-1.760686	0.112712
1	-4.238717	-1.056362	-0.726942
1	-4.723857	-2.680458	-0.240703
6	-5.040726	-1.165934	1.274220
1	-4.589328	-0.226614	1.615644
1	-6.075681	-0.957848	0.983002
1	-5.065431	-1.846808	2.132300
1	0.892319	-0.476028	1.678344

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2 [L1′=L2′=AcO^{-}, L=BS]

Number of imaginary frequencies : 0
Electronic energy : HF=-2073.6569782
Zero-point correction= 0.354093 (Hartree/Particle)
Thermal correction to Energy= 0.382894
Thermal correction to Enthalpy= 0.383838
Thermal correction to Gibbs Free Energy= 0.291916
Sum of electronic and zero-point Energies= -2073.302885
Sum of electronic and thermal Energies= -2073.274084
Sum of electronic and thermal Enthalpies= -2073.273140
Sum of electronic and thermal Free Energies= -2073.365062

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Cartesian Coordinates

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46	-0.007988	0.814765	-0.121789
8	-2.923394	1.756297	0.158644
8	-0.915335	2.589907	-0.440834
8	1.504110	1.954302	0.615454
6	-2.200355	2.680276	-0.216204
6	-2.742827	4.075669	-0.482863
1	-3.791827	4.126306	-0.189683
1	-2.156882	4.817019	0.066516
1	-2.644871	4.301277	-1.549075
6	2.159640	1.489992	1.647094
8	2.001011	0.373765	2.148553
6	3.220078	2.452297	2.156879
1	3.548698	2.147369	3.150966
1	4.073739	2.419369	1.471071
1	2.840011	3.475815	2.170209
16	1.192942	-1.158317	-0.005956
16	-1.692166	-0.443525	-1.136087
6	-0.822795	-2.049841	-1.591276
1	-1.248367	-2.305301	-2.564203
1	-1.096850	-2.800656	-0.848546
6	0.682962	-1.860919	-1.641868
1	1.207156	-2.813618	-1.755480
1	1.000944	-1.161175	-2.420079
6	-2.919583	-1.103028	0.010201
6	-4.258454	-0.991621	-0.346584
6	-2.499493	-1.669699	1.214125

6	-5.218421	-1.492547	0.533290
1	-4.527403	-0.505901	-1.277927
6	-3.475127	-2.160090	2.082225
1	-1.445727	-1.733432	1.473504
6	-4.828337	-2.073413	1.742292
1	-6.271053	-1.417599	0.278264
1	-3.174759	-2.604735	3.025868
1	-5.581149	-2.454272	2.426043
8	-2.345802	0.075795	-2.374796
8	0.899092	-2.232818	0.994444
6	2.962246	-0.982699	-0.271674
6	3.439700	0.042015	-1.090140
6	3.803833	-1.884186	0.374321
6	4.818077	0.145210	-1.280408
1	2.759763	0.762060	-1.534530
6	5.179110	-1.764857	0.172196
1	3.380716	-2.637298	1.030494
6	5.683098	-0.756185	-0.653151
1	5.214027	0.937176	-1.908341
1	5.856253	-2.453466	0.667905
1	6.755018	-0.664870	-0.800475

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2 [L1′=L2′=AcO^{-}, L=BQ]

Number of imaginary frequencies : 0
Electronic energy : HF=-966.4035138
Zero-point correction= 0.189562 (Hartree/Particle)
Thermal correction to Energy= 0.208122
Thermal correction to Enthalpy= 0.209066
Thermal correction to Gibbs Free Energy= 0.139518
Sum of electronic and zero-point Energies= -966.213952
Sum of electronic and thermal Energies= -966.195392
Sum of electronic and thermal Enthalpies= -966.194448
Sum of electronic and thermal Free Energies= -966.263996

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Cartesian Coordinates

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46	0.592453	-0.307571	-0.413419
8	2.461001	0.596209	-0.251925
8	2.182616	-1.508181	0.258547
8	-0.788116	-1.747471	-0.510074
6	-1.132263	0.904660	-1.310383
6	-0.132589	1.768878	-0.915680
1	-1.190358	0.491838	-2.313518
1	0.663957	2.085723	-1.583797
6	-2.373947	0.759562	-0.479215
6	-0.244127	2.556832	0.361999
8	0.611691	3.378819	0.652901
8	-3.323653	0.114283	-0.894894
6	-2.411989	1.472276	0.820946

6	-1.436025	2.314078	1.202354
1	-1.468452	2.856008	2.142207
1	-3.288747	1.280253	1.429799
6	2.966570	-0.504776	0.175748
6	4.399578	-0.587857	0.588275
1	4.992605	0.140623	0.032347
1	4.470021	-0.351949	1.655641
1	4.775312	-1.600595	0.431405
6	-1.490419	-1.918863	0.595329
8	-1.419919	-1.186266	1.577224
6	-2.457522	-3.080835	0.492117
1	-3.353766	-2.719025	-0.023305
1	-2.035308	-3.901797	-0.090450
1	-2.730661	-3.415677	1.493747

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2 [L1′=DBPO^{-}, L2′=AcO^{-}, L=AcOH]

Number of imaginary frequencies : 0
Electronic energy : HF=-1543.6635319
Zero-point correction= 0.383439 (Hartree/Particle)
Thermal correction to Energy= 0.412032
Thermal correction to Enthalpy= 0.412976
Thermal correction to Gibbs Free Energy= 0.318579
Sum of electronic and zero-point Energies= -1543.280093
Sum of electronic and thermal Energies= -1543.251500
Sum of electronic and thermal Enthalpies= -1543.250556
Sum of electronic and thermal Free Energies= -1543.344953

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Cartesian Coordinates

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46	1.272864	-0.855779	0.680759
8	3.258117	-0.648562	1.232090
8	1.371124	-2.516419	-0.525261
8	-0.807388	-3.116196	-0.455920
8	1.720691	0.740074	1.914729
6	2.958284	0.411439	1.885593
6	4.005866	1.255448	2.534650
1	4.352903	1.995874	1.805057
1	3.585260	1.783382	3.392333
1	4.854936	0.637825	2.832649
6	0.419400	-3.261683	-0.855770
6	0.669127	-4.407734	-1.787819
1	0.065103	-5.268792	-1.495053
1	0.351689	-4.095587	-2.788742
1	1.729240	-4.657511	-1.808276
8	-0.744308	-0.725591	0.391103
8	-0.692777	1.673349	-0.409585
15	-1.128066	0.184143	-0.867273
8	-2.736966	0.197246	-0.817648
8	-0.597434	-0.245631	-2.184250

6	0.072235	2.514502	-1.306015
1	-0.248139	3.538116	-1.087269
1	-0.181251	2.277775	-2.344084
6	1.565175	2.345257	-1.058572
1	1.842093	1.313520	-1.309586
1	1.753035	2.476422	0.013255
6	2.422095	3.318718	-1.873728
1	2.231852	3.168474	-2.944607
1	2.122517	4.351559	-1.648756
6	3.917530	3.144550	-1.588823
1	4.244613	2.124948	-1.822201
1	4.526158	3.836374	-2.179812
1	4.137172	3.329773	-0.530012
6	-3.423145	0.629560	0.381296
1	-3.153357	-0.037660	1.208336
1	-3.093844	1.644055	0.636254
6	-4.916434	0.589431	0.104444
1	-5.193086	-0.429866	-0.192107
1	-5.133991	1.237285	-0.753609
6	-5.742056	1.027843	1.320031
1	-5.505018	0.380392	2.175118
1	-5.446270	2.043681	1.615249
6	-7.249575	0.990442	1.050774
1	-7.576345	-0.020966	0.784120
1	-7.821098	1.306349	1.929415
1	-7.517286	1.653558	0.220441
1	-0.917082	-2.198105	-0.012340

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2 [L1′=DBPO^{-}, L2′=AcO^{-}, L=POH]

Number of imaginary frequencies : 0
Electronic energy : HF=-2273.2765103
Zero-point correction= 0.600265 (Hartree/Particle)
Thermal correction to Energy= 0.640700
Thermal correction to Enthalpy= 0.641645
Thermal correction to Gibbs Free Energy= 0.521576
Sum of electronic and zero-point Energies= -2272.676245
Sum of electronic and thermal Energies= -2272.635810
Sum of electronic and thermal Enthalpies= -2272.634866
Sum of electronic and thermal Free Energies= -2272.754935

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Cartesian Coordinates

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46	-1.347373	-0.269535	0.630176
8	-3.135535	-1.079913	1.307263
8	0.011779	-1.765876	1.014076
8	1.254737	-1.309733	-1.201885
8	-3.037708	0.901968	0.401121
8	0.127208	0.791001	-0.301079
8	0.684121	3.246115	0.153310

15	1.044731	1.738695	0.606599
8	2.517947	1.564615	-0.018213
8	0.991334	1.467273	2.064220
6	-0.638515	3.752333	0.471528
1	-0.497037	4.806663	0.728243
1	-1.021860	3.240709	1.362630
6	-1.590944	3.588899	-0.705849
1	-1.621520	2.532159	-0.984625
1	-1.192983	4.140637	-1.567120
6	-3.006184	4.072284	-0.368766
1	-3.343927	3.567698	0.544867
1	-2.990879	5.148758	-0.149729
6	-4.001748	3.781891	-1.495438
1	-4.067981	2.702750	-1.672704
1	-5.004639	4.147678	-1.250335
1	-3.692661	4.258233	-2.432929
6	2.775637	1.910444	-1.403558
1	1.852283	1.825779	-1.987668
1	3.101726	2.955618	-1.433793
6	3.841621	0.972017	-1.943927
1	3.454412	-0.052977	-1.908959
1	4.715810	1.012465	-1.281864
6	4.250665	1.324684	-3.379121
1	3.362796	1.305185	-4.025598
1	4.630153	2.354897	-3.409730
6	5.310006	0.368491	-3.935746
1	4.941103	-0.663223	-3.944354
1	5.589335	0.633453	-4.960427
1	6.219185	0.390174	-3.324314
15	0.942070	-2.349815	-0.052135
8	2.312351	-2.869192	0.536694
8	0.352880	-3.672093	-0.708244
1	0.879535	-0.393698	-0.958518
6	-1.092024	-3.890636	-0.681644
1	-1.450579	-3.708287	0.335817
1	-1.210171	-4.951084	-0.913889
6	-1.833387	-3.008827	-1.680556
1	-1.528581	-1.965619	-1.532020
1	-1.542001	-3.276458	-2.702902
6	-3.354665	-3.097517	-1.498755
1	-3.704595	-4.105217	-1.757988
1	-3.593985	-2.939492	-0.440051
6	-4.096663	-2.052461	-2.338852
1	-3.877254	-2.166574	-3.406199
1	-5.181276	-2.134899	-2.211485
1	-3.796401	-1.038579	-2.047237
6	3.334776	-1.893496	0.950070
1	4.255040	-2.480657	0.985270
1	3.427977	-1.139415	0.163492
6	3.014325	-1.249603	2.289517

1	2.955651	-2.027973	3.060228
1	2.036468	-0.762503	2.243715
6	4.066797	-0.195689	2.661169
1	4.124947	0.542099	1.851622
1	5.057640	-0.665490	2.740725
6	3.712075	0.523298	3.966417
1	4.473881	1.264837	4.229514
1	2.753110	1.037772	3.855784
1	3.632205	-0.184864	4.799749
6	-3.752384	-0.028066	0.918004
6	-5.237875	0.093596	1.015638
1	-5.533612	1.142146	0.957885
1	-5.686579	-0.449655	0.176785
1	-5.589626	-0.360817	1.944180

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2 **[**L1′=DBPO^{-}, L2′=AcO^{-}, L=BS]

Number of imaginary frequencies : 0
Electronic energy : HF=-2803.2632733
Zero-point correction= 0.571089 (Hartree/Particle)
Thermal correction to Energy= 0.611969
Thermal correction to Enthalpy= 0.612913
Thermal correction to Gibbs Free Energy= 0.492803
Sum of electronic and zero-point Energies= -2802.692184
Sum of electronic and thermal Energies= -2802.651304
Sum of electronic and thermal Enthalpies= -2802.650360
Sum of electronic and thermal Free Energies= -2802.770470

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Cartesian Coordinates

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46	-0.761449	-0.377429	-0.808856
8	-2.809154	1.580660	-0.122397
8	-1.891571	0.787909	-2.020297
8	0.738551	0.974562	-1.066827
6	-2.687906	1.582093	-1.349858
6	-3.452436	2.541769	-2.246122
1	-4.284119	2.979262	-1.692839
1	-2.774930	3.340108	-2.564379
1	-3.809692	2.029268	-3.142065
8	1.382526	0.511630	1.394365
16	0.428224	-1.900924	0.496204
16	-2.470710	-1.913274	-0.776587
6	-1.704779	-3.470243	-0.077037
1	-2.209184	-4.275853	-0.615533
1	-1.943300	-3.508984	0.987530
6	-0.200914	-3.453854	-0.299795
1	0.286987	-4.290956	0.206248
1	0.076297	-3.438552	-1.357771
6	-3.681521	-1.495387	0.487324
6	-5.024338	-1.504210	0.122496

6	-3.239556	-1.109974	1.755241
6	-5.968748	-1.128461	1.079963
1	-5.308889	-1.788584	-0.885099
6	-4.198511	-0.743369	2.696124
1	-2.181192	-1.087226	2.001886
6	-5.556319	-0.750783	2.359093
1	-7.023256	-1.125618	0.822169
1	-3.882605	-0.436666	3.688049
1	-6.294906	-0.452348	3.097045
8	-3.162804	-2.251054	-2.056435
8	0.099839	-2.082559	1.945393
6	2.187886	-2.065976	0.180382
6	2.696761	-1.713498	-1.069262
6	2.986856	-2.554793	1.211835
6	4.061621	-1.893377	-1.296158
1	2.059234	-1.262098	-1.822908
6	4.350276	-2.719651	0.967605
1	2.544544	-2.768539	2.179116
6	4.883620	-2.395450	-0.283754
1	4.483848	-1.614851	-2.256110
1	4.996743	-3.091197	1.756583
1	5.947325	-2.516757	-0.464487
15	1.556825	1.402082	0.197817
8	3.083567	1.481815	-0.329554
8	1.266803	2.960381	0.488998
6	4.143448	1.227229	0.614706
1	4.135328	1.994372	1.399670
1	3.976836	0.255049	1.090382
6	5.458432	1.245946	-0.146700
1	5.373901	0.556999	-0.995142
1	5.620418	2.245739	-0.567567
6	6.642823	0.838777	0.736250
1	6.718509	1.523947	1.591189
1	6.448617	-0.156405	1.159363
6	7.969621	0.820924	-0.028569
1	8.803413	0.526372	0.617132
1	7.929498	0.115596	-0.867178
1	8.199336	1.809056	-0.442524
6	-0.083011	3.356768	0.846541
1	-0.733779	2.483587	0.962069
1	-0.006134	3.858307	1.815708
6	-0.631296	4.279985	-0.233321
1	0.083237	5.098585	-0.389517
1	-0.665687	3.707153	-1.167110
6	-2.022532	4.843773	0.098510
1	-2.406736	5.359620	-0.790818
1	-2.705365	4.009094	0.292380
6	-2.035928	5.819708	1.282320
1	-1.748866	5.330092	2.218854
1	-1.340250	6.651274	1.117884

1	-3.034471	6.244396	1.431191

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2 [L1′=DBPO^{-}, L2′=AcO^{-}, L=BQ]

Number of imaginary frequencies : 0
Electronic energy : HF=-1696.0149349
Zero-point correction= 0.406425 (Hartree/Particle)
Thermal correction to Energy= 0.437183
Thermal correction to Enthalpy= 0.438128
Thermal correction to Gibbs Free Energy= 0.339597
Sum of electronic and zero-point Energies= -1695.608510
Sum of electronic and thermal Energies= -1695.577751
Sum of electronic and thermal Enthalpies= -1695.576807
Sum of electronic and thermal Free Energies= -1695.675338

Cartesian Coordinates

46	0.924029	-0.332592	1.077888
8	2.412642	0.319795	2.326207
8	0.492359	1.374241	2.334209
8	-0.760162	-0.762759	0.110559
8	-0.774410	1.637228	-0.672397
15	-1.132205	0.121088	-1.149283
8	-2.738294	0.064096	-1.180211
8	-0.529103	-0.234214	-2.460416
6	0.016643	2.485458	-1.539456
1	-0.246464	3.510159	-1.260660
1	-0.267633	2.315084	-2.582427
6	1.503549	2.219349	-1.344430
1	1.693018	1.166867	-1.576882
1	1.755146	2.379174	-0.286794
6	2.403427	3.081943	-2.234415
1	2.110026	2.942318	-3.282933
1	2.250116	4.145583	-2.006182
6	3.881669	2.714435	-2.066160
1	4.041974	1.657766	-2.306829
1	4.524084	3.314405	-2.718593
1	4.211099	2.876330	-1.032478
6	-3.497428	0.423457	-0.000354
1	-3.249674	-0.274093	0.807644
1	-3.211764	1.434405	0.314843
6	-4.972723	0.355765	-0.356733
1	-5.203319	-0.655911	-0.712608
1	-5.166428	1.037049	-1.194401
6	-5.870821	0.713695	0.833566
1	-5.657643	0.033113	1.668940
1	-5.620417	1.722249	1.189663
6	-7.361216	0.647898	0.485840
1	-7.644025	-0.358422	0.157006
1	-7.985100	0.906356	1.347492

1	-7.606640	1.341797	-0.326049
6	1.673916	-2.366200	0.761669
6	2.298979	-1.533688	-0.162124
1	2.101270	-2.568499	1.741517
1	3.235735	-1.028887	0.062923
6	0.601919	-3.327357	0.317934
6	1.978834	-1.639673	-1.629409
8	2.653011	-1.019152	-2.436939
8	0.070590	-4.062509	1.136258
6	0.282277	-3.362727	-1.122331
6	0.905275	-2.578751	-2.021590
1	0.651709	-2.581962	-3.074323
1	-0.508386	-4.049243	-1.407527
6	1.675839	1.279694	2.783581
6	2.234395	2.250692	3.773049
1	2.991669	1.766019	4.392142
1	2.708454	3.073028	3.225951
1	1.430625	2.660467	4.386958

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2 [L1′= L2′= $DBPO^{-}$,L=AcOH]

Number of imaginary frequencies : 0
Electronic energy : HF=-2273.267084
Zero-point correction= 0.599986 (Hartree/Particle)
Thermal correction to Energy= 0.640975
Thermal correction to Enthalpy= 0.641919
Thermal correction to Gibbs Free Energy= 0.517551
Sum of electronic and zero-point Energies= -2272.667098
Sum of electronic and thermal Energies= -2272.626109
Sum of electronic and thermal Enthalpies= -2272.625165
Sum of electronic and thermal Free Energies= -2272.749533

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Cartesian Coordinates

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46	-0.127055	-0.789617	-0.869732
8	1.877801	-1.388176	-0.923424
8	-0.616134	-1.378203	-2.772285
8	-2.841723	-1.612172	-2.452710
8	0.722704	-0.288311	0.963743
6	-1.771170	-1.635876	-3.186303
6	-1.974424	-1.989536	-4.627419
1	-2.746165	-2.755857	-4.722681
1	-2.327348	-1.086684	-5.137792
1	-1.036668	-2.313905	-5.077022
8	-2.040431	-0.193119	-0.513209
8	-1.403590	2.249313	-0.040396
15	-2.337586	1.319203	-0.970975
8	-3.801193	1.588758	-0.368204
8	-2.230566	1.562790	-2.430163
6	-0.157510	2.778047	-0.551890

1	-0.374882	3.674769	-1.143539
1	0.317716	2.047183	-1.217778
6	0.742669	3.080148	0.633170
1	0.853374	2.160916	1.216518
1	0.250773	3.820944	1.276468
6	2.121003	3.588419	0.197041
1	2.587762	2.834781	-0.450459
1	2.011141	4.498067	-0.409158
6	3.037767	3.868004	1.391298
1	3.179036	2.959164	1.985536
1	4.025077	4.216597	1.069879
1	2.608807	4.634542	2.046588
6	-4.047884	1.415616	1.048347
1	-3.769987	0.395826	1.338911
1	-3.417646	2.117651	1.606553
6	-5.522828	1.678476	1.299987
1	-6.114390	0.985620	0.688776
1	-5.765571	2.690610	0.953792
6	-5.892296	1.523914	2.780164
1	-5.631056	0.511764	3.117885
1	-5.284197	2.212727	3.382030
6	-7.378074	1.785623	3.045793
1	-8.007280	1.089398	2.479843
1	-7.621659	1.670484	4.106926
1	-7.657952	2.801775	2.745891
1	-2.640906	-1.118822	-1.573367
15	2.091939	-0.854354	0.518499
8	3.195586	0.284278	0.635630
8	2.675982	-1.996039	1.472407
6	4.562977	0.015090	0.204042
1	4.540341	-0.317592	-0.839854
1	4.970712	-0.789954	0.824929
6	5.360534	1.296500	0.359356
1	4.888885	2.082448	-0.241296
1	5.304892	1.623188	1.404183
6	6.824291	1.118918	-0.062190
1	6.866443	0.777949	-1.105319
1	7.285771	0.324512	0.539680
6	7.630743	2.412645	0.088402
1	8.672406	2.271243	-0.216005
1	7.206821	3.213467	-0.527649
1	7.628575	2.758348	1.128119
6	2.082071	-3.328859	1.443748
1	2.831724	-3.971759	1.912211
1	1.962343	-3.634213	0.398672
6	0.758885	-3.383516	2.196010
1	0.918767	-3.026640	3.220653
1	0.046131	-2.693274	1.731308
6	0.173740	-4.801244	2.209823
1	0.046071	-5.151663	1.176412

1	0.886326	-5.490750	2.682755
6	-1.170761	-4.866739	2.941053
1	-1.067233	-4.547207	3.983940
1	-1.906858	-4.209561	2.464646
1	-1.576757	-5.883166	2.939900

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2 [L1′= L2′= $DBPO^{-}$, L=DBPOH]

Number of imaginary frequencies : 0
Electronic energy : HF=-3002.8835411
Zero-point correction= 0.817524 (Hartree/Particle)
Thermal correction to Energy= 0.870052
Thermal correction to Enthalpy= 0.870996
Thermal correction to Gibbs Free Energy= 0.723409
Sum of electronic and zero-point Energies= -3002.066017
Sum of electronic and thermal Energies= -3002.013489
Sum of electronic and thermal Enthalpies= -3002.012545
Sum of electronic and thermal Free Energies= -3002.160132

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Cartesian Coordinates

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46	0.443894	-0.144462	-0.366365
8	2.381491	-0.944784	-0.228457
8	-0.624336	-1.891155	-0.558797
8	-2.445230	-1.035234	1.079287
8	1.767949	1.451294	-0.178053
8	-1.304092	0.880330	-0.130923
8	-1.878715	3.093166	-1.256795
15	-2.011167	1.495714	-1.428703
8	-3.585320	1.278059	-1.151151
8	-1.573542	0.921117	-2.723416
6	-0.564914	3.671611	-1.023745
1	-0.547594	4.600599	-1.601495
1	0.217678	3.013036	-1.413776
6	-0.356665	3.936745	0.460454
1	-0.434077	2.982471	0.990376
1	-1.171046	4.578029	0.822715
6	1.002031	4.582466	0.752824
1	1.791966	3.919170	0.382797
1	1.091168	5.526115	0.197008
6	1.209356	4.845851	2.247667
1	1.152447	3.912289	2.818252
1	2.187171	5.297998	2.443553
1	0.441897	5.521880	2.642276
6	-4.202011	1.863670	0.023746
1	-3.445194	2.035105	0.797762
1	-4.616732	2.835990	-0.263049
6	-5.278897	0.918995	0.530797
1	-4.808754	-0.033212	0.801966
1	-5.983731	0.713837	-0.284760

6	-6.023756	1.491426	1.742823
1	-5.301665	1.711071	2.541096
1	-6.484046	2.451268	1.472255
6	-7.097149	0.536094	2.273261
1	-6.654889	-0.418487	2.579596
1	-7.616655	0.958588	3.139251
1	-7.847592	0.321822	1.503953
15	2.927612	0.467696	0.119696
8	4.216964	0.893576	-0.696448
8	3.434590	0.524982	1.640048
6	5.427022	0.081373	-0.626889
1	5.172001	-0.949808	-0.896694
1	5.797587	0.099305	0.403736
6	6.435113	0.672528	-1.594870
1	5.995815	0.680426	-2.599445
1	6.618063	1.717891	-1.318483
6	7.753081	-0.112524	-1.599226
1	7.553508	-1.160005	-1.862281
1	8.174814	-0.125389	-0.585123
6	8.778169	0.474941	-2.574237
1	9.710789	-0.097648	-2.563965
1	8.392747	0.470257	-3.599761
1	9.018200	1.512084	-2.315060
6	2.571801	-0.031819	2.683320
1	3.236033	-0.178328	3.537388
1	2.230850	-1.012895	2.343732
6	1.382491	0.877545	3.016962
1	1.668042	1.610709	3.780394
1	1.121494	1.450380	2.123871
6	0.146501	0.084420	3.466915
1	-0.060285	-0.703189	2.731542
1	0.348311	-0.427130	4.417774
6	-1.095581	0.970616	3.596119
1	-0.939045	1.777073	4.321484
1	-1.334951	1.428186	2.630015
1	-1.964897	0.387665	3.914493
15	-1.806567	-2.267693	0.334532
8	-2.934353	-3.021773	-0.485794
8	-1.414915	-3.299282	1.475940
1	-2.084563	-0.168147	0.672104
6	-0.282964	-4.205744	1.280075
1	-0.228510	-4.504556	0.228295
1	-0.527902	-5.085804	1.879311
6	1.011511	-3.546944	1.728810
1	1.152412	-2.634892	1.144283
1	0.914098	-3.256559	2.782630
6	2.237440	-4.446367	1.532553
1	2.142173	-5.354834	2.142401
1	2.278123	-4.775385	0.485785
6	3.537469	-3.711894	1.879928

1	3.537354	-3.384309	2.926330
1	4.411945	-4.353502	1.732079
1	3.650869	-2.824305	1.248453
6	-3.725897	-2.276050	-1.480394
1	-4.626650	-2.882126	-1.602123
1	-4.008628	-1.313003	-1.045249
6	-2.988405	-2.080836	-2.795003
1	-2.720893	-3.060505	-3.210497
1	-2.061219	-1.530003	-2.618057
6	-3.848025	-1.286075	-3.788276
1	-4.145504	-0.341905	-3.317114
1	-4.770473	-1.840954	-4.012371
6	-3.084788	-0.977108	-5.079136
1	-3.715160	-0.434391	-5.791501
1	-2.214488	-0.355842	-4.850269
1	-2.741184	-1.896532	-5.568340

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2 [L1′= L2′= $DBPO^{-}$, L=BS]

Number of imaginary frequencies : 0
Electronic energy : HF=-3532.8766882
Zero-point correction= 0.788770 (Hartree/Particle)
Thermal correction to Energy= 0.841438
Thermal correction to Enthalpy= 0.842382
Thermal correction to Gibbs Free Energy= 0.696910
Sum of electronic and zero-point Energies= -3532.087918
Sum of electronic and thermal Energies= -3532.035250
Sum of electronic and thermal Enthalpies= -3532.034306
Sum of electronic and thermal Free Energies= -3532.179778

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Cartesian Coordinates

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46	-0.282711	-0.798932	-0.350593
8	-1.837309	1.903123	0.622946
8	-1.446620	0.408991	-1.474740
8	1.246202	0.499352	-0.682295
8	2.384282	-0.263759	1.514514
16	0.940184	-2.437430	0.768697
16	-2.072284	-2.259504	-0.324938
6	-1.388618	-3.791423	0.471905
1	-2.009362	-4.606156	0.091632
1	-1.501871	-3.692120	1.554332
6	0.073209	-3.928058	0.083853
1	0.539702	-4.794776	0.558748
1	0.225394	-3.963201	-0.998994
6	-3.386544	-1.823538	0.817318
6	-4.524905	-2.637019	0.819311
6	-3.262849	-0.701040	1.634449
6	-5.562967	-2.322124	1.691041
1	-4.605132	-3.471824	0.130409

6	-4.322629	-0.395739	2.492849
1	-2.403872	-0.039116	1.577066
6	-5.460463	-1.202215	2.524988
1	-6.457013	-2.937326	1.708708
1	-4.255237	0.488734	3.117467
1	-6.280590	-0.952275	3.191286
8	-2.644696	-2.657824	-1.647935
8	0.853354	-2.615909	2.247290
6	2.596128	-2.745061	0.136149
6	2.887194	-2.461599	-1.197237
6	3.535258	-3.271845	1.019079
6	4.170202	-2.747657	-1.665375
1	2.152803	-1.986371	-1.840480
6	4.813927	-3.545881	0.534006
1	3.266815	-3.426426	2.058638
6	5.128468	-3.288645	-0.804136
1	4.424348	-2.525072	-2.696583
1	5.567360	-3.949276	1.203398
1	6.128799	-3.494324	-1.172702
15	2.370450	0.723683	0.385986
8	3.729879	0.748461	-0.484483
8	2.290653	2.257967	0.883004
6	4.967358	0.406501	0.176246
1	5.218947	1.182781	0.910368
1	4.838310	-0.540397	0.710841
6	6.046369	0.292422	-0.887372
1	5.690967	-0.396285	-1.662537
1	6.186047	1.267201	-1.370398
6	7.373058	-0.214259	-0.311650
1	7.719643	0.469525	0.474734
1	7.203720	-1.182651	0.178973
6	8.460041	-0.363573	-1.380210
1	9.399094	-0.728496	-0.951533
1	8.149950	-1.070226	-2.159193
1	8.665469	0.594710	-1.870122
6	1.101842	2.607522	1.646719
1	0.289140	2.810608	0.949706
1	0.802022	1.749426	2.256071
6	1.410657	3.814761	2.517021
1	2.044416	3.504246	3.357253
1	1.994608	4.530285	1.926787
6	0.127160	4.490090	3.029821
1	0.405540	5.287585	3.729976
1	-0.376381	4.981688	2.187022
6	-0.862603	3.524934	3.697924
1	-1.286040	2.831675	2.964203
1	-0.374427	2.940947	4.487841
1	-1.693740	4.073669	4.153676
15	-2.109851	1.684373	-0.830149
8	-3.692202	1.561835	-1.107767

8	-1.726815	2.905621	-1.814613
6	-4.165553	1.185758	-2.423639
1	-4.027025	2.035544	-3.101523
1	-3.571731	0.340093	-2.789169
6	-5.631396	0.800840	-2.300616
1	-6.006389	0.577819	-3.309050
1	-6.200185	1.664948	-1.933701
6	-5.851450	-0.400952	-1.376677
1	-5.471332	-0.148556	-0.382033
1	-5.242371	-1.242359	-1.732892
6	-7.319190	-0.821588	-1.278445
1	-7.443237	-1.673083	-0.600511
1	-7.940030	-0.002079	-0.897801
1	-7.719391	-1.111761	-2.257060
6	-0.332423	3.298890	-1.907630
1	-0.107247	3.377757	-2.976516
1	0.312726	2.518301	-1.490963
6	-0.125436	4.631340	-1.200801
1	-0.511644	4.539705	-0.179223
1	-0.732498	5.400372	-1.695425
6	1.350027	5.047229	-1.169852
1	1.933202	4.267366	-0.665316
1	1.736305	5.105881	-2.196960
6	1.562249	6.391178	-0.465907
1	1.195845	6.354331	0.566406
1	2.622080	6.664893	-0.434353
1	1.022248	7.196713	-0.977029

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2 [L1′= L2′= $DBPO^{-}$, L=BQ]

Number of imaginary frequencies : 0
Electronic energy : HF=-2425.6315803
Zero-point correction= 0.624241 (Hartree/Particle)
Thermal correction to Energy= 0.666744
Thermal correction to Enthalpy= 0.667688
Thermal correction to Gibbs Free Energy= 0.542340
Sum of electronic and zero-point Energies= -2425.007340
Sum of electronic and thermal Energies= -2424.964836
Sum of electronic and thermal Enthalpies= -2424.963892
Sum of electronic and thermal Free Energies= -2425.089240

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Cartesian Coordinates

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46	-0.328938	-0.394359	-0.703240
8	-2.357882	-0.803235	-0.787039
8	-1.373281	1.290078	0.060514
8	1.518989	0.364569	-0.605906
8	2.322747	2.063690	1.148419
15	2.189505	0.489535	0.825940
8	3.737473	0.110867	0.606095

8	1.542507	-0.339818	1.884312
6	1.123712	2.860393	1.328870
1	1.362000	3.568611	2.128838
1	0.299469	2.225980	1.669200
6	0.751187	3.583500	0.042485
1	0.578722	2.834900	-0.736413
1	1.601571	4.199000	-0.278574
6	-0.501390	4.449758	0.214478
1	-1.318478	3.816819	0.579842
1	-0.320793	5.214494	0.982883
6	-0.928555	5.121689	-1.093694
1	-1.160053	4.368648	-1.855549
1	-1.820074	5.742160	-0.954178
1	-0.132581	5.762768	-1.490128
6	4.452621	0.641948	-0.536341
1	3.966181	0.293067	-1.454493
1	4.407457	1.736988	-0.512075
6	5.888067	0.151601	-0.455453
1	5.887184	-0.945870	-0.417357
1	6.329781	0.496033	0.487513
6	6.728773	0.630653	-1.644735
1	6.265207	0.286957	-2.579032
1	6.714854	1.728234	-1.681474
6	8.177482	0.137801	-1.577177
1	8.220531	-0.957315	-1.571394
1	8.760194	0.490497	-2.434114
1	8.672268	0.492807	-0.666112
15	-2.705548	0.511823	-0.011957
8	-3.362009	0.165539	1.394688
8	-3.803858	1.408804	-0.715158
6	-2.744029	-0.834483	2.278839
1	-2.414449	-1.683355	1.670737
1	-3.565615	-1.163493	2.919671
6	-1.598743	-0.249932	3.088893
1	-0.797463	0.081594	2.422402
1	-1.965030	0.629754	3.633428
6	-1.021951	-1.284837	4.065347
1	-0.655690	-2.146445	3.494531
1	-1.819006	-1.654077	4.727004
6	0.127133	-0.705859	4.896645
1	0.520012	-1.451334	5.595959
1	0.939605	-0.388183	4.237804
1	-0.205932	0.159332	5.482805
6	-5.228827	1.100583	-0.671772
1	-5.708337	2.001693	-1.060822
1	-5.524807	0.967026	0.373211
6	-5.574162	-0.119190	-1.514835
1	-5.191529	0.033850	-2.531013
1	-5.055997	-0.998766	-1.113447
6	-7.086182	-0.376417	-1.548327

1	-7.457215	-0.506749	-0.522825
1	-7.598766	0.507695	-1.950613
6	-7.449264	-1.606745	-2.385652
1	-7.116124	-1.488779	-3.422671
1	-6.973519	-2.508800	-1.985095
1	-8.530538	-1.775021	-2.397691
6	0.525397	-2.109788	-1.820959
6	-0.065790	-2.567039	-0.648427
1	-0.012113	-2.075055	-2.765568
1	-1.104366	-2.884319	-0.619621
6	2.023921	-2.043998	-1.922403
6	0.753258	-2.985342	0.539519
8	0.196382	-3.451393	1.522321
8	2.565507	-1.709558	-2.965089
6	2.799372	-2.457043	-0.728994
6	2.220031	-2.869717	0.413063
1	2.794561	-3.125783	1.295970
1	3.875708	-2.366967	-0.823703

2' mode **a**

Number of imaginary frequencies : 0
Electronic energy : = -1181.5511328
Zero-point correction= 0.388831 (Hartree/Particle)
Thermal correction to Energy= 0.416021
Thermal correction to Enthalpy= 0.416965
Thermal correction to Gibbs Free Energy= 0.329309
Sum of electronic and zero-point Energies= -1181.162302
Sum of electronic and thermal Energies= -1181.135112
Sum of electronic and thermal Enthalpies= -1181.134168
Sum of electronic and thermal Free Energies= -1181.221823

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Cartesian Coordinates

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46	1.202612	0.909713	-0.364344
6	2.244377	0.133678	-2.110056
6	1.343470	-0.868316	-1.778302
6	1.756081	-2.136310	-1.083439
6	0.599555	-2.915126	-0.403706
6	-0.139766	-3.828927	-1.390702
8	0.235164	2.636472	0.627895
8	2.700093	0.216984	0.788724
8	1.243542	-0.615230	2.304875
7	-0.304629	-2.064093	0.365924
8	-0.188908	1.985027	-1.426802
1	1.993023	0.878073	-2.860375
1	0.340514	-0.842762	-2.203737
1	3.289590	0.049279	-1.822464

1	2.546365	-1.902850	-0.365628
1	2.211589	-2.789989	-1.842122
1	0.035405	-1.710980	1.258551
1	1.070127	-3.565633	0.343110
1	-0.562537	-3.267932	-2.223981
1	0.555823	-4.580852	-1.777151
1	-0.960544	-4.345929	-0.886146
6	-1.429995	-1.464580	-0.119251
8	-1.782517	-1.436635	-1.295026
8	-2.109987	-0.917704	0.917878
6	-3.389896	-0.235266	0.721909
6	-3.164990	1.054536	-0.068365
1	-2.723219	0.841139	-1.042248
1	-4.116694	1.577406	-0.209681
1	-2.494260	1.706497	0.496644
6	-4.404126	-1.166000	0.048376
1	-5.393449	-0.697229	0.064064
1	-4.121803	-1.375346	-0.982636
1	-4.464596	-2.110927	0.597512
6	-3.817979	0.078658	2.157520
1	-4.762156	0.632066	2.156638
1	-3.953998	-0.844886	2.727407
1	-3.055367	0.682161	2.657737
6	-0.377067	2.826054	-0.464328
6	-1.283011	3.999940	-0.680320
1	-0.739699	4.770251	-1.237986
1	-2.148230	3.695731	-1.272733
1	-1.596517	4.410666	0.280389
6	2.380709	-0.308145	1.948749
6	3.588278	-0.498995	2.852260
1	3.879932	0.473438	3.262078
1	3.331027	-1.170947	3.671942
1	4.439012	-0.887086	2.286743

TS[2'-4] mode **a**

Number of imaginary frequencies : 1
Electronic energy : = -1181.5182838
Zero-point correction= 0.383043 (Hartree/Particle)
Thermal correction to Energy= 0.409918
Thermal correction to Enthalpy= 0.410862
Thermal correction to Gibbs Free Energy= 0.323595
Sum of electronic and zero-point Energies= -1181.135241
Sum of electronic and thermal Energies= -1181.108366
Sum of electronic and thermal Enthalpies= -1181.107421
Sum of electronic and thermal Free Energies= -1181.194689

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Cartesian Coordinates

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46	1.766555	0.672057	-0.300243
6	2.048213	-0.686595	-1.868629
6	0.768755	-1.296141	-1.666848
6	0.571003	-2.501607	-0.973455
6	-0.824326	-3.116501	-0.795231
6	-1.540193	-3.442011	-2.112920
8	1.113837	2.709572	0.637619
8	2.708406	-0.492116	1.143011
8	1.096346	-2.031210	1.533109
7	-1.669279	-2.323676	0.116914
8	0.909966	2.105123	-1.476246
1	2.138558	-0.003654	-2.712271
1	-0.108013	-0.728736	-1.977065
1	2.930214	-1.298877	-1.678247
1	0.858153	-2.099723	0.279847
1	1.391554	-3.222275	-1.048195
1	-1.477033	-2.446138	1.102098
1	-0.675099	-4.060501	-0.259846
1	-1.725269	-2.535459	-2.688944
1	-0.920603	-4.122711	-2.704961
1	-2.501063	-3.925851	-1.913199
6	-2.187986	-1.095501	-0.193745
8	-2.254778	-0.617032	-1.319934
8	-2.637458	-0.509183	0.939820
6	-3.250369	0.825948	0.909740
6	-2.233673	1.857528	0.414726
1	-1.954363	1.664451	-0.621538
1	-2.671639	2.858867	0.485257
1	-1.331258	1.837865	1.031699
6	-4.521289	0.801100	0.055388
1	-5.043947	1.758284	0.150528
1	-4.282038	0.628929	-0.993878
1	-5.191572	0.008189	0.401745
6	-3.589217	1.064441	2.382552
1	-4.058905	2.044839	2.504946
1	-4.279516	0.298058	2.746787
1	-2.682092	1.033528	2.992735
6	0.751641	2.983155	-0.535280
6	0.106034	4.291210	-0.898252
1	0.577061	4.705491	-1.793304
1	-0.948605	4.111885	-1.128859
1	0.183752	4.990674	-0.065221
6	2.147198	-1.379405	1.851045
6	2.759453	-1.679344	3.199308
1	2.178181	-1.153673	3.964889
1	2.705767	-2.749089	3.410809
1	3.789170	-1.322156	3.237530

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4 [L1=AcO^-, L2=AcOH]

Number of imaginary frequencies : 0

Electronic energy : = -1181.5429601
Zero-point correction= 0.388597 (Hartree/Particle)
Thermal correction to Energy= 0.416176
Thermal correction to Enthalpy= 0.417120
Thermal correction to Gibbs Free Energy= 0.327908
Sum of electronic and zero-point Energies= -1181.154363
Sum of electronic and thermal Energies= -1181.126784
Sum of electronic and thermal Enthalpies= -1181.125840
Sum of electronic and thermal Free Energies= -1181.215052

Cartesian Coordinates

46	1.498909	-0.968455	-0.158198
6	0.676973	-2.233776	-1.539623
6	-0.652275	-1.656700	-1.767089
6	-1.768199	-2.050748	-1.119978
6	-3.067671	-1.268059	-1.098976
6	-3.614580	-0.867347	-2.472929
8	2.812659	0.805107	0.634748
8	0.523551	-2.099334	1.395332
8	-0.940585	-0.630736	2.320751
7	-2.912072	-0.096115	-0.188857
8	2.677652	0.128607	-1.471735
1	1.362413	-2.171733	-2.386884
1	-0.701091	-0.792536	-2.426289
1	0.672065	-3.225829	-1.078624
1	-0.726529	0.007525	1.598927
1	-1.702853	-2.902156	-0.441634
1	-2.898575	-0.336508	0.794217
1	-3.832329	-1.880319	-0.608572
1	-2.902767	-0.257325	-3.026730
1	-3.833954	-1.771988	-3.047323
1	-4.536007	-0.289666	-2.354940
6	-2.071456	0.942030	-0.499840
8	-1.844729	1.375135	-1.612960
8	-1.514589	1.432026	0.657752
6	-0.989342	2.818906	0.723252
6	0.274663	2.952625	-0.124279
1	0.064356	2.735178	-1.170801
1	0.651588	3.977724	-0.039219
1	1.047350	2.274242	0.241443
6	-2.095330	3.780988	0.286748
1	-1.768787	4.811098	0.457624
1	-2.322034	3.659068	-0.773422
1	-3.005274	3.606844	0.869646

6	-0.669069	2.975704	2.209868
1	-0.273015	3.977229	2.400020
1	-1.566116	2.831466	2.819025
1	0.087621	2.247788	2.518265
6	3.158119	0.916056	-0.574378
6	4.097153	2.008350	-1.021593
1	4.693377	1.678616	-1.874661
1	3.500061	2.871464	-1.336784
1	4.739098	2.314050	-0.193838
6	-0.310940	-1.792046	2.245369
6	-0.722900	-2.746617	3.330746
1	-0.516158	-2.297560	4.306570
1	-1.800989	-2.923703	3.273892
1	-0.179304	-3.683891	3.224307

2' mode **b**

Number of imaginary frequencies : 0 Electronic energy : = -1911.152145
Zero-point correction= 0.605808 (Hartree/Particle)
Thermal correction to Energy= 0.645175
Thermal correction to Enthalpy= 0.646119
Thermal correction to Gibbs Free Energy= 0.528508
Sum of electronic and zero-point Energies= -1910.546337
Sum of electronic and thermal Energies= -1910.506970
Sum of electronic and thermal Enthalpies= -1910.506026
Sum of electronic and thermal Free Energies= -1910.623637

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Cartesian Coordinates

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46	-1.510385	-1.688486	-1.051121
6	-1.059519	-1.304940	-3.149049
6	0.173509	-1.637609	-2.603051
6	1.238075	-0.647131	-2.250696
6	2.274667	-1.089968	-1.185361
6	1.713356	-1.914279	-0.015613
8	-2.266394	-2.643814	0.777453
8	-1.990624	0.261684	-0.924651
15	-1.180440	1.305782	-0.064437
8	0.256350	0.997207	0.187395
7	2.917153	0.120324	-0.694377
8	-1.303144	-3.729723	-0.866008
8	-2.066328	1.562153	1.268736
8	-1.341331	2.714240	-0.819146
1	-1.655836	-2.054437	-3.663083
1	0.453004	-2.691441	-2.605003
1	-1.330804	-0.263319	-3.295854
1	1.784182	-0.429523	-3.181337
1	2.304729	0.788850	-0.235448

1	3.058438	-1.677208	-1.672229
1	0.995014	-1.319452	0.553559
1	1.235018	-2.840595	-0.351187
1	2.540273	-2.185327	0.647571
6	4.249819	0.145257	-0.408860
8	5.046928	-0.731762	-0.718070
8	4.547425	1.298061	0.243379
6	5.921954	1.597744	0.647373
6	6.420815	0.544893	1.642854
1	6.507669	-0.429731	1.162538
1	7.400076	0.840930	2.033156
1	5.725138	0.465780	2.484294
6	6.825690	1.699787	-0.586106
1	7.820171	2.047322	-0.287438
1	6.918924	0.731596	-1.078050
1	6.408837	2.420750	-1.296396
6	5.777315	2.961564	1.326726
1	6.750807	3.309241	1.685591
1	5.379393	3.698264	0.622982
1	5.092960	2.894413	2.177234
1	0.776740	0.290557	-1.938378
6	-2.542709	0.449258	2.058014
6	-1.419014	-0.322804	2.740574
1	-3.135196	-0.218023	1.421445
1	-3.209524	0.899814	2.799657
6	-1.959318	-1.383257	3.706469
1	-0.805811	-0.810056	1.976470
1	-0.765034	0.384634	3.263515
6	-0.853899	-2.310104	4.221130
1	-2.459767	-0.893041	4.552550
1	-2.717935	-1.981997	3.190054
1	-1.244047	-3.054544	4.923309
1	-0.384470	-2.845346	3.386928
1	-0.066119	-1.746053	4.732874
6	-2.654264	3.228124	-1.147274
6	-3.074250	4.303351	-0.155049
1	-3.381241	2.408739	-1.176375
1	-2.569598	3.637806	-2.159567
6	-4.440758	4.906476	-0.501435
1	-3.095946	3.859811	0.846052
1	-2.306970	5.087369	-0.141265
6	-4.874199	5.988837	0.492140
1	-4.410770	5.329208	-1.515275
1	-5.195379	4.108173	-0.525980
1	-5.852744	6.404818	0.231096
1	-4.941616	5.583799	1.508090
1	-4.153639	6.814167	0.513436
6	-1.834950	-3.741158	0.310178
6	-1.893683	-5.010083	1.100855
1	-1.111523	-4.977735	1.866976

1	-2.857270	-5.080173	1.610408
1	-1.730772	-5.874794	0.456234

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4 [L1=DBPO^{-}, L2=AcOH]

Number of imaginary frequencies : 0
Electronic energy : = -1911.1606176
Zero-point correction= 0.605253 (Hartree/Particle)
Thermal correction to Energy= 0.644076
Thermal correction to Enthalpy= 0.645020
Thermal correction to Gibbs Free Energy= 0.530741
Sum of electronic and zero-point Energies= -1910.555365
Sum of electronic and thermal Energies= -1910.516541
Sum of electronic and thermal Enthalpies= -1910.515597
Sum of electronic and thermal Free Energies= -1910.629877

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Cartesian Coordinates

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46	0.120470	-1.765653	-0.401427
6	0.038258	-1.646786	-2.434228
6	0.947408	-0.531183	-2.720967
6	0.593075	0.765734	-2.667965
6	1.557145	1.929487	-2.697133
6	2.878063	1.676500	-3.432334
7	1.808738	2.407275	-1.313631
8	1.772615	-3.119643	-0.474791
1	0.351780	-2.614087	-2.832473
1	1.992215	-0.786297	-2.882379
1	-1.017872	-1.439913	-2.620159
1	-0.442072	1.012269	-2.435099
1	1.406218	3.283121	-1.016068
1	1.057355	2.778110	-3.179340
1	3.468935	0.917125	-2.918012
1	2.680162	1.339853	-4.453716
1	3.466472	2.597634	-3.472075
6	2.332927	1.630744	-0.332039
8	2.794360	0.504859	-0.533546
8	2.288136	2.272771	0.844580
6	2.874462	1.712762	2.084551
6	2.087969	0.480271	2.521344
1	2.193174	-0.345063	1.820668
1	2.455028	0.144220	3.496266
1	1.023875	0.698491	2.616581
6	4.363928	1.426873	1.876746
1	4.817253	1.177014	2.840853
1	4.522462	0.592128	1.194296
1	4.870051	2.312399	1.479592
6	2.673897	2.863132	3.072429

1	3.066693	2.582699	4.053745
1	3.193654	3.762965	2.730680
1	1.609849	3.092250	3.179211
8	-1.625073	-0.545316	-0.175019
8	-0.406215	-1.356256	1.902963
8	3.562803	-1.859201	0.127644
1	3.054976	-1.027263	-0.103189
6	2.942829	-2.992796	-0.092917
6	3.790532	-4.214640	0.145400
1	4.756691	-3.950841	0.574725
1	3.249827	-4.895852	0.806637
1	3.938590	-4.730262	-0.808195
15	-1.563750	-0.532791	1.377869
8	-1.536287	1.026792	1.848959
8	-2.934226	-1.035577	2.052765
6	-1.011746	2.016429	0.940042
6	-2.132662	2.662263	0.137126
1	-0.282982	1.561968	0.265713
1	-0.487826	2.752223	1.558376
6	-1.615082	3.730977	-0.832735
1	-2.646472	1.871290	-0.420970
1	-2.861022	3.102954	0.830053
6	-2.740671	4.422962	-1.607288
1	-1.032943	4.481586	-0.278579
1	-0.922559	3.261329	-1.544058
1	-2.350642	5.171918	-2.304302
1	-3.319337	3.694507	-2.186041
1	-3.433017	4.928384	-0.924910
6	-4.193674	-0.448284	1.657036
6	-4.767440	-1.134831	0.422760
1	-4.063673	0.627996	1.488559
1	-4.855082	-0.572894	2.520230
6	-6.121137	-0.545275	0.010354
1	-4.045784	-1.040178	-0.395580
1	-4.869973	-2.206385	0.634985
6	-6.703507	-1.230007	-1.230108
1	-6.831734	-0.629079	0.844411
1	-6.005550	0.530016	-0.185039
1	-7.667383	-0.795424	-1.514810
1	-6.024741	-1.133206	-2.084934
1	-6.857504	-2.300143	-1.051522

TS[2'-4] mode **b**

Number of imaginary frequencies : 1
The smallest frequency is : -886.4862 cm(-1)

Hartree-Fock electronic energy : = -1911.1303647

Zero-point correction= 0.599454 (Hartree/Particle)
Thermal correction to Energy= 0.638734
Thermal correction to Enthalpy= 0.639678
Thermal correction to Gibbs Free Energy= 0.520779
Sum of electronic and zero-point Energies= -1910.530911
Sum of electronic and thermal Energies= -1910.491630
Sum of electronic and thermal Enthalpies= -1910.490686
Sum of electronic and thermal Free Energies= -1910.609586

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Cartesian Coordinates

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46	-2.418024	-1.028389	-1.094114
6	-1.212465	-1.576524	-2.709098
6	-0.130945	-2.063199	-1.913807
6	1.057199	-1.360503	-1.652916
6	2.252379	-1.997463	-0.938914
6	1.853280	-2.905103	0.233890
8	-4.059461	-1.252143	0.489306
8	-1.689799	0.912722	-1.142700
15	-0.624678	1.393618	-0.141106
8	0.465952	0.366941	0.202777
7	3.122723	-0.910043	-0.494437
8	-3.323357	-2.854550	-0.834201
8	-1.303510	1.947840	1.203854
8	0.099723	2.689847	-0.725565
1	-1.852567	-2.328072	-3.170585
1	-0.295952	-3.017153	-1.413718
1	-1.021966	-0.693578	-3.318031
1	1.335906	-0.621955	-2.410356
1	2.695713	-0.122739	-0.021389
1	2.846412	-2.582235	-1.649704
1	1.241917	-2.351558	0.954670
1	1.292534	-3.784482	-0.099688
1	2.759107	-3.259358	0.731687
6	4.452458	-1.135065	-0.282137
8	5.038882	-2.157830	-0.609998
8	5.003592	-0.052547	0.320369
6	6.434321	-0.019949	0.640040
6	6.776711	-1.134895	1.633703
1	6.647067	-2.115267	1.175324
1	7.815547	-1.028427	1.962516
1	6.129417	-1.064862	2.513613
6	7.262854	-0.115824	-0.645023
1	8.322317	0.032109	-0.411833
1	7.134215	-1.090315	-1.116099
1	6.954022	0.663147	-1.349116
6	6.596577	1.355687	1.290190
1	7.638955	1.512871	1.583083
1	6.306031	2.145654	0.591707
1	5.966817	1.434853	2.181029

1	0.632489	-0.534385	-0.744108
6	-2.322898	1.188986	1.911596
6	-1.783246	-0.092382	2.536052
1	-3.148430	0.970227	1.227471
1	-2.680810	1.876021	2.683288
6	-2.827201	-0.764223	3.436847
1	-1.489772	-0.787419	1.741049
1	-0.872634	0.140079	3.100798
6	-2.378719	-2.152755	3.902486
1	-3.026324	-0.125464	4.307897
1	-3.766885	-0.854984	2.881909
1	-3.122507	-2.616084	4.559235
1	-2.227384	-2.817765	3.043471
1	-1.431124	-2.105184	4.451057
6	-0.683331	3.815334	-1.208357
6	-0.801043	4.893850	-0.140882
1	-1.666957	3.463488	-1.538485
1	-0.144681	4.184379	-2.086307
6	-1.566275	6.122041	-0.648968
1	-1.302936	4.468584	0.734851
1	0.207718	5.181970	0.179527
6	-1.691904	7.215203	0.416853
1	-1.061337	6.529384	-1.535608
1	-2.567780	5.816218	-0.981005
1	-2.242373	8.082311	0.038154
1	-2.220581	6.841979	1.301089
1	-0.704751	7.560899	0.743555
6	-4.091070	-2.461112	0.127036
6	-4.971924	-3.465321	0.815771
1	-4.518621	-3.723652	1.778992
1	-5.949299	-3.020337	1.015141
1	-5.075013	-4.369902	0.214919

2' mode **c**

Number of imaginary frequencies : 0 Electronic energy : = -1911.1632462
Zero-point correction= 0.606560 (Hartree/Particle)
Thermal correction to Energy= 0.645457
Thermal correction to Enthalpy= 0.646401
Thermal correction to Gibbs Free Energy= 0.531797
Sum of electronic and zero-point Energies= -1910.556686
Sum of electronic and thermal Energies= -1910.517789
Sum of electronic and thermal Enthalpies= -1910.516845
Sum of electronic and thermal Free Energies= -1910.631450

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Cartesian Coordinates

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46	1.194459	-0.639846	-0.702016
6	1.237688	-1.889691	-2.474796
6	0.291861	-0.910896	-2.747035

6	-1.190954	-1.152573	-2.811262
6	-2.136533	0.036601	-2.476965
6	-1.573060	1.398474	-2.897226
8	2.078328	0.377427	0.993131
8	0.090898	-2.092741	0.156585
8	-0.916890	-0.418083	1.268688
7	-2.538479	0.046639	-1.081401
8	2.408909	0.906903	-1.389345
1	2.265021	-1.771624	-2.808363
1	0.654273	0.002036	-3.215987
1	0.928012	-2.880648	-2.153864
1	-1.377259	-1.430163	-3.860652
1	-1.853290	0.123941	-0.332498
1	-3.063457	-0.139459	-3.027625
1	-0.692329	1.662547	-2.303393
1	-1.283005	1.401453	-3.954055
1	-2.327752	2.173729	-2.744536
6	-3.820589	-0.263793	-0.723417
8	-4.739781	-0.454694	-1.509183
8	-3.908636	-0.326508	0.628280
6	-5.198450	-0.529472	1.293090
6	-6.161519	0.606787	0.934908
1	-6.421993	0.576173	-0.123135
1	-7.075555	0.515592	1.530534
1	-5.700079	1.573065	1.160765
6	-5.767746	-1.904300	0.927668
1	-6.676594	-2.093511	1.508093
1	-6.005316	-1.953661	-0.134818
1	-5.043036	-2.689590	1.166903
6	-4.818855	-0.472799	2.774406
1	-5.704478	-0.636717	3.395748
1	-4.077587	-1.241665	3.008519
1	-4.388704	0.500796	3.022498
8	4.304243	1.594512	0.281375
8	2.273155	2.910727	0.296934
15	2.739864	1.411017	0.056625
1	-1.463485	-2.018184	-2.201072
6	5.180921	0.453971	0.057153
6	5.261927	-0.449329	1.280483
1	6.152942	0.895689	-0.177575
1	4.833998	-0.094279	-0.826881
6	6.233367	-1.615344	1.061007
1	5.579834	0.152974	2.140190
1	4.260665	-0.828294	1.511587
6	6.320756	-2.539000	2.280016
1	5.914024	-2.196198	0.184354
1	7.231939	-1.224431	0.822018
1	7.013487	-3.368181	2.104393
1	6.668887	-1.991965	3.163190
1	5.339995	-2.964551	2.519636

6	0.882470	3.269469	0.021429
6	-0.067571	2.818803	1.122906
1	0.606514	2.841253	-0.948608
1	0.900148	4.357320	-0.081204
6	-1.527326	3.153177	0.785162
1	0.026770	1.740701	1.272769
1	0.226188	3.301146	2.063218
6	-2.495097	2.623366	1.849085
1	-1.648707	4.239103	0.666568
1	-1.787274	2.704158	-0.182268
1	-3.531949	2.868945	1.595371
1	-2.412686	1.536314	1.928681
1	-2.276500	3.059635	2.830804
6	-0.732488	-1.620279	1.059487
6	-1.517721	-2.679600	1.804500
1	-1.540601	-2.421913	2.865823
1	-2.546392	-2.642825	1.432190
1	-1.106680	-3.679313	1.660551

TS[2'-4] mode **c**

Number of imaginary frequencies : 1 The smallest frequency is : -1535.9144 cm(-1)

Electronic energy : = -1911.1242387
Zero-point correction= 0.600079 (Hartree/Particle)
Thermal correction to Energy= 0.638911
Thermal correction to Enthalpy= 0.639855
Thermal correction to Gibbs Free Energy= 0.525514
Sum of electronic and zero-point Energies= -1910.524160
Sum of electronic and thermal Energies= -1910.485328
Sum of electronic and thermal Enthalpies= -1910.484383
Sum of electronic and thermal Free Energies= -1910.598725

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Cartesian Coordinates

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46	-1.812989	1.051326	-0.287305
6	-1.108429	2.390987	-1.733451
6	0.077931	1.627432	-1.975747
6	1.329852	1.847697	-1.385947
6	2.594040	1.100278	-1.814951
6	2.345908	-0.121983	-2.709012
8	-2.683331	-0.630874	0.874497
8	-1.043728	2.181519	1.280762
8	0.970194	1.175795	1.112459
7	3.356472	0.740439	-0.612052
8	-2.570830	-0.373640	-1.594244
1	-1.879223	2.334594	-2.500900
1	-0.055436	0.739465	-2.592025

1	-0.986309	3.374339	-1.279695
1	1.510733	2.869223	-1.037927
1	2.899573	0.689393	0.287524
1	3.227758	1.791434	-2.385514
1	1.663157	-0.836106	-2.238840
1	1.925048	0.178135	-3.674197
1	3.299318	-0.619299	-2.894530
6	4.661047	0.360094	-0.687591
8	5.315381	0.345204	-1.721540
8	5.102763	0.008106	0.548595
6	6.468383	-0.492803	0.741182
6	6.667102	-1.784909	-0.057465
1	6.624511	-1.588705	-1.128885
1	7.640130	-2.222909	0.186915
1	5.889093	-2.509631	0.202961
6	7.485098	0.587654	0.359335
1	8.494380	0.249434	0.615263
1	7.441029	0.800918	-0.708554
1	7.280596	1.508489	0.914563
6	6.511905	-0.771320	2.245077
1	7.501012	-1.142403	2.529456
1	6.305553	0.142527	2.809567
1	5.765884	-1.522446	2.520489
8	-4.331203	-2.042457	-0.626630
8	-2.005013	-2.716362	-0.570638
15	-2.888715	-1.390413	-0.445943
1	0.986094	1.375471	-0.138724
6	-5.483986	-1.160528	-0.732205
6	-5.979450	-0.706155	0.634718
1	-6.239748	-1.755542	-1.251986
1	-5.222478	-0.307615	-1.369283
6	-7.232237	0.171121	0.522972
1	-6.190309	-1.593304	1.244330
1	-5.176792	-0.158497	1.140085
6	-7.734431	0.647294	1.889719
1	-7.012115	1.042051	-0.109737
1	-8.029080	-0.385849	0.011148
1	-8.625636	1.275461	1.791916
1	-7.991351	-0.202466	2.531947
1	-6.965479	1.231997	2.406789
6	-0.559544	-2.581474	-0.654032
6	0.095971	-2.331764	0.700587
1	-0.324594	-1.775563	-1.359616
1	-0.219184	-3.524636	-1.089736
6	1.623602	-2.263950	0.580176
1	-0.281541	-1.393093	1.116456
1	-0.202017	-3.129316	1.391764
6	2.311514	-1.908031	1.901363
1	2.011632	-3.219456	0.201392
1	1.895198	-1.508797	-0.165313

1	3.392052	-1.804965	1.763065
1	1.936411	-0.951007	2.278856
1	2.129317	-2.671105	2.666387
6	0.079097	1.845290	1.751865
6	0.401432	2.224223	3.173878
1	0.362358	1.315302	3.784231
1	1.416711	2.622363	3.236120
1	-0.326046	2.940998	3.554843

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4 [L1=AcO^{-}, L2=DBPOH]

Number of imaginary frequencies : 0
Electronic energy : = -1911.1507955
Zero-point correction= 0.604949 (Hartree/Particle)
Thermal correction to Energy= 0.644572
Thermal correction to Enthalpy= 0.645517
Thermal correction to Gibbs Free Energy= 0.529335
Sum of electronic and zero-point Energies= -1910.545847
Sum of electronic and thermal Energies= -1910.506223
Sum of electronic and thermal Enthalpies= -1910.505279
Sum of electronic and thermal Free Energies= -1910.621460

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Cartesian Coordinates

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46	0.187190	0.742358	1.700812
6	-0.669373	-0.892993	2.573753
6	-0.201709	-2.012224	1.746263
6	-0.976811	-2.750509	0.916474
6	-0.447649	-3.796350	-0.063475
6	0.185842	-5.012097	0.628288
8	1.994516	2.223619	1.249265
8	-1.620467	1.147012	0.642440
8	-1.268359	-0.690819	-1.132608
7	0.445816	-3.207590	-1.087256
8	2.003038	0.516837	2.661064
1	-0.233073	-0.866678	3.575258
1	0.868084	-2.209375	1.766293
1	-1.754334	-0.754218	2.587069
1	-0.987883	-1.188919	-0.326670
1	-2.059628	-2.611213	0.944369
1	-0.017887	-2.729524	-1.848497
1	-1.303711	-4.158922	-0.642567
1	1.042552	-4.712349	1.230413
1	-0.557211	-5.488751	1.274696
1	0.521966	-5.737376	-0.118806
6	1.693508	-2.712515	-0.804589
8	2.362570	-3.001853	0.176649
8	2.071764	-1.865416	-1.793725

6	3.402021	-1.236293	-1.767490
6	3.537107	-0.346668	-0.528923
1	3.546707	-0.938589	0.385890
1	4.466436	0.228883	-0.594649
1	2.707236	0.361254	-0.469420
6	4.490401	-2.311442	-1.835716
1	5.469634	-1.834126	-1.943729
1	4.491096	-2.921098	-0.932283
1	4.326628	-2.958576	-2.703056
6	3.394026	-0.392053	-3.043499
1	4.348287	0.131570	-3.151182
1	3.239966	-1.024892	-3.922188
1	2.594929	0.352929	-3.008844
6	2.597595	1.510722	2.093982
6	4.042688	1.755966	2.448407
1	4.181864	1.696729	3.530537
1	4.654334	0.971593	1.991055
1	4.362808	2.728550	2.072581
15	-1.850236	0.761432	-0.801123
8	-3.392636	0.786623	-1.180570
8	-1.278081	1.703781	-1.930129
6	0.172084	1.842880	-2.101166
6	0.654309	3.143520	-1.485534
1	0.328302	1.816875	-3.183006
1	0.673352	0.972300	-1.665052
6	2.157754	3.351381	-1.708476
1	0.084306	3.972621	-1.922325
1	0.447862	3.126233	-0.411919
6	2.672915	4.609686	-1.005437
1	2.698957	2.484977	-1.314336
1	2.369206	3.402330	-2.786035
1	3.739389	4.764341	-1.200835
1	2.137445	5.504501	-1.343716
1	2.534451	4.507965	0.074675
6	-4.345285	0.206575	-0.245635
6	-5.738792	0.451569	-0.794426
1	-4.206740	0.674197	0.734564
1	-4.139971	-0.868152	-0.153684
6	-6.824991	-0.128268	0.120368
1	-5.882306	1.532005	-0.914551
1	-5.809416	0.008156	-1.794918
6	-8.236785	0.122630	-0.418282
1	-6.663706	-1.208065	0.241338
1	-6.730329	0.310176	1.122794
1	-8.997067	-0.298422	0.246789
1	-8.434668	1.195669	-0.517008
1	-8.367689	-0.330825	-1.407148

2' mode **d**

Number of imaginary frequencies : 0 Electronic energy : = -2640.7764108
Zero-point correction= 0.824204 (Hartree/Particle)
Thermal correction to Energy= 0.874887
Thermal correction to Enthalpy= 0.875832
Thermal correction to Gibbs Free Energy= 0.736768
Sum of electronic and zero-point Energies= -2639.952207
Sum of electronic and thermal Energies= -2639.901523
Sum of electronic and thermal Enthalpies= -2639.900579
Sum of electronic and thermal Free Energies= -2640.039643

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Cartesian Coordinates

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46	-1.088211	0.545868	-1.350561
6	-0.339886	1.744739	-2.993843
6	0.382965	0.560582	-3.061888
6	1.839560	0.419548	-2.713398
6	2.380014	-1.007376	-2.391659
6	1.619336	-2.123410	-3.117302
8	-2.592832	-0.265259	0.007526
8	-0.016129	1.787920	-0.171980
15	0.777372	1.061832	0.978577
8	0.595293	-0.421743	1.038127
7	2.456595	-1.298668	-0.972687
8	-2.344560	-0.713812	-2.403277
8	0.405778	1.862061	2.330224
8	2.332024	1.439679	0.793542
1	-1.230591	1.879975	-3.601598
1	-0.050062	-0.234664	-3.664994
1	0.092816	2.630094	-2.536813
1	2.364398	0.766361	-3.617652
1	1.625899	-1.254582	-0.382837
1	3.418634	-1.016277	-2.729643
1	0.593939	-2.211672	-2.742790
1	1.572725	-1.944281	-4.197636
1	2.120810	-3.079040	-2.947768
6	3.650812	-1.182545	-0.310048
8	4.713124	-0.864485	-0.835326
8	3.474018	-1.512407	0.984521
6	4.576276	-1.485541	1.945431
6	5.627729	-2.526859	1.550423
1	6.094874	-2.258727	0.602182
1	6.398973	-2.588329	2.325266
1	5.160567	-3.511831	1.450891
6	5.165887	-0.076774	2.049717
1	5.891466	-0.044105	2.869217
1	5.663629	0.203408	1.121553
1	4.366619	0.639480	2.254335

6	3.880542	-1.872422	3.252422
1	4.600925	-1.873906	4.076230
1	3.082631	-1.159660	3.477995
1	3.436618	-2.867968	3.170921
8	-4.742485	-0.904164	-1.333387
8	-3.156124	-2.686310	-0.906189
15	-3.178767	-1.118016	-1.138616
1	2.116827	1.107503	-1.911809
6	-5.293526	0.429820	-1.133285
6	-5.786085	0.589461	0.296116
1	-6.107348	0.512916	-1.858171
1	-4.538734	1.186688	-1.376973
6	-6.374119	1.981758	0.554720
1	-6.535430	-0.184993	0.499925
1	-4.942228	0.407943	0.967915
6	-6.877794	2.142704	1.992833
1	-5.608997	2.742556	0.347171
1	-7.196641	2.173029	-0.147932
1	-7.295443	3.140496	2.160295
1	-7.659495	1.409134	2.219479
1	-6.064696	1.993470	2.710897
6	-1.876484	-3.397218	-0.918597
6	-1.101375	-3.210785	0.377137
1	-1.303018	-3.055803	-1.787171
1	-2.153106	-4.441996	-1.079369
6	0.225485	-3.981801	0.356350
1	-0.895966	-2.149859	0.545432
1	-1.725759	-3.552075	1.212311
6	1.019163	-3.786669	1.652221
1	0.034771	-5.050649	0.183612
1	0.834646	-3.634422	-0.488469
1	1.970655	-4.327025	1.614573
1	1.238415	-2.727990	1.807745
1	0.453928	-4.155845	2.516245
6	-0.994241	2.075483	2.644694
6	-1.715846	0.789336	3.030486
1	-1.477851	2.545539	1.779886
1	-0.989813	2.793337	3.470336
6	-3.201288	1.036465	3.313249
1	-1.624416	0.069142	2.213601
1	-1.223243	0.348825	3.905908
6	-3.958633	-0.266634	3.585874
1	-3.318823	1.723040	4.163422
1	-3.646490	1.541924	2.445669
1	-5.024436	-0.086797	3.762714
1	-3.865883	-0.947748	2.732986
1	-3.553941	-0.778832	4.465824
6	2.733142	2.759498	0.359474
6	4.177567	2.681959	-0.111800
1	2.612997	3.461335	1.193397

1	2.073313	3.083686	-0.454088
6	4.621243	3.961887	-0.829046
1	4.828760	2.491257	0.747705
1	4.288087	1.813086	-0.772285
6	6.085054	3.899713	-1.276123
1	3.976319	4.132278	-1.702580
1	4.473916	4.827536	-0.168556
1	6.385746	4.814901	-1.796413
1	6.751624	3.767455	-0.416653
1	6.251520	3.054810	-1.953437

TS[2'-4] mode **d**

Number of imaginary frequencies : 1 The smallest frequency is : -1310.2955 cm(-1)

Electronic energy : = -2640.7413265
Zero-point correction= 0.816779 (Hartree/Particle)
Thermal correction to Energy= 0.868054
Thermal correction to Enthalpy= 0.868998
Thermal correction to Gibbs Free Energy= 0.724964
Sum of electronic and zero-point Energies= -2639.924547
Sum of electronic and thermal Energies= -2639.873272
Sum of electronic and thermal Enthalpies= -2639.872328
Sum of electronic and thermal Free Energies= -2640.016362

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Cartesian Coordinates

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46	-1.652169	0.773763	-1.113541
6	-0.699194	1.291935	-2.897229
6	0.257284	0.232741	-2.802029
6	1.565294	0.328426	-2.303485
6	2.579710	-0.810556	-2.458605
6	1.986918	-2.136397	-2.954804
8	-2.818784	-0.222713	0.552409
8	-0.626949	2.317567	-0.160171
15	0.602254	1.904514	0.663057
8	1.192700	0.524525	0.286234
7	3.291797	-0.991536	-1.189396
8	-2.684555	-0.876454	-1.853042
8	0.298420	1.981722	2.227128
8	1.778180	2.970328	0.474306
1	-1.495006	1.152881	-3.628281
1	-0.122399	-0.753792	-3.061618
1	-0.331747	2.312703	-2.801027
1	2.005803	1.329747	-2.326477
1	2.893202	-0.649721	-0.325969
1	3.331814	-0.500103	-3.195178
1	1.175431	-2.482463	-2.307179

1	1.600948	-2.038853	-3.974827
1	2.776314	-2.889935	-2.960031
6	4.473543	-1.662640	-1.133526
8	5.049996	-2.124487	-2.110063
8	4.892303	-1.736594	0.156473
6	6.134327	-2.433457	0.503217
6	6.028539	-3.913369	0.121034
1	5.972714	-4.030361	-0.961244
1	6.904125	-4.454110	0.494493
1	5.134373	-4.354721	0.572886
6	7.328481	-1.746746	-0.167359
1	8.260396	-2.195655	0.191310
1	7.275874	-1.851816	-1.250947
1	7.339737	-0.682221	0.086592
6	6.195365	-2.266912	2.023070
1	7.098124	-2.743006	2.417260
1	6.212277	-1.206714	2.291248
1	5.323057	-2.726664	2.496587
8	-4.796633	-1.583618	-0.464503
8	-2.731573	-2.783933	-0.079763
15	-3.222802	-1.311339	-0.452975
1	1.260599	0.374189	-0.982744
6	-5.679392	-0.436198	-0.579408
6	-7.073310	-0.874878	-0.166516
1	-5.661958	-0.086724	-1.618867
1	-5.307824	0.367024	0.066858
6	-8.090302	0.268583	-0.269676
1	-7.383422	-1.715097	-0.799683
1	-7.031458	-1.251700	0.862620
6	-9.498495	-0.160031	0.154178
1	-7.758228	1.109424	0.354154
1	-8.114831	0.644045	-1.301586
1	-10.209249	0.668605	0.074411
1	-9.866119	-0.979027	-0.474111
1	-9.506838	-0.510210	1.192466
6	-1.339157	-3.156630	-0.263833
6	-0.434384	-2.568496	0.812435
1	-1.021970	-2.853854	-1.268199
1	-1.343049	-4.249034	-0.219567
6	0.985798	-3.147491	0.761108
1	-0.386568	-1.481334	0.700553
1	-0.890872	-2.769518	1.788395
6	1.902074	-2.559732	1.839121
1	0.942813	-4.240507	0.863857
1	1.429750	-2.948220	-0.220657
1	2.920566	-2.946503	1.743872
1	1.954849	-1.470479	1.750020
1	1.534412	-2.795911	2.844279
6	-0.902259	1.345634	2.771075
6	-0.531384	0.062477	3.496128

1	-1.616398	1.148568	1.968987
1	-1.338054	2.083369	3.450896
6	-1.776567	-0.715696	3.940180
1	0.065480	-0.555487	2.819452
1	0.107931	0.298712	4.356133
6	-1.421767	-1.981102	4.726642
1	-2.415965	-0.069498	4.557690
1	-2.363306	-0.973159	3.050293
1	-2.319254	-2.537090	5.016113
1	-0.792136	-2.651452	4.130591
1	-0.867135	-1.737929	5.640341
6	1.498835	4.383330	0.659023
6	2.742431	5.157603	0.259231
1	1.242982	4.554734	1.711082
1	0.638004	4.658858	0.039290
6	2.559673	6.670747	0.429993
1	3.586452	4.807807	0.865988
1	2.984322	4.922139	-0.784640
6	3.808836	7.460244	0.026532
1	1.702695	7.005348	-0.169992
1	2.306145	6.891854	1.475512
1	3.659729	8.536820	0.155783
1	4.672827	7.166034	0.632806
1	4.065213	7.280935	-1.023595

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4 [L1=DBPO^{-}, L2=DBPOH]

Number of imaginary frequencies : 0

Electronic energy : = -2640.7529508
Zero-point correction= 0.821307 (Hartree/Particle)
Thermal correction to Energy= 0.873495
Thermal correction to Enthalpy= 0.874439
Thermal correction to Gibbs Free Energy= 0.725917
Sum of electronic and zero-point Energies= -2639.931644
Sum of electronic and thermal Energies= -2639.879456
Sum of electronic and thermal Enthalpies= -2639.878512
Sum of electronic and thermal Free Energies= -2640.027034

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Cartesian Coordinates

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46	0.450958	0.963915	-0.971928
6	1.347963	0.209984	-2.644344
6	1.712094	-1.162918	-2.272044
6	2.968785	-1.635362	-2.104498
6	3.329562	-3.015830	-1.560886
6	3.616209	-4.031736	-2.677535
8	-1.120517	1.486155	0.698493

8	2.323088	1.645012	-0.222024
8	3.114432	-0.658113	0.607735
7	2.360288	-3.504667	-0.567385
8	-1.491566	0.285159	-1.488912
1	0.538170	0.266853	-3.376169
1	0.872832	-1.824789	-2.073548
1	2.194419	0.851667	-2.903957
1	2.860037	-0.846856	-0.332147
1	3.812945	-1.006615	-2.395097
1	2.408395	-3.033104	0.327092
1	4.258902	-2.893045	-0.989754
1	2.729153	-4.189313	-3.288908
1	4.429431	-3.657729	-3.307830
1	3.919518	-4.989800	-2.245309
6	1.089304	-3.916495	-0.893145
8	0.751234	-4.373428	-1.973666
8	0.281108	-3.735687	0.179977
6	-1.146125	-4.092808	0.111922
6	-1.840035	-3.321926	-1.016465
1	-1.499284	-3.663257	-1.993089
1	-2.920492	-3.486589	-0.947205
1	-1.652178	-2.248812	-0.927378
6	-1.279927	-5.608960	-0.049992
1	-2.336228	-5.893231	-0.004838
1	-0.868568	-5.929725	-1.007710
1	-0.749963	-6.124414	0.757191
6	-1.663801	-3.631581	1.475659
1	-2.719177	-3.900944	1.583355
1	-1.101452	-4.110281	2.282718
1	-1.572836	-2.547203	1.573025
15	2.878352	0.885126	0.966820
8	4.263429	1.498694	1.445965
8	2.073020	0.907675	2.319707
6	0.965966	-0.023518	2.581011
6	-0.018753	0.666151	3.502004
1	1.404549	-0.922582	3.025375
1	0.476868	-0.287422	1.640323
6	-1.231697	-0.230773	3.780879
1	0.483992	0.943074	4.437098
1	-0.350480	1.580992	3.004326
6	-2.308709	0.488515	4.598004
1	-1.665716	-0.542621	2.825674
1	-0.911641	-1.142828	4.303760
1	-3.164446	-0.167033	4.792835
1	-1.920493	0.828546	5.565173
1	-2.675700	1.367188	4.056576
6	5.256074	1.854129	0.443267
6	6.436082	2.480133	1.164001
1	4.803338	2.548675	-0.271697
1	5.557268	0.944551	-0.092304

6	7.551683	2.885707	0.192470
1	6.081792	3.355924	1.720611
1	6.818948	1.766810	1.903733
6	8.745547	3.524961	0.908373
1	7.888464	2.002575	-0.367246
1	7.150644	3.586069	-0.552375
1	9.530192	3.807363	0.199636
1	8.441722	4.427547	1.449985
1	9.183942	2.833429	1.636473
15	-2.146948	0.776748	-0.169418
8	-3.453095	1.658684	-0.523935
8	-2.810847	-0.424587	0.666259
6	-4.140978	-0.936314	0.418679
6	-5.136439	-0.300653	1.378054
1	-4.070240	-2.015565	0.577898
1	-4.425758	-0.761187	-0.623834
6	-6.547883	-0.876401	1.214973
1	-4.779068	-0.456739	2.403856
1	-5.145754	0.780339	1.202085
6	-7.553998	-0.240789	2.179553
1	-6.885340	-0.725634	0.180466
1	-6.522548	-1.963395	1.373234
1	-8.555874	-0.662505	2.049803
1	-7.254599	-0.401230	3.221403
1	-7.621528	0.840983	2.018601
6	-3.302465	2.758909	-1.452822
6	-4.679912	3.348100	-1.703736
1	-2.852106	2.383360	-2.378715
1	-2.626898	3.504163	-1.014671
6	-4.635596	4.533545	-2.675204
1	-5.332658	2.560078	-2.099997
1	-5.109309	3.662729	-0.744344
6	-6.021681	5.131090	-2.936205
1	-3.970122	5.309207	-2.273220
1	-4.189523	4.209901	-3.625236
1	-5.968720	5.975220	-3.631034
1	-6.697234	4.383825	-3.367723
1	-6.476632	5.490380	-2.006240

2' mode **e**

Number of imaginary frequencies : 0

Electronic energy : = -2670.2666745
Zero-point correction= 0.639651 (Hartree/Particle)
Thermal correction to Energy= 0.685032
Thermal correction to Enthalpy= 0.685976
Thermal correction to Gibbs Free Energy= 0.558615

Sum of electronic and zero-point Energies= -2669.627023
Sum of electronic and thermal Energies= -2669.581643
Sum of electronic and thermal Enthalpies= -2669.580699
Sum of electronic and thermal Free Energies= -2669.708059

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Cartesian Coordinates

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6	2.148810	-2.260658	0.577975
6	0.895237	-2.882144	0.511851
6	0.758678	-4.229614	0.166079
6	1.908899	-4.963460	-0.129083
6	3.164655	-4.354507	-0.073438
6	3.288513	-3.007623	0.279139
16	-0.488068	-1.806085	0.917517
8	-0.551943	-1.541991	2.387806
6	-1.981167	-2.815277	0.539749
6	-3.216573	-1.962260	0.820687
16	-3.615247	-0.880263	-0.636118
8	-4.316509	-1.789035	-1.625591
6	-4.840641	0.139989	0.222297
6	-6.192785	-0.076896	-0.030014
6	-7.130602	0.738465	0.607403
6	-6.705399	1.749877	1.472301
6	-5.341273	1.958959	1.700922
6	-4.389508	1.157973	1.068478
46	-0.579059	0.061373	-0.561914
6	-0.561327	-1.101377	-2.496750
6	0.759375	-0.783316	-2.265956
6	1.500338	0.363705	-2.893295
6	2.527176	1.044712	-1.968752
6	3.130155	2.283972	-2.636714
8	-1.011310	1.175105	1.106973
8	-1.051979	1.652753	-1.722931
8	0.425580	3.054833	-0.724699
7	3.544424	0.061230	-1.577556
8	1.169185	0.834813	1.554805
1	-3.078578	-1.344386	1.712167
1	-4.097711	-2.597555	0.949087
1	-1.953765	-3.173558	-0.492689
1	-1.934120	-3.663921	1.227684
1	-3.324401	1.318981	1.226454
1	-6.484629	-0.863887	-0.719406
1	-5.016348	2.753083	2.366715
1	-8.190676	0.585994	0.426560
1	-7.438100	2.383487	1.963675
1	-0.210559	-4.711986	0.122635
1	2.214084	-1.206083	0.831655
1	1.819145	-6.010302	-0.402884
1	4.257304	-2.519080	0.291391
1	4.053154	-4.931530	-0.312193

1	-0.942770	-2.087941	-2.251621
1	1.384986	-1.504544	-1.744635
1	-1.187480	-0.483274	-3.132953
1	0.792559	1.106728	-3.263904
1	2.029589	-0.041858	-3.772539
1	3.915203	-0.561919	-2.281882
1	2.022330	1.361768	-1.053956
1	3.604971	2.033765	-3.593470
1	2.350472	3.031406	-2.808956
1	3.879481	2.725141	-1.975814
6	4.382806	0.197115	-0.498331
8	5.292503	-0.592545	-0.260726
8	4.046460	1.269946	0.230515
6	4.648899	1.542540	1.546381
6	4.356526	0.381653	2.500338
1	4.853334	-0.530695	2.166403
1	4.728720	0.633050	3.498969
1	3.277600	0.221606	2.560713
6	6.147383	1.805195	1.379807
1	6.569019	2.129667	2.336690
1	6.665525	0.905626	1.046860
1	6.310971	2.601471	0.646569
6	3.902396	2.804031	1.981290
1	4.233563	3.109611	2.978801
1	4.095736	3.623377	1.282464
1	2.830074	2.601677	1.996991
6	-0.533135	2.832653	-1.453479
6	-1.275236	3.945803	-2.185484
1	-1.427108	3.682809	-3.235758
1	-2.264261	4.071493	-1.733394
1	-0.714492	4.877677	-2.102867
6	0.086891	1.377663	1.791781
6	-0.076446	2.398191	2.899584
1	0.719091	2.276748	3.635834
1	0.000930	3.392070	2.446421
1	-1.055838	2.311891	3.374899

TS[2'-4] mode **e**

Number of imaginary frequencies : 1
The smallest frequency is : -1359.7203 cm(-1)

Electronic energy : = -2670.2256093
Zero-point correction= 0.633191 (Hartree/Particle)
Thermal correction to Energy= 0.678440
Thermal correction to Enthalpy= 0.679384
Thermal correction to Gibbs Free Energy= 0.551020
Sum of electronic and zero-point Energies= -2669.592418

Sum of electronic and thermal Energies= -2669.547170
Sum of electronic and thermal Enthalpies= -2669.546226
Sum of electronic and thermal Free Energies= -2669.674589

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Cartesian Coordinates

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6	1.606281	-1.438428	1.503137
6	0.667839	-2.187237	0.780489
6	1.052077	-3.207972	-0.091900
6	2.415300	-3.468514	-0.257751
6	3.366825	-2.714263	0.430757
6	2.959606	-1.711901	1.317637
16	-1.008675	-1.547413	0.884855
8	-1.470732	-1.503621	2.306427
6	-2.062818	-2.799166	0.044028
6	-3.506325	-2.308246	0.132056
16	-3.884595	-1.088005	-1.224412
8	-4.309905	-1.927024	-2.411138
6	-5.360118	-0.393669	-0.428902
6	-6.612345	-0.734713	-0.932736
6	-7.746850	-0.172182	-0.343254
6	-7.611716	0.717683	0.725010
6	-6.342888	1.056583	1.206752
6	-5.197768	0.508538	0.627317
46	-1.070357	0.432105	-0.322030
6	-0.142419	-0.361581	-2.107706
6	1.141443	0.019167	-1.645220
6	1.863442	1.198026	-1.925502
6	3.269425	1.303371	-1.335351
6	3.948366	2.619943	-1.724626
8	-2.021412	1.303254	1.331027
8	-1.264711	2.247924	-1.339777
8	0.675380	3.269079	-0.835760
7	4.076153	0.130937	-1.719025
8	0.028402	1.258177	2.261797
1	-3.708665	-1.856327	1.106404
1	-4.205043	-3.131874	-0.040836
1	-1.736865	-2.932496	-0.990709
1	-1.919556	-3.728193	0.603307
1	-4.206163	0.778059	0.988056
1	-6.676786	-1.421168	-1.771992
1	-6.242718	1.755351	2.032209
1	-8.733615	-0.426682	-0.719181
1	-8.496224	1.154931	1.179263
1	0.323149	-3.783686	-0.650251
1	1.275377	-0.613515	2.128508
1	2.730847	-4.247792	-0.944295
1	3.698512	-1.104340	1.827041
1	4.422969	-2.879117	0.246753
1	-0.357215	-1.428574	-2.113025

1	1.607948	-0.652638	-0.929950
1	-0.590401	0.195512	-2.927233
1	1.195356	2.192304	-1.327718
1	1.732608	1.605558	-2.934173
1	3.903010	-0.306415	-2.611916
1	3.181584	1.267023	-0.245007
1	4.065525	2.687441	-2.812120
1	3.346798	3.469293	-1.386711
1	4.937786	2.681271	-1.264544
6	5.168236	-0.358481	-1.068003
8	5.833221	-1.302441	-1.475458
8	5.381906	0.318864	0.090258
6	6.635966	0.154722	0.837414
6	6.779217	-1.275463	1.368902
1	6.880781	-1.983426	0.547122
1	7.666767	-1.337867	2.006717
1	5.912020	-1.551486	1.976182
6	7.815923	0.546988	-0.056567
1	8.741745	0.535557	0.526986
1	7.915751	-0.148647	-0.890741
1	7.670590	1.557811	-0.450267
6	6.463151	1.148448	1.986981
1	7.346305	1.136905	2.632439
1	6.324787	2.161691	1.599611
1	5.587604	0.890305	2.590267
6	-0.594019	3.204257	-0.821855
6	-1.363894	4.318793	-0.163725
1	-2.124587	4.688914	-0.856878
1	-1.887908	3.879806	0.691018
1	-0.708629	5.128444	0.157709
6	-1.189056	1.456779	2.327041
6	-1.858889	1.874112	3.624944
1	-1.128847	2.329519	4.295661
1	-2.692673	2.555939	3.441685
1	-2.257383	0.968635	4.094870

2' mode **f**

Number of imaginary frequencies : 0
Electronic energy : = -3399.8701567
Zero-point correction= 0.858214 (Hartree/Particle)
Thermal correction to Energy= 0.914985
Thermal correction to Enthalpy= 0.915929
Thermal correction to Gibbs Free Energy= 0.765100
Sum of electronic and zero-point Energies= -3399.011943
Sum of electronic and thermal Energies= -3398.955172
Sum of electronic and thermal Enthalpies= -3398.954228
Sum of electronic and thermal Free Energies= -3399.105057

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Cartesian Coordinates

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6	-1.291566	3.298728	0.532338
6	0.025154	3.759656	0.460149
6	0.327980	5.125500	0.532948
6	-0.715997	6.043173	0.623408
6	-2.041058	5.596532	0.657223
6	-2.326986	4.231564	0.619493
16	1.362777	2.549164	0.419686
8	2.157760	2.561884	1.688014
6	2.499190	3.251980	-0.862985
6	3.838130	2.526481	-0.776966
16	3.762852	0.778015	-1.434768
8	4.365592	0.822289	-2.823499
6	4.960956	0.060534	-0.281756
6	6.196232	-0.355234	-0.770839
6	7.086211	-0.981894	0.105328
6	6.725423	-1.189766	1.438764
6	5.473367	-0.775255	1.905442
6	4.571588	-0.149633	1.044769
46	0.743591	0.436927	-0.420268
6	0.491597	0.814827	-2.711359
6	-0.681818	1.228124	-2.130169
6	-1.888790	0.367807	-1.872557
6	-3.245572	0.852810	-2.470733
6	-3.385410	2.367627	-2.654283
8	1.205512	-0.311098	1.404471
8	0.401375	-1.482810	-1.045413
15	-0.503848	-2.385275	-0.143429
8	-1.548909	-1.754354	0.710609
7	-4.340240	0.293721	-1.658990
8	-0.496743	0.927321	2.223669
8	0.433241	-3.333526	0.774388
6	1.636573	-3.932506	0.244048
6	2.823654	-2.973857	0.294492
6	4.165160	-3.656730	-0.011224
6	4.685420	-4.546932	1.124038
8	-1.118690	-3.386047	-1.277698
6	-2.328201	-4.101865	-0.952411
6	-3.562006	-3.275616	-1.301155
6	-4.874902	-4.028693	-1.061556
6	-6.101310	-3.203093	-1.465882
1	4.185658	2.510934	0.257854
1	4.585454	3.011533	-1.412112
1	2.009421	3.171108	-1.836313
1	2.638077	4.308520	-0.625275
1	3.585225	0.148637	1.393049
1	6.434323	-0.192913	-1.817945
1	5.191089	-0.951123	2.939054

1	8.055683	-1.312948	-0.255192
1	7.415716	-1.685956	2.114508
1	1.354402	5.476169	0.541373
1	-1.515153	2.240453	0.561640
1	-0.493660	7.104601	0.674717
1	-3.344891	3.862207	0.663794
1	-2.850071	6.317720	0.727658
1	1.458729	-4.285979	-0.779720
1	1.809578	-4.810223	0.873849
1	2.643187	-2.167423	-0.419332
1	2.847810	-2.506053	1.284143
1	4.076666	-4.245806	-0.935209
1	4.908924	-2.880329	-0.217186
1	5.655965	-4.987145	0.871188
1	4.813708	-3.960360	2.040967
1	4.000557	-5.370919	1.351654
1	-2.339521	-4.376239	0.109547
1	-2.294339	-5.025176	-1.540670
1	-3.538377	-2.364604	-0.695360
1	-3.487340	-2.980467	-2.357751
1	-4.866946	-4.977032	-1.616450
1	-4.948992	-4.295510	0.001314
1	-6.067052	-2.949640	-2.533106
1	-7.032723	-3.751058	-1.289041
1	-6.145346	-2.270719	-0.894763
1	1.256463	1.523556	-3.012766
1	-0.796985	2.288512	-1.913058
1	0.617038	-0.207365	-3.053062
1	-2.021739	0.309388	-0.788567
1	-1.690071	-0.652388	-2.204222
1	-4.612689	-0.653952	-1.883455
1	-3.363881	0.394265	-3.458498
1	-3.205627	2.902095	-1.722212
1	-2.680796	2.722605	-3.414109
1	-4.398215	2.600486	-2.993793
6	-4.412718	0.591047	-0.316667
8	-3.914809	1.589427	0.188600
8	-5.108779	-0.356652	0.335201
6	-5.231936	-0.327416	1.811714
6	-3.850404	-0.307964	2.470441
1	-3.346217	0.649044	2.344306
1	-3.972062	-0.498855	3.542346
1	-3.206925	-1.078972	2.042804
6	-6.098749	0.867521	2.212888
1	-6.285505	0.838333	3.291082
1	-5.594909	1.803546	1.969597
1	-7.062365	0.834019	1.694320
6	-5.945875	-1.649803	2.095827
1	-6.130395	-1.749150	3.169355
1	-6.904452	-1.696062	1.570386

1	-5.327277	-2.490919	1.770370
6	0.322100	0.019012	2.327423
6	0.399600	-0.893295	3.533478
1	1.437786	-1.080592	3.817511
1	-0.157196	-0.458561	4.364065
1	-0.050254	-1.845427	3.235989

TS[2'-4] mode **f**

Number of imaginary frequencies : 1
The smallest frequency is : -1091.5306 cm(-1)

Electronic energy : = -3399.8459947
Zero-point correction= 0.851376 (Hartree/Particle)
Thermal correction to Energy= 0.907995
Thermal correction to Enthalpy= 0.908939
Thermal correction to Gibbs Free Energy= 0.757440
Sum of electronic and zero-point Energies= -3398.994619
Sum of electronic and thermal Energies= -3398.938000
Sum of electronic and thermal Enthalpies= -3398.937056
Sum of electronic and thermal Free Energies= -3399.088555

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Cartesian Coordinates

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6	-0.907940	3.319300	1.125553
6	0.365644	3.746775	0.729765
6	0.606951	5.063154	0.324210
6	-0.459078	5.964130	0.300643
6	-1.736585	5.551961	0.688488
6	-1.959204	4.235780	1.100149
16	1.655555	2.486491	0.814495
8	2.174152	2.321734	2.206779
6	3.066551	3.203412	-0.133187
6	4.213940	2.194737	-0.108245
16	4.011775	0.868172	-1.403844
8	4.759512	1.366264	-2.623942
6	5.031919	-0.383775	-0.570939
6	6.231264	-0.758862	-1.170686
6	6.987659	-1.775871	-0.582783
6	6.534852	-2.402252	0.580545
6	5.322000	-2.017102	1.161788
6	4.551786	-1.005870	0.585960
46	0.956151	0.606661	-0.329163
6	0.446351	1.637987	-2.149499
6	-0.942016	1.835034	-1.911203
6	-1.995094	0.966704	-2.247717
6	-3.468748	1.441689	-2.277027
6	-3.668675	2.953137	-2.104785

8	1.428716	-0.516124	1.364551
8	0.482669	-1.180311	-1.389286
15	-0.765744	-1.848342	-0.813336
8	-1.869979	-0.876570	-0.375710
7	-4.344462	0.692237	-1.361246
8	-0.331177	0.472412	2.370399
8	-0.505683	-2.789034	0.462907
6	0.414932	-3.914548	0.392787
6	1.873759	-3.490405	0.248290
6	2.855407	-4.647274	0.489847
6	2.945975	-5.088080	1.956667
8	-1.281314	-2.851694	-1.974035
6	-2.465909	-3.655880	-1.734987
6	-3.752342	-2.844858	-1.851716
6	-5.016437	-3.691703	-1.671546
6	-6.280649	-2.824829	-1.709444
1	4.305498	1.741714	0.881971
1	5.158242	2.679320	-0.373762
1	2.747818	3.464775	-1.145157
1	3.352442	4.108050	0.410518
1	3.598591	-0.720935	1.025824
1	6.547273	-0.256939	-2.080486
1	4.968317	-2.510418	2.062241
1	7.927562	-2.079437	-1.034768
1	7.123291	-3.195289	1.033013
1	1.594213	5.395592	0.025909
1	-1.076713	2.287448	1.421562
1	-0.287713	6.986690	-0.021708
1	-2.949797	3.891053	1.373902
1	-2.561086	6.258448	0.661862
1	0.110346	-4.574158	-0.429680
1	0.244791	-4.443554	1.333334
1	2.026207	-3.068216	-0.749054
1	2.060046	-2.673904	0.949928
1	2.591037	-5.507483	-0.141450
1	3.846981	-4.319877	0.157776
1	3.708309	-5.862241	2.093129
1	3.209093	-4.239496	2.599116
1	1.999515	-5.495215	2.328575
1	-2.395516	-4.124410	-0.745297
1	-2.424907	-4.446697	-2.489786
1	-3.738439	-2.062816	-1.090042
1	-3.763159	-2.350712	-2.832921
1	-5.068963	-4.470490	-2.444226
1	-4.965449	-4.215883	-0.707204
1	-6.374941	-2.312663	-2.675049
1	-7.186007	-3.422680	-1.564125
1	-6.247039	-2.062812	-0.923352
1	1.037041	2.552637	-2.159334
1	-1.201713	2.711660	-1.323075

1	0.730678	0.913600	-2.910093
1	-1.905018	0.129147	-1.224133
1	-1.750558	0.244056	-3.031377
1	-4.758013	-0.156744	-1.717201
1	-3.845089	1.181930	-3.272721
1	-3.353421	3.282910	-1.115395
1	-3.100334	3.500460	-2.863686
1	-4.729296	3.192763	-2.219887
6	-4.156777	0.713456	-0.002372
8	-3.484731	1.547517	0.587427
8	-4.850239	-0.302498	0.557309
6	-4.779781	-0.576904	2.004336
6	-3.347654	-0.920181	2.415216
1	-2.667976	-0.080478	2.284581
1	-3.343161	-1.215190	3.470353
1	-2.964893	-1.749454	1.816374
6	-5.339465	0.617362	2.782247
1	-5.419694	0.357827	3.842655
1	-4.685283	1.482679	2.678822
1	-6.337428	0.876876	2.414202
6	-5.695519	-1.794856	2.143392
1	-5.739260	-2.112268	3.189291
1	-6.709818	-1.559943	1.806423
1	-5.314548	-2.627409	1.544074
6	0.570595	-0.365229	2.339277
6	0.741014	-1.387629	3.451440
1	1.796178	-1.607290	3.630070
1	0.262721	-1.030141	4.364246
1	0.248457	-2.310560	3.127107

2' mode **g**

Number of imaginary frequencies : 0

Electronic energy : = -3399.8614119
Zero-point correction= 0.855803 (Hartree/Particle)
Thermal correction to Energy= 0.913696
Thermal correction to Enthalpy= 0.914640
Thermal correction to Gibbs Free Energy= 0.758033
Sum of electronic and zero-point Energies= -3399.005609
Sum of electronic and thermal Energies= -3398.947716
Sum of electronic and thermal Enthalpies= -3398.946772
Sum of electronic and thermal Free Energies= -3399.103379

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Cartesian Coordinates

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6	1.970296	-2.267003	1.983392
6	0.780962	-2.996601	1.870164

6	0.743077	-4.386752	2.013949
6	1.937626	-5.062119	2.266562
6	3.137086	-4.351897	2.370617
6	3.153648	-2.962531	2.229145
16	-0.657211	-1.988293	1.502588
8	-1.088135	-1.198538	2.695898
6	-2.033831	-3.170900	1.198538
6	-3.243056	-2.360642	0.725211
16	-3.226359	-2.195789	-1.124306
8	-3.721202	-3.531917	-1.643075
6	-4.566796	-0.980573	-1.219760
6	-5.835605	-1.411362	-1.600207
6	-6.856889	-0.465839	-1.716004
6	-6.593169	0.882962	-1.464058
6	-5.307518	1.295309	-1.099423
6	-4.274252	0.365032	-0.976322
46	-0.326354	-0.826031	-0.555811
6	0.224044	-2.719327	-1.640737
6	1.434483	-2.087366	-1.453727
6	2.180307	-1.349647	-2.529124
6	3.664015	-1.814158	-2.718266
6	3.958780	-3.244676	-2.244423
8	-1.344262	0.711695	0.384808
8	-0.476047	0.229759	-2.270379
8	1.283010	1.546086	-1.737821
7	4.626192	-0.863791	-2.146756
8	0.958582	0.973945	1.618676
1	-3.263985	-1.364524	1.175220
1	-4.172922	-2.887623	0.956758
1	-1.751842	-3.942336	0.477301
1	-2.222083	-3.630110	2.172823
1	-3.271970	0.677191	-0.691122
1	-5.997557	-2.465042	-1.808444
1	-5.103691	2.344941	-0.915226
1	-7.854536	-0.781048	-2.007804
1	-7.388042	1.616970	-1.559926
1	-0.184747	-4.941869	1.934522
1	1.969860	-1.187304	1.845335
1	1.929413	-6.142048	2.377683
1	4.085777	-2.411716	2.271667
1	4.063834	-4.887241	2.554693
1	-0.107131	-3.489598	-0.951589
1	1.987134	-2.249581	-0.535163
1	-0.287773	-2.680931	-2.598335
1	2.194441	-0.287385	-2.277598
1	1.636166	-1.450553	-3.473122
1	5.071526	-0.211713	-2.774990
1	3.856621	-1.775482	-3.795044
1	3.913099	-3.307096	-1.155062
1	3.234979	-3.948896	-2.668339

1	4.961726	-3.544230	-2.560486
6	4.553967	-0.450592	-0.844643
8	3.855984	-0.989559	0.006195
8	5.381402	0.595429	-0.654164
6	5.257467	1.452721	0.540248
6	3.867179	2.085490	0.562991
1	3.072209	1.355200	0.713254
1	3.818935	2.808834	1.383624
1	3.675410	2.613001	-0.375644
6	5.558378	0.654304	1.812006
1	5.656343	1.342810	2.657318
1	4.756680	-0.051139	2.024799
1	6.499890	0.106550	1.702208
6	6.339794	2.505754	0.294506
1	6.344200	3.231768	1.112639
1	7.328328	2.040347	0.234024
1	6.147988	3.038308	-0.641384
15	-0.382719	1.549547	1.301076
8	-1.197992	1.879834	2.663340
8	-0.330645	2.972585	0.521782
6	-2.626214	1.762442	2.737046
6	-3.349980	2.908297	2.035987
1	-2.858987	1.760734	3.806924
1	-2.931677	0.795562	2.323704
6	-4.872580	2.796949	2.173366
1	-2.997398	3.857603	2.458890
1	-3.068112	2.914913	0.976285
6	-5.609850	3.995640	1.568436
1	-5.212193	1.872944	1.687765
1	-5.141670	2.704861	3.234731
1	-6.696339	3.877760	1.637724
1	-5.338471	4.924085	2.083279
1	-5.354315	4.126731	0.510460
6	0.679001	3.936987	0.883207
6	1.208818	4.584426	-0.386952
1	1.487895	3.434904	1.422846
1	0.223597	4.678247	1.553520
6	2.318620	5.602752	-0.104943
1	1.573733	3.785335	-1.039678
1	0.376810	5.072019	-0.912916
6	2.886676	6.215940	-1.388689
1	1.938056	6.399818	0.548806
1	3.127652	5.110190	0.450892
1	3.680759	6.939287	-1.175082
1	3.305059	5.438218	-2.037866
1	2.105542	6.733746	-1.957267
6	0.224081	1.341629	-2.328705
6	-0.425974	2.402888	-3.197992
1	-1.051688	1.965228	-3.977961
1	-1.059954	3.003540	-2.536791

1	0.339192	3.052121	-3.627352

TS[2'-4] mode **g**

Number of imaginary frequencies : 1 The smallest frequency is : -958.0464 cm(-1)

Electronic energy : = -3399.8408801
Zero-point correction= 0.850724 (Hartree/Particle)
Thermal correction to Energy= 0.907736
Thermal correction to Enthalpy= 0.908680
Thermal correction to Gibbs Free Energy= 0.754904
Sum of electronic and zero-point Energies= -3398.990156
Sum of electronic and thermal Energies= -3398.933145
Sum of electronic and thermal Enthalpies= -3398.932200
Sum of electronic and thermal Free Energies= -3399.085976

Cartesian Coordinates

6	1.857780	-1.990629	2.193589
6	0.715472	-2.797156	2.136626
6	0.746200	-4.158473	2.452566
6	1.965492	-4.725933	2.826393
6	3.119899	-3.939099	2.880683
6	3.065720	-2.578994	2.566748
16	-0.754704	-1.931475	1.570687
8	-1.263345	-0.986100	2.610937
6	-2.064043	-3.213681	1.403921
6	-3.312190	-2.526505	0.848403
16	-3.292528	-2.500006	-1.013294
8	-3.905920	-3.820179	-1.434278
6	-4.532376	-1.187878	-1.198315
6	-5.824889	-1.540957	-1.578236
6	-6.766865	-0.528171	-1.773278
6	-6.401492	0.809372	-1.601928
6	-5.093113	1.142126	-1.236757
6	-4.139536	0.143737	-1.031184
46	-0.298647	-1.080784	-0.533317
6	0.333308	-2.978879	-1.291318
6	1.731872	-2.745253	-1.218431
6	2.554638	-2.316184	-2.281108
6	4.095358	-2.407912	-2.164038
6	4.593476	-3.499541	-1.202347
8	-1.137347	0.754918	0.100134
8	-0.113441	-0.280517	-2.442617
8	2.063964	0.253237	-2.654507
7	4.744331	-1.128972	-1.852118
8	1.092233	1.058207	1.443147
1	-3.409502	-1.508805	1.235015

1	-4.210627	-3.097091	1.101156
1	-1.724407	-4.036730	0.770254
1	-2.234310	-3.576320	2.421583
1	-3.121978	0.403006	-0.745798
1	-6.066039	-2.589985	-1.723886
1	-4.807617	2.182100	-1.117385
1	-7.781705	-0.783101	-2.064795
1	-7.133641	1.595747	-1.761375
1	-0.144946	-4.773902	2.410246
1	1.809782	-0.940694	1.909605
1	2.011471	-5.782750	3.070715
1	3.961098	-1.967824	2.570464
1	4.065976	-4.392951	3.160814
1	-0.039668	-3.714918	-0.581354
1	2.188486	-2.828475	-0.236626
1	-0.121649	-3.047454	-2.277676
1	2.270556	-1.073417	-2.351648
1	2.169977	-2.594797	-3.267321
1	5.211879	-0.625422	-2.589666
1	4.457090	-2.659630	-3.165793
1	4.356225	-3.238994	-0.168575
1	4.131146	-4.463592	-1.438165
1	5.679348	-3.599876	-1.285196
6	4.405927	-0.395062	-0.750680
8	3.611838	-0.774399	0.100804
8	5.114965	0.751866	-0.740311
6	4.674562	1.931309	0.024539
6	3.372484	2.443161	-0.588931
1	2.549105	1.763803	-0.370904
1	3.134049	3.419999	-0.159721
1	3.480036	2.550982	-1.671499
6	4.519698	1.624950	1.517774
1	4.450720	2.570811	2.066200
1	3.616365	1.049218	1.709395
1	5.395707	1.080804	1.885264
6	5.825530	2.910489	-0.216102
1	5.611670	3.865884	0.271970
1	6.760495	2.512751	0.190033
1	5.960648	3.088063	-1.287139
15	-0.241569	1.602640	1.043054
8	-1.097332	2.025135	2.353729
8	-0.116556	3.012477	0.218813
6	-2.531326	1.947568	2.370717
6	-3.189359	3.097832	1.614624
1	-2.806374	1.977512	3.430054
1	-2.846882	0.981023	1.965993
6	-4.714686	3.085945	1.765350
1	-2.781808	4.045336	1.990555
1	-2.911328	3.035630	0.555355
6	-5.392288	4.246317	1.030245

1	-5.109351	2.133174	1.389844
1	-4.976583	3.128287	2.831467
1	-6.481361	4.210070	1.138123
1	-5.048048	5.211933	1.417581
1	-5.161987	4.226551	-0.041399
6	0.541774	4.112300	0.870477
6	0.800291	5.189841	-0.170247
1	1.479788	3.762864	1.318625
1	-0.098201	4.488981	1.678908
6	1.567333	6.386327	0.402851
1	1.365449	4.745913	-0.998951
1	-0.160314	5.518317	-0.587077
6	1.828463	7.474129	-0.643339
1	1.007088	6.811859	1.246390
1	2.523529	6.038232	0.817412
1	2.380141	8.318285	-0.217042
1	2.414472	7.079281	-1.481147
1	0.887752	7.860358	-1.052039
6	0.833931	0.552219	-2.674747
6	0.441841	1.970731	-2.995976
1	-0.438250	1.969123	-3.643712
1	0.160864	2.453564	-2.053596
1	1.266560	2.514782	-3.458314

2' mode **h**

Number of imaginary frequencies : 0
Electronic energy : = -4129.4815397
Zero-point correction= 1.075193 (Hartree/Particle)
Thermal correction to Energy= 1.144333
Thermal correction to Enthalpy= 1.145278
Thermal correction to Gibbs Free Energy= 0.965849
Sum of electronic and zero-point Energies= -4128.406347
Sum of electronic and thermal Energies= -4128.337206
Sum of electronic and thermal Enthalpies= -4128.336262
Sum of electronic and thermal Free Energies= -4128.515690

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Cartesian Coordinates

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6	-1.294486	-3.159366	-1.912404
6	-0.173706	-3.810860	-1.382012
6	-0.159825	-5.187169	-1.133255
6	-1.309791	-5.925076	-1.418429
6	-2.441064	-5.291215	-1.938932
6	-2.433761	-3.916223	-2.185462
16	1.226845	-2.734093	-1.030377
8	1.937732	-2.336733	-2.283606
6	2.419282	-3.769797	-0.088296

6	3.666906	-2.928082	0.177557
16	3.405860	-1.793785	1.623450
8	3.439122	-2.708136	2.834520
6	4.979242	-0.918676	1.468148
6	6.040693	-1.270007	2.298781
6	7.233954	-0.552248	2.197308
6	7.342036	0.498711	1.282948
6	6.259179	0.845728	0.468992
6	5.057647	0.141303	0.559967
46	0.591346	-0.995931	0.444268
6	0.047331	-2.105333	2.403568
6	-0.949906	-2.453077	1.522802
6	-2.235351	-1.719802	1.305449
6	-3.529307	-2.414636	1.819203
6	-3.700676	-3.863950	1.365093
8	1.528962	0.235297	-0.898851
8	0.310025	0.611202	1.669620
15	-0.855020	1.631114	1.486965
8	-1.922525	1.382255	0.478164
7	-4.668915	-1.561428	1.429746
8	-0.625223	-0.190297	-2.330641
8	-0.211400	3.097160	1.270623
6	1.082883	3.415285	1.829720
6	2.187523	3.131223	0.817662
6	3.593514	3.399868	1.370657
6	3.889077	4.875183	1.667639
8	-1.450271	1.676843	3.011204
6	-2.641914	2.465669	3.217668
6	-3.898254	1.635246	2.978354
6	-5.193704	2.429219	3.174031
6	-6.439637	1.562548	2.959833
1	3.940209	-2.337807	-0.701268
1	4.501889	-3.574115	0.463275
1	1.954217	-4.127786	0.834573
1	2.663789	-4.615169	-0.736844
1	4.196380	0.412855	-0.047951
1	5.911605	-2.078566	3.012408
1	6.345568	1.675802	-0.223540
1	8.074791	-0.808709	2.834986
1	8.269373	1.059349	1.211541
1	0.710220	-5.686182	-0.722901
1	-1.270388	-2.085240	-2.096243
1	-1.319516	-6.993827	-1.227900
1	-3.324851	-3.414024	-2.543460
1	-3.336498	-5.870986	-2.141534
1	1.247861	2.844995	2.752026
1	1.031401	4.476089	2.092194
1	2.095645	2.086603	0.511853
1	2.005370	3.732831	-0.080772
1	3.751927	2.799211	2.277226

1	4.326344	3.029704	0.644652
1	4.925655	5.016532	1.992042
1	3.730441	5.490636	0.774213
1	3.242952	5.271092	2.458390
1	-2.630465	3.346608	2.562896
1	-2.592822	2.819632	4.252963
1	-3.854043	1.251054	1.954910
1	-3.876510	0.776583	3.665833
1	-5.215621	2.871693	4.179582
1	-5.207970	3.269188	2.466523
1	-6.471673	0.736301	3.680987
1	-7.360348	2.142306	3.082882
1	-6.441512	1.129500	1.954471
1	0.879547	-2.770697	2.621219
1	-0.862586	-3.408871	1.010351
1	-0.050717	-1.227517	3.034361
1	-2.358831	-1.574554	0.227611
1	-2.185871	-0.729155	1.754083
1	-4.769412	-0.751969	2.029476
1	-3.517210	-2.396372	2.915214
1	-3.673978	-3.936258	0.278905
1	-2.907420	-4.491954	1.785488
1	-4.662902	-4.248505	1.714033
6	-4.799785	-1.213970	0.092419
8	-4.585890	-1.975362	-0.839225
8	-5.188666	0.070202	-0.006421
6	-5.187669	0.780679	-1.306062
6	-3.866922	0.575869	-2.053720
1	-3.783426	-0.427297	-2.467770
1	-3.825124	1.293248	-2.880601
1	-3.015227	0.758176	-1.396305
6	-6.399009	0.305059	-2.106855
1	-6.466702	0.863639	-3.045887
1	-6.300916	-0.757918	-2.336822
1	-7.322273	0.464174	-1.540731
6	-5.318457	2.239307	-0.864075
1	-5.379716	2.892257	-1.739484
1	-6.217430	2.384917	-0.257312
1	-4.439838	2.521342	-0.277122
15	0.603935	0.629180	-2.109165
8	1.546260	0.611978	-3.427381
8	0.303765	2.195115	-1.849314
6	2.979115	0.648658	-3.339211
6	3.511710	1.988880	-2.840029
1	3.329799	0.454364	-4.358077
1	3.317728	-0.173443	-2.699428
6	5.041502	2.053839	-2.901514
1	3.073161	2.791578	-3.445539
1	3.170085	2.151763	-1.811461
6	5.596900	3.383371	-2.380711

1	5.463707	1.221551	-2.321904
1	5.375701	1.898727	-3.936256
1	6.691695	3.405215	-2.411494
1	5.229110	4.222673	-2.981035
1	5.283499	3.565712	-1.346488
6	-0.737972	2.837978	-2.621087
6	-1.457844	3.844518	-1.739667
1	-1.438606	2.078481	-2.981292
1	-0.269557	3.320336	-3.489565
6	-2.589763	4.554448	-2.489572
1	-1.851160	3.306872	-0.874134
1	-0.735614	4.576790	-1.357747
6	-3.365874	5.520409	-1.589043
1	-2.186892	5.098258	-3.355583
1	-3.280871	3.803134	-2.895970
1	-4.172950	6.022853	-2.133207
1	-3.811874	4.986431	-0.742691
1	-2.704878	6.293061	-1.179874

TS[2'-4] mode **h**

Number of imaginary frequencies : 1 The smallest frequency is : -755.9583 cm(-1)

Electronic energy : = -4129.461803
Zero-point correction= 1.069513 (Hartree/Particle)
Thermal correction to Energy= 1.137788
Thermal correction to Enthalpy= 1.138732
Thermal correction to Gibbs Free Energy= 0.962852
Sum of electronic and zero-point Energies= -4128.392290
Sum of electronic and thermal Energies= -4128.324015
Sum of electronic and thermal Enthalpies= -4128.323071
Sum of electronic and thermal Free Energies= -4128.498951

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Cartesian Coordinates

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6	0.980511	-2.985017	2.229384
6	-0.150467	-3.669005	1.764372
6	-0.193625	-5.062558	1.669018
6	0.937722	-5.790188	2.044015
6	2.077502	-5.126909	2.505929
6	2.098083	-3.732640	2.599480
16	-1.503108	-2.596391	1.260578
8	-2.153790	-1.955826	2.443398
6	-2.792853	-3.702668	0.551629
6	-3.927511	-2.811258	0.044059
16	-3.615317	-2.248164	-1.703821
8	-4.203862	-3.331927	-2.584350
6	-4.757321	-0.837714	-1.663918

6	-5.956703	-0.934368	-2.365178
6	-6.811004	0.170782	-2.389456
6	-6.451350	1.347953	-1.729008
6	-5.235075	1.427762	-1.042978
6	-4.369321	0.333678	-1.006243
46	-0.720657	-1.222981	-0.429980
6	-0.032633	-2.859711	-1.640399
6	1.323163	-2.931268	-1.225630
6	2.416471	-2.265236	-1.819315
6	3.880270	-2.707191	-1.559446
6	4.035388	-3.997845	-0.744932
8	-1.572011	0.406877	0.615779
8	-0.155379	0.007048	-2.042325
15	1.101791	0.848973	-1.790609
8	2.158624	0.196022	-0.901333
7	4.718992	-1.633800	-1.008165
8	0.444145	0.135569	2.273938
8	0.825245	2.283708	-1.142086
6	-0.097275	3.238956	-1.731098
6	-1.554809	2.796497	-1.660371
6	-2.525536	3.955412	-1.936428
6	-2.601675	4.984181	-0.799352
8	1.673861	1.161025	-3.276341
6	2.851342	1.997733	-3.404977
6	4.134281	1.252345	-3.050009
6	5.395478	2.103445	-3.229199
6	6.652419	1.343677	-2.788599
1	-4.069114	-1.945833	0.696544
1	-4.863010	-3.374895	-0.017919
1	-2.376137	-4.338260	-0.233435
1	-3.124131	-4.321269	1.390476
1	-3.421938	0.399641	-0.475786
1	-6.194665	-1.859611	-2.881933
1	-4.952817	2.344485	-0.537566
1	-7.752817	0.113393	-2.927521
1	-7.114319	2.207996	-1.753680
1	-1.075059	-5.583113	1.312725
1	0.993567	-1.895323	2.270383
1	0.925577	-6.873391	1.971457
1	2.993019	-3.208714	2.913469
1	2.957014	-5.700337	2.783601
1	0.208684	3.436606	-2.766723
1	0.068897	4.143234	-1.144806
1	-1.721118	1.984030	-2.373555
1	-1.729073	2.377208	-0.667870
1	-2.257217	4.459467	-2.876089
1	-3.522369	3.530596	-2.101667
1	-3.360716	5.747119	-1.003222
1	-2.854044	4.497487	0.148560
1	-1.649699	5.504794	-0.648831

1	2.738558	2.887751	-2.773171
1	2.856244	2.320614	-4.450287
1	4.068175	0.927427	-2.009425
1	4.194633	0.349920	-3.674227
1	5.494968	2.423622	-4.275101
1	5.299433	3.021123	-2.632796
1	6.791990	0.436287	-3.389470
1	7.554528	1.953553	-2.900239
1	6.572889	1.045391	-1.737445
1	-0.644137	-3.709309	-1.342594
1	1.519484	-3.484179	-0.310530
1	-0.235085	-2.495254	-2.645278
1	2.271023	-1.133865	-1.264160
1	2.234922	-1.953338	-2.852211
1	5.149227	-1.006851	-1.672078
1	4.310087	-2.900319	-2.548566
1	3.661685	-3.871524	0.270519
1	3.496409	-4.820076	-1.227214
1	5.094991	-4.260817	-0.686480
6	4.448748	-1.072677	0.216677
8	3.738604	-1.588389	1.066871
8	5.112596	0.098510	0.323776
6	4.951002	0.963892	1.506441
6	3.494524	1.400289	1.658832
1	2.823932	0.569694	1.871831
1	3.432919	2.121918	2.480387
1	3.141192	1.876795	0.742637
6	5.476638	0.238435	2.748104
1	5.485271	0.927849	3.598365
1	4.841662	-0.613134	2.991964
1	6.499338	-0.113999	2.578856
6	5.840164	2.158332	1.153657
1	5.813380	2.895302	1.961698
1	6.876883	1.842513	1.001895
1	5.484059	2.636848	0.236220
15	-0.789035	0.879262	1.877715
8	-1.826898	0.941285	3.126090
8	-0.514061	2.451955	1.550748
6	-3.243375	1.021554	2.921125
6	-3.692300	2.390860	2.417224
1	-3.686514	0.811854	3.900394
1	-3.555430	0.229863	2.231942
6	-5.218348	2.529056	2.387921
1	-3.254900	3.163302	3.062385
1	-3.280033	2.554204	1.414866
6	-5.675728	3.902533	1.885920
1	-5.643568	1.743677	1.749675
1	-5.620666	2.356064	3.395278
1	-6.767700	3.978038	1.854349
1	-5.301736	4.701971	2.535411

1	-5.296814	4.104522	0.877283
6	0.354458	3.191520	2.426325
6	1.079566	4.243913	1.601444
1	1.071150	2.508396	2.894001
1	-0.248831	3.653812	3.219764
6	2.069601	5.068756	2.429271
1	1.601039	3.730736	0.786650
1	0.335693	4.906683	1.138725
6	2.849192	6.073318	1.575324
1	1.534847	5.598068	3.229657
1	2.775445	4.392231	2.929311
1	3.549142	6.660298	2.179108
1	3.426431	5.557858	0.798918
1	2.171707	6.773648	1.073093

2' mode **i**

Number of imaginary frequencies : 0
Electronic energy : = -1563.0126639
Zero-point correction= 0.475863 (Hartree/Particle)
Thermal correction to Energy= 0.510625
Thermal correction to Enthalpy= 0.511569
Thermal correction to Gibbs Free Energy= 0.410210
Sum of electronic and zero-point Energies= -1562.536801
Sum of electronic and thermal Energies= -1562.502039
Sum of electronic and thermal Enthalpies= -1562.501094
Sum of electronic and thermal Free Energies= -1562.602453

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Cartesian Coordinates

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46	-0.942703	-0.977091	0.240243
6	-0.597516	-2.946571	1.251189
6	0.657991	-2.384153	1.322456
6	1.791150	-2.802219	0.422017
6	3.076667	-1.936924	0.391427
6	3.567089	-1.522470	1.786342
8	-1.833667	0.426240	-0.955675
8	-0.840609	-2.103226	-1.425822
8	0.738255	-0.789189	-2.387731
7	3.046728	-0.804135	-0.527375
8	-3.798891	-0.575779	-0.476395
1	-1.283257	-2.910997	2.091975
1	0.921571	-1.812985	2.208603
1	-0.848779	-3.645572	0.459127
1	1.423497	-2.973441	-0.592501
1	2.101662	-3.786188	0.807481
1	3.311495	-0.965716	-1.487181
1	3.842014	-2.595935	-0.035231

1	2.905285	-0.786871	2.244728
1	3.628952	-2.397833	2.441592
1	4.563889	-1.080010	1.708538
6	2.362953	0.356244	-0.324859
8	1.659527	0.587913	0.658003
8	2.643425	1.210550	-1.321921
6	1.984916	2.516130	-1.451383
6	0.467631	2.356253	-1.498281
1	0.075334	2.031220	-0.539039
1	0.006886	3.314463	-1.760999
1	0.184493	1.602936	-2.233501
6	2.445313	3.420853	-0.304621
1	2.019484	4.422051	-0.427503
1	2.121073	3.011835	0.652299
1	3.536325	3.507958	-0.299986
6	2.517781	3.017114	-2.794817
1	2.119994	4.014004	-3.006869
1	3.610478	3.071379	-2.780963
1	2.212250	2.338363	-3.595674
6	-2.151334	0.573042	1.853628
6	-1.180863	-0.060016	2.570987
1	-3.116078	0.125791	1.630427
1	-1.352408	-1.020905	3.044265
8	0.898280	0.069402	3.684945
6	-1.991273	2.017240	1.474926
8	-2.892244	2.616154	0.907261
6	0.065877	0.645961	2.996268
6	0.213015	2.060410	2.590093
6	-0.740584	2.694101	1.887808
1	-0.644177	3.729299	1.577130
1	1.139840	2.538841	2.886522
6	-3.128186	0.248960	-1.094703
6	-3.739493	1.241923	-2.068268
1	-3.846308	2.194733	-1.539800
1	-3.086715	1.400670	-2.929309
1	-4.722332	0.890075	-2.384829
6	-0.113135	-1.666303	-2.433358
6	-0.458711	-2.405513	-3.720405
1	-0.604383	-3.472309	-3.535611
1	-1.401613	-2.005430	-4.106910
1	0.330422	-2.245149	-4.456342

TS[2'-4] mode **i**

Number of imaginary frequencies : 1 The smallest frequency is : -1097.3913 cm(-1)

Electronic energy : = -1562.9833745
Zero-point correction= 0.471002 (Hartree/Particle)

Thermal correction to Energy= 0.504830
Thermal correction to Enthalpy= 0.505775
Thermal correction to Gibbs Free Energy= 0.406313
Sum of electronic and zero-point Energies= -1562.512372
Sum of electronic and thermal Energies= -1562.478544
Sum of electronic and thermal Enthalpies= -1562.477600
Sum of electronic and thermal Free Energies= -1562.577062

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Cartesian Coordinates

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46	1.248394	-0.945882	0.469264
6	0.175209	-2.811473	0.839865
6	-1.133908	-2.306363	0.597477
6	-2.030147	-1.818131	1.568706
6	-3.482318	-1.441130	1.198968
6	-4.124394	-2.326877	0.122673
8	2.071629	0.983885	0.526726
8	0.857561	-0.575773	2.488044
8	-1.118963	0.491781	2.447921
7	-3.629886	-0.012501	0.852393
8	4.120326	0.078039	0.791757
1	0.519957	-3.535536	0.107101
1	-1.432549	-2.216868	-0.441048
1	0.450154	-3.028393	1.870007
1	-1.496578	-0.687499	1.907186
1	-1.915243	-2.278314	2.555031
1	-3.834849	0.618440	1.614325
1	-4.069548	-1.553987	2.115355
1	-3.640276	-2.177700	-0.843754
1	-4.041482	-3.381962	0.400926
1	-5.182457	-2.072315	0.014642
6	-2.882923	0.556855	-0.141558
8	-2.258900	-0.078081	-0.987076
8	-2.964200	1.900671	-0.060215
6	-2.039211	2.761013	-0.816316
6	-0.599960	2.418049	-0.429338
1	-0.348575	1.399885	-0.717834
1	0.102275	3.096871	-0.921112
1	-0.470277	2.502151	0.651297
6	-2.302636	2.621437	-2.318499
1	-1.677740	3.333287	-2.867947
1	-2.080430	1.610007	-2.655930
1	-3.351054	2.842237	-2.540817
6	-2.414154	4.160988	-0.328802
1	-1.783302	4.908022	-0.819485
1	-3.460759	4.381770	-0.557888
1	-2.271470	4.239236	0.752565
6	2.379577	-0.778074	-1.545580
6	1.655123	-1.951468	-1.568280
1	3.397258	-0.738154	-1.168994

1	2.107085	-2.894947	-1.279263
8	-0.247653	-3.103169	-2.378024
6	1.898413	0.431526	-2.290099
8	2.584175	1.439806	-2.364301
6	0.365650	-2.043131	-2.314847
6	-0.127371	-0.811562	-2.974569
6	0.587270	0.326369	-2.972169
1	0.236785	1.231275	-3.457091
1	-1.100240	-0.889135	-3.446502
6	3.364955	1.046578	0.725793
6	3.876489	2.478684	0.792992
1	3.882073	2.872459	-0.228580
1	3.217894	3.112706	1.391670
1	4.889591	2.491601	1.196561
6	0.116016	0.439642	2.732670
6	0.752058	1.637138	3.382535
1	1.525503	1.314930	4.082784
1	1.245823	2.188623	2.575168
1	0.011269	2.271700	3.870336

2' mode **j**

Number of imaginary frequencies : 0
Electronic energy : = -2292.6217184
Zero-point correction= 0.693612 (Hartree/Particle)
Thermal correction to Energy= 0.740216
Thermal correction to Enthalpy= 0.741160
Thermal correction to Gibbs Free Energy= 0.612297
Sum of electronic and zero-point Energies= -2291.928106
Sum of electronic and thermal Energies= -2291.881503
Sum of electronic and thermal Enthalpies= -2291.880559
Sum of electronic and thermal Free Energies= -2292.009421

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Cartesian Coordinates

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46	-0.591985	-0.829760	-0.932973
6	-0.562212	-0.121836	-3.074935
6	0.787842	-0.131515	-2.799027
6	1.562318	1.128449	-2.528932
6	2.949183	1.032414	-1.848598
6	3.841202	-0.077522	-2.424014
8	-1.254755	-1.220552	0.955771
8	-0.788394	1.154415	-0.598472
15	-0.863629	1.860487	0.811781
8	0.254228	1.656614	1.769056
7	2.903269	1.005689	-0.386488
8	-3.334819	-1.391113	0.098508
8	-2.295113	1.524381	1.473098

6	-3.550478	2.050310	0.982055
6	-3.801378	1.813513	-0.506243
6	-5.270066	2.047591	-0.896430
6	-6.236383	1.008734	-0.308041
8	-1.053641	3.418071	0.351668
6	-0.021634	4.363372	0.688374
6	1.177174	4.235842	-0.244775
6	2.294243	5.234325	0.073547
6	3.524398	5.038205	-0.819064
1	-3.593686	3.120816	1.215814
1	-4.298123	1.533303	1.587368
1	-3.147509	2.473145	-1.085893
1	-3.523718	0.783578	-0.742884
1	-5.584391	3.059960	-0.604514
1	-5.338146	2.016981	-1.991089
1	-7.237843	1.111452	-0.739252
1	-5.875867	-0.006967	-0.502454
1	-6.339954	1.113381	0.777165
1	0.292176	4.213771	1.727125
1	-0.488534	5.349810	0.599200
1	1.557864	3.214337	-0.149530
1	0.838688	4.359662	-1.281786
1	1.918717	6.260055	-0.039770
1	2.586300	5.128994	1.126872
1	3.264334	5.141783	-1.878806
1	4.309984	5.766349	-0.593856
1	3.955630	4.038349	-0.682566
1	-1.041144	-0.942176	-3.600517
1	1.361910	-1.032051	-3.004983
1	-1.132222	0.799220	-2.997208
1	0.929269	1.842053	-1.998455
1	1.746395	1.548829	-3.530935
1	3.244996	1.807358	0.119737
1	3.429251	1.991849	-2.071323
1	3.470588	-1.067632	-2.154844
1	3.884368	-0.003188	-3.515901
1	4.858067	0.023006	-2.033955
6	2.615931	-0.082946	0.378605
8	2.158614	-1.134165	-0.071860
8	2.944426	0.164508	1.651482
6	2.705827	-0.800909	2.737996
6	1.246086	-1.246183	2.786328
1	0.987240	-1.859892	1.928072
1	1.084811	-1.828182	3.700770
1	0.587029	-0.378172	2.783438
6	3.671423	-1.974199	2.551245
1	3.568698	-2.678193	3.383375
1	3.453183	-2.497006	1.618485
1	4.707189	-1.621285	2.523244
6	3.054966	0.025276	3.975949

1	2.950456	-0.586750	4.876823
1	4.084349	0.392557	3.919730
1	2.378379	0.880890	4.046630
6	-1.143194	-3.229648	-0.977348
6	-0.127244	-3.014062	-1.867923
1	-2.193762	-3.112126	-1.224352
1	-0.319906	-2.801794	-2.914029
8	2.159986	-3.250997	-2.401058
6	-0.849513	-3.879740	0.348012
8	-1.759656	-4.248163	1.073278
6	1.289154	-3.375566	-1.549562
6	1.560445	-3.918907	-0.202241
6	0.569771	-4.145999	0.676016
1	0.751290	-4.552516	1.665516
1	2.601788	-4.118465	0.024032
6	-2.563817	-1.336105	1.055120
6	-3.014026	-1.425897	2.497953
1	-2.658548	-0.543593	3.034381
1	-4.102079	-1.489448	2.536533
1	-2.571757	-2.316200	2.953867

TS[2'-4] mode **j**

Number of imaginary frequencies : 1
The smallest frequency is : -1045.3486 cm(-1)

Electronic energy : = -2292.5950465
Zero-point correction= 0.688457 (Hartree/Particle)
Thermal correction to Energy= 0.734219
Thermal correction to Enthalpy= 0.735163
Thermal correction to Gibbs Free Energy= 0.608404
Sum of electronic and zero-point Energies= -2291.906590
Sum of electronic and thermal Energies= -2291.860828
Sum of electronic and thermal Enthalpies= -2291.859884
Sum of electronic and thermal Free Energies= -2291.986643

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Cartesian Coordinates

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46	-1.330050	-0.082705	-1.233694
6	-0.134536	-0.808590	-2.910197
6	0.784389	-1.571121	-2.129283
6	2.042523	-1.149430	-1.661829
6	3.041852	-2.142420	-1.022081
6	3.027910	-3.548653	-1.635096
8	-1.977265	0.713415	0.584053
8	0.046149	1.490549	-1.324875
15	1.017338	1.710822	-0.161908
8	1.643672	0.423651	0.402947

7	2.929379	-2.213644	0.448843
8	-3.528890	2.040428	-0.374083
8	0.413371	2.483234	1.094766
6	-0.106823	3.844472	1.036316
6	-0.770768	4.246381	-0.279595
6	-1.527972	5.580144	-0.151695
6	-2.834033	5.468746	0.647297
8	2.147349	2.683166	-0.788770
6	3.401300	2.829672	-0.078503
6	4.422243	1.808552	-0.564914
6	5.789539	1.970285	0.108057
6	6.792911	0.909938	-0.356781
1	0.724637	4.521081	1.268287
1	-0.818672	3.882068	1.862500
1	-0.002073	4.326121	-1.055361
1	-1.467348	3.467871	-0.598141
1	-0.875400	6.347029	0.290123
1	-1.761574	5.930079	-1.163814
1	-3.391145	6.411046	0.623758
1	-3.467423	4.678388	0.230952
1	-2.651898	5.227508	1.700548
1	3.238088	2.734425	1.002010
1	3.735792	3.851475	-0.281694
1	4.025195	0.808088	-0.362777
1	4.520486	1.903651	-1.653587
1	6.187575	2.972275	-0.100587
1	5.668869	1.908542	1.198069
1	6.953470	0.967535	-1.439183
1	7.763806	1.032345	0.133179
1	6.429878	-0.099567	-0.129748
1	-0.779297	-1.406369	-3.548363
1	0.448733	-2.552725	-1.810608
1	0.226979	0.118117	-3.350345
1	1.728796	-0.395805	-0.630687
1	2.504900	-0.358078	-2.258429
1	3.463099	-1.527907	0.964902
1	4.035889	-1.715417	-1.190977
1	2.089345	-4.059110	-1.413705
1	3.152555	-3.490367	-2.720772
1	3.844485	-4.143524	-1.216435
6	1.734427	-2.514853	1.052314
8	0.783939	-3.037756	0.478899
8	1.789271	-2.178914	2.354417
6	0.566326	-2.109651	3.173768
6	-0.419492	-1.125130	2.544778
1	-0.746121	-1.469434	1.566244
1	-1.302812	-1.019417	3.181734
1	0.039011	-0.144514	2.410412
6	-0.024126	-3.512513	3.344374
1	-0.865473	-3.473641	4.044143

1	-0.368630	-3.902613	2.387206
1	0.729044	-4.195094	3.750062
6	1.094045	-1.575475	4.505625
1	0.270833	-1.475365	5.219116
1	1.841639	-2.254709	4.926197
1	1.554670	-0.594021	4.363403
6	-3.375778	-1.078433	-0.891262
6	-2.768357	-1.731655	-1.944595
1	-4.011488	-0.209162	-1.035944
1	-2.957724	-1.441764	-2.973337
8	-1.617581	-3.659077	-2.696668
6	-3.431267	-1.714325	0.466821
8	-4.093683	-1.220941	1.366607
6	-2.112901	-3.059227	-1.748506
6	-2.086042	-3.610796	-0.374090
6	-2.703002	-2.992321	0.646477
1	-2.695532	-3.390495	1.655488
1	-1.531865	-4.534004	-0.247918
6	-2.929929	1.603203	0.610626
6	-3.275603	2.019500	2.033500
1	-2.370664	2.118897	2.637472
1	-3.846790	2.948049	2.030084
1	-3.880949	1.216304	2.465653

2' mode **k**

Number of imaginary frequencies : 0
Electronic energy : = -2292.673142
Zero-point correction= 0.692931 (Hartree/Particle)
Thermal correction to Energy= 0.739815
Thermal correction to Enthalpy= 0.740759
Thermal correction to Gibbs Free Energy= 0.610489
Sum of electronic and zero-point Energies= -2291.980211
Sum of electronic and thermal Energies= -2291.933327
Sum of electronic and thermal Enthalpies= -2291.932383
Sum of electronic and thermal Free Energies= -2292.062653

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Cartesian Coordinates

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46	0.400132	-1.043317	0.027235
6	0.714116	-3.091131	-0.629024
6	1.584863	-2.292512	-1.410653
6	1.053624	-1.185918	-2.094267
6	1.892102	-0.056698	-2.676171
6	1.395099	0.312788	-4.078670
8	0.313355	1.109420	0.068858
8	-2.027302	-2.089891	-1.559472
8	-3.329374	-0.333979	-2.091280

7	3.318522	-0.360452	-2.693608
8	-1.215274	1.122752	-2.036494
1	1.151775	-3.804303	0.063693
1	2.658424	-2.364349	-1.253515
1	-0.304063	-3.283031	-0.956763
1	-2.449701	0.178776	-2.111219
1	0.004895	-1.207982	-2.392604
1	3.649836	-0.995951	-3.406919
1	1.753675	0.810134	-2.023822
1	1.475275	-0.536538	-4.767777
1	0.349265	0.622574	-4.014953
1	1.988188	1.140479	-4.475394
6	4.143272	-0.337636	-1.591256
8	5.209290	-0.932882	-1.550902
8	3.605933	0.418633	-0.613282
6	4.243851	0.514700	0.710365
6	4.228282	-0.863131	1.375806
1	4.833363	-1.571634	0.807694
1	4.636057	-0.790302	2.388452
1	3.206479	-1.244088	1.457233
6	5.659359	1.085125	0.583585
1	6.049134	1.306004	1.582617
1	6.326073	0.382824	0.084948
1	5.635546	2.018205	0.012094
6	3.330761	1.495065	1.446129
1	3.643097	1.580672	2.491257
1	3.382744	2.485304	0.984312
1	2.291224	1.168841	1.395481
6	-3.136536	-1.591069	-1.734261
6	-4.417070	-2.358547	-1.518465
1	-4.631477	-2.339080	-0.445026
1	-5.250942	-1.908011	-2.058367
1	-4.276869	-3.398881	-1.817333
15	-0.786421	1.797814	-0.752562
8	-0.304825	3.295034	-1.113799
8	-2.019699	1.979513	0.292474
6	-0.422148	4.431129	-0.231746
1	-1.448164	4.490719	0.151891
1	-0.257293	5.287735	-0.890869
6	0.582820	4.460054	0.921704
1	1.559882	4.145577	0.535297
6	-3.362783	2.248501	-0.182173
1	-3.591233	3.300387	0.029764
1	-3.410155	2.098406	-1.264159
6	-4.323869	1.310861	0.530552
1	-4.362944	1.570048	1.596776
1	-3.918169	0.297636	0.469444
6	-5.728270	1.338645	-0.080922
1	-6.129154	2.361713	-0.061857
1	-5.651768	1.050739	-1.136995

6	-6.692701	0.393086	0.641544
1	-6.806447	0.672778	1.695131
1	-7.686740	0.404468	0.182509
1	-6.319632	-0.636832	0.614049
1	0.689403	5.512655	1.221578
6	0.206995	3.632696	2.158855
1	0.185470	2.572919	1.896657
1	-0.811888	3.897824	2.471475
6	1.179281	3.859828	3.320633
1	0.909564	3.253019	4.191667
1	2.202601	3.594353	3.034634
1	1.187011	4.910017	3.636111
6	0.279448	-1.210042	2.304879
6	-0.995782	-0.956382	1.837285
1	-1.377709	0.054256	1.720819
1	0.952527	-0.408568	2.594748
6	-2.003586	-2.054433	1.743049
6	0.693994	-2.588961	2.696717
6	-0.317807	-3.670864	2.550865
6	-1.558625	-3.426385	2.098102
8	1.815142	-2.822250	3.128876
8	-3.167100	-1.827930	1.435198
1	0.016534	-4.664905	2.833468
1	-2.306414	-4.206038	1.988449

TS[2'-4] mode **k**

Number of imaginary frequencies : 1 The smallest frequency is : -1076.9170 cm(-1)

Electronic energy : = -2292.5927531
Zero-point correction= 0.686381 (Hartree/Particle)
Thermal correction to Energy= 0.733113
Thermal correction to Enthalpy= 0.734058
Thermal correction to Gibbs Free Energy= 0.602010
Sum of electronic and zero-point Energies= -2291.906372
Sum of electronic and thermal Energies= -2291.859640
Sum of electronic and thermal Enthalpies= -2291.858696
Sum of electronic and thermal Free Energies= -2291.990743

Cartesian Coordinates

46	-1.471087	-0.212944	1.308400
6	-1.178718	1.353085	2.748950
6	0.031354	1.644067	2.049594
6	1.315151	1.149981	2.382238
6	2.482086	1.475823	1.442020
6	3.806648	0.940737	1.995278
8	-1.318978	-1.768093	-0.165797

8	-0.760732	-1.573620	2.705269
8	1.463252	-1.474181	2.401051
7	2.546297	2.901637	1.128109
8	0.489706	-0.054642	-0.944930
1	-2.007033	2.048058	2.651546
1	-0.045679	2.221231	1.127784
1	-1.102450	0.864312	3.717888
1	1.256983	-0.119606	2.326905
1	1.530673	1.147952	3.459413
1	2.476190	3.580862	1.871633
1	2.263242	0.977659	0.494767
1	4.072671	1.441649	2.933865
1	3.735562	-0.134617	2.188106
1	4.607780	1.119704	1.273516
6	2.583466	3.453246	-0.129225
8	2.441513	4.648761	-0.333118
8	2.817888	2.499382	-1.055635
6	2.457191	2.709424	-2.466302
6	0.966094	3.042828	-2.552106
1	0.748642	4.000908	-2.077329
1	0.660307	3.092597	-3.602319
1	0.392694	2.257165	-2.054629
6	3.345873	3.794514	-3.079105
1	3.149150	3.863611	-4.154270
1	3.153510	4.760707	-2.613451
1	4.401201	3.539068	-2.939302
6	2.742171	1.340154	-3.086367
1	2.524621	1.365530	-4.158776
1	3.795951	1.074796	-2.953254
1	2.116187	0.580336	-2.612868
6	0.390618	-2.121931	2.573634
6	0.449691	-3.622965	2.614057
1	0.333008	-3.955648	1.577120
1	1.414295	-3.968165	2.989355
1	-0.374246	-4.020932	3.208783
15	-0.039445	-1.459772	-0.993583
8	-0.337080	-1.859721	-2.533009
8	1.044328	-2.555194	-0.476612
6	-1.004002	-3.106520	-2.840513
1	-1.281543	-3.624417	-1.916143
1	-0.289216	-3.730982	-3.387189
6	-2.239284	-2.816531	-3.682367
1	-1.927806	-2.304257	-4.601701
6	2.441426	-2.317113	-0.773393
1	2.624680	-2.545412	-1.831887
1	2.666393	-1.258142	-0.609674
6	3.283305	-3.194716	0.136278
1	3.026551	-4.247964	-0.036684
1	3.017741	-2.959144	1.171834
6	4.784624	-2.973645	-0.081312

1	5.042741	-3.182218	-1.128515
1	5.020984	-1.914066	0.086752
6	5.643761	-3.841865	0.842902
1	5.448265	-4.907403	0.676497
1	6.712081	-3.668057	0.678701
1	5.426878	-3.626591	1.895386
1	-2.677032	-3.777131	-3.987403
6	-3.287479	-1.971694	-2.949570
1	-2.821496	-1.025906	-2.651691
1	-3.572249	-2.482024	-2.020122
6	-4.530143	-1.695064	-3.799434
1	-5.258573	-1.083511	-3.256317
1	-4.267657	-1.162130	-4.720490
1	-5.029509	-2.627060	-4.088006
6	-2.354650	1.165906	-0.294509
6	-3.327458	0.274508	0.130199
1	-3.424654	-0.711284	-0.313644
1	-1.638288	0.929356	-1.076300
6	-4.467204	0.719429	0.992771
6	-2.452985	2.611509	0.075382
6	-3.627699	3.041325	0.879133
6	-4.545146	2.164879	1.323586
8	-1.598882	3.416281	-0.270369
8	-5.321837	-0.070465	1.365356
1	-3.675707	4.103211	1.102453
1	-5.393784	2.464228	1.931703

2' mode **l**

Number of imaginary frequencies :
0 Electronic energy : = -3022.2350747
Zero-point correction= 0.911210 (Hartree/Particle)
Thermal correction to Energy= 0.969896
Thermal correction to Enthalpy= 0.970840
Thermal correction to Gibbs Free Energy= 0.814406
Sum of electronic and zero-point Energies= -3021.323865
Sum of electronic and thermal Energies= -3021.265179
Sum of electronic and thermal Enthalpies= -3021.264235
Sum of electronic and thermal Free Energies= -3021.420669

Cartesian Coordinates

46	-0.052809	-0.676938	-0.954693
6	0.562557	-1.334005	-3.018350
6	1.405326	-2.118401	-2.262104
6	2.876859	-1.821100	-2.153318
6	3.703987	-2.515447	-1.046779
6	3.399248	-4.010846	-0.883762

8	-1.026958	0.626742	0.279886
8	1.433500	0.651851	-1.180592
15	1.489704	2.086038	-0.503487
8	1.569654	2.176395	0.979248
7	3.682855	-1.806666	0.229751
8	-2.676242	1.087203	-1.723043
8	0.281955	2.978949	-1.063549
6	0.113541	3.432036	-2.424684
6	-0.034602	2.297084	-3.433097
6	-0.588489	2.770323	-4.786976
6	-2.055546	3.219189	-4.720145
8	2.802687	2.695277	-1.255874
6	3.989569	2.903698	-0.458658
6	4.605444	1.588916	0.009157
6	5.859449	1.787892	0.866607
6	6.387241	0.462520	1.427155
1	0.954041	4.086354	-2.685133
1	-0.797683	4.030777	-2.379390
1	0.942468	1.820337	-3.570382
1	-0.720569	1.558911	-3.008079
1	0.037389	3.578223	-5.192197
1	-0.502403	1.938439	-5.497614
1	-2.457460	3.402317	-5.722276
1	-2.668669	2.456522	-4.229097
1	-2.173383	4.145451	-4.148497
1	3.740113	3.527559	0.406452
1	4.675518	3.457157	-1.107296
1	3.852561	1.058877	0.600314
1	4.836699	0.972436	-0.870730
1	6.644078	2.286441	0.281868
1	5.619749	2.459923	1.701030
1	6.664190	-0.227110	0.618562
1	7.277698	0.608156	2.046823
1	5.624734	-0.024127	2.046566
1	-0.382081	-1.699325	-3.404040
1	1.073163	-3.102925	-1.947928
1	0.931421	-0.404238	-3.438732
1	3.025717	-0.738802	-2.105014
1	3.295230	-2.158727	-3.114704
1	4.432074	-1.159368	0.418194
1	4.745961	-2.430813	-1.375559
1	2.407642	-4.162123	-0.456246
1	3.456620	-4.518705	-1.852588
1	4.129021	-4.467516	-0.209999
6	2.591836	-1.695051	1.038142
8	1.550679	-2.332168	0.877312
8	2.847207	-0.813265	2.012551
6	1.983338	-0.653227	3.207111
6	0.536424	-0.340157	2.836189
1	0.026588	-1.215449	2.441235

1	0.013661	-0.020840	3.743844
1	0.498313	0.472419	2.112989
6	2.103131	-1.933002	4.034019
1	1.554171	-1.817659	4.973692
1	1.673128	-2.776956	3.488710
1	3.150914	-2.147479	4.267675
6	2.626939	0.554155	3.888693
1	2.105010	0.774141	4.824846
1	3.680304	0.358733	4.114471
1	2.552815	1.420712	3.226083
15	-2.378341	1.209102	-0.264305
8	-2.501465	2.714292	0.278409
8	-3.447958	0.351006	0.632921
6	-1.718604	3.178414	1.416283
6	-2.070175	2.478211	2.723488
1	-1.939656	4.248040	1.473589
1	-0.660900	3.048462	1.188413
6	-1.143353	2.942002	3.854329
1	-3.121004	2.666267	2.981031
1	-1.959965	1.397265	2.591120
6	-1.478663	2.286715	5.197212
1	-0.108303	2.711112	3.573314
1	-1.199659	4.034696	3.956876
1	-0.788559	2.608268	5.984503
1	-2.495536	2.540195	5.518916
1	-1.421053	1.194442	5.127096
6	-4.854365	0.596066	0.442463
6	-5.622380	-0.485710	1.184951
1	-5.084835	0.582350	-0.630043
1	-5.100514	1.592138	0.832987
6	-7.141068	-0.307525	1.078884
1	-5.330115	-1.463818	0.780506
1	-5.313332	-0.476104	2.237806
6	-7.915288	-1.400385	1.822346
1	-7.420305	0.677034	1.477480
1	-7.434797	-0.302906	0.020584
1	-8.996846	-1.255444	1.734911
1	-7.677141	-2.392625	1.422392
1	-7.662811	-1.405067	2.888745
6	-1.595150	-2.180385	0.203448
6	-1.930136	-2.157141	-1.129862
1	-1.946766	-1.420722	0.891332
1	-2.573312	-1.386923	-1.553893
8	-2.012970	-3.391229	-3.156401
6	-0.994094	-3.397433	0.835660
8	-0.930610	-3.496614	2.049923
6	-1.670031	-3.360870	-1.981063
6	-0.971163	-4.514016	-1.357795
6	-0.619783	-4.517209	-0.060106
1	-0.108774	-5.351964	0.409283

1	-0.763616	-5.347095	-2.023225

TS[2'-4] mode **l**

Number of imaginary frequencies : 1
The smallest frequency is : -836.1962 cm(-1)

Electronic energy : = -3022.2026149
Zero-point correction= 0.906296 (Hartree/Particle)
Thermal correction to Energy= 0.964122
Thermal correction to Enthalpy= 0.965066
Thermal correction to Gibbs Free Energy= 0.811305
Sum of electronic and zero-point Energies= -3021.296319
Sum of electronic and thermal Energies= -3021.238493
Sum of electronic and thermal Enthalpies= -3021.237549
Sum of electronic and thermal Free Energies= -3021.391310

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Cartesian Coordinates

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46	-0.164508	-0.416690	-1.615578
6	1.355156	-0.832296	-3.105428
6	2.324521	-1.384735	-2.218385
6	3.385956	-0.678529	-1.611060
6	4.537151	-1.402467	-0.869857
6	4.952098	-2.744342	-1.486112
8	-1.338116	0.273640	-0.025244
8	0.800669	1.427120	-1.572879
15	1.573481	1.823856	-0.305269
8	2.299325	0.660996	0.388239
7	4.292924	-1.537263	0.579980
8	-2.604992	2.114892	-1.451191
8	0.712668	2.539740	0.824080
6	0.086692	3.860865	0.701709
6	-0.268274	4.304474	-0.713630
6	-1.146917	5.569236	-0.694866
6	-2.586004	5.317165	-0.222284
8	2.633150	2.920393	-0.848125
6	3.677636	3.366616	0.049773
6	4.920714	2.495038	-0.084595
6	6.076158	2.958590	0.808290
6	7.289800	2.028549	0.709715
1	0.772705	4.572896	1.176004
1	-0.810058	3.772000	1.313210
1	0.652989	4.499245	-1.272631
1	-0.809490	3.503645	-1.222955
1	-0.674159	6.349113	-0.078983
1	-1.173853	5.969661	-1.715298
1	-3.188075	6.228448	-0.308319

1	-3.046419	4.525075	-0.819064
1	-2.626958	4.991233	0.821721
1	3.311481	3.366728	1.084066
1	3.887170	4.402248	-0.234325
1	4.641547	1.469318	0.175750
1	5.232648	2.488534	-1.136774
1	6.369330	3.980752	0.534480
1	5.734257	3.005515	1.850973
1	7.668981	1.982364	-0.317450
1	8.108286	2.364495	1.353771
1	7.026918	1.007477	1.011668
1	0.926886	-1.536395	-3.813184
1	2.193396	-2.420857	-1.921677
1	1.552088	0.161784	-3.500169
1	2.774483	-0.090669	-0.656769
1	3.697200	0.212689	-2.163283
1	4.549274	-0.736843	1.141926
1	5.397126	-0.728240	-0.931712
1	4.157640	-3.484122	-1.378867
1	5.179821	-2.617560	-2.549102
1	5.841834	-3.125722	-0.977483
6	3.158975	-2.158655	1.038732
8	2.478015	-2.926721	0.365216
8	2.936881	-1.817608	2.320982
6	1.627143	-2.071525	2.949672
6	0.521454	-1.416343	2.121456
1	0.519895	-1.803482	1.105216
1	-0.453360	-1.623721	2.566964
1	0.667795	-0.337765	2.056962
6	1.428338	-3.579466	3.127153
1	0.488254	-3.766492	3.656297
1	1.405310	-4.079605	2.159508
1	2.246821	-4.002986	3.717516
6	1.762685	-1.378497	4.305334
1	0.833527	-1.491947	4.871962
1	2.582010	-1.814060	4.884987
1	1.959465	-0.311949	4.166817
15	-2.544832	1.225243	-0.258278
8	-2.690863	2.085255	1.113355
8	-3.813202	0.187769	-0.221988
6	-2.186591	1.575061	2.370093
6	-2.878790	0.299797	2.836717
1	-2.350792	2.389967	3.083558
1	-1.108714	1.411502	2.271511
6	-2.352099	-0.162582	4.201162
1	-3.961997	0.469045	2.885814
1	-2.717237	-0.486015	2.094506
6	-2.850377	-1.564867	4.566616
1	-1.254212	-0.161183	4.183615
1	-2.643240	0.554708	4.980510

1	-2.451683	-1.897832	5.531133
1	-3.944203	-1.589006	4.630212
1	-2.554508	-2.291484	3.801296
6	-5.133647	0.736541	-0.383004
6	-6.111125	-0.420864	-0.509171
1	-5.156341	1.380282	-1.270633
1	-5.372211	1.355160	0.492695
6	-7.564008	0.050970	-0.634326
1	-5.835433	-1.020834	-1.386699
1	-5.996643	-1.073679	0.365242
6	-8.552171	-1.110129	-0.780725
1	-7.828594	0.650330	0.247283
1	-7.655717	0.723112	-1.498204
1	-9.583000	-0.751400	-0.866584
1	-8.329611	-1.705415	-1.673682
1	-8.501915	-1.781509	0.084124
6	-1.865002	-2.033476	-1.360931
6	-1.123546	-2.379796	-2.467202
1	-2.731990	-1.382506	-1.408589
1	-1.389882	-2.034836	-3.462500
8	0.480749	-3.848989	-3.406896
6	-1.712633	-2.789738	-0.072088
8	-2.456877	-2.584392	0.873400
6	-0.139406	-3.505373	-2.406639
6	0.053123	-4.177110	-1.102673
6	-0.673941	-3.844698	-0.023963
1	-0.542229	-4.327918	0.937481
1	0.822872	-4.940456	-1.072407

2' mode **m**

Number of imaginary frequencies : 0

Electronic energy : = -2670.2793045
Zero-point correction= 0.637341 (Hartree/Particle)
Thermal correction to Energy= 0.682601
Thermal correction to Enthalpy= 0.683545
Thermal correction to Gibbs Free Energy= 0.555560
Sum of electronic and zero-point Energies= -2669.641963
Sum of electronic and thermal Energies= -2669.596703
Sum of electronic and thermal Enthalpies= -2669.595759
Sum of electronic and thermal Free Energies= -2669.723745

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Cartesian Coordinates

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6	1.428466	2.030905	-1.472510
6	0.190810	2.630573	-1.215305
6	0.071019	4.006616	-1.008925

6	1.222617	4.795208	-1.058866
6	2.464092	4.211313	-1.321235
6	2.565819	2.833279	-1.528445
16	-1.184637	1.468842	-1.157047
8	-1.458073	0.945244	-2.538595
6	-2.640293	2.494626	-0.701567
6	-3.852074	1.566633	-0.650423
16	-3.965145	0.671910	0.980307
8	-4.725711	1.604087	1.900820
6	-5.099149	-0.616509	0.386265
6	-6.425429	-0.578929	0.807924
6	-7.291642	-1.590728	0.386755
6	-6.821068	-2.617223	-0.435380
6	-5.481356	-2.642334	-0.837071
6	-4.600401	-1.642352	-0.422915
46	-0.721094	-0.103169	0.463071
6	-0.264501	1.321317	1.900602
6	1.190738	1.540397	1.899572
6	2.064324	0.840368	2.640626
6	3.569470	0.978020	2.614289
6	4.095959	2.286190	2.009607
8	-1.325881	-1.654973	-0.982430
6	-0.445331	-1.849175	-1.877614
6	-0.924474	-2.236491	-3.257344
8	0.018562	-1.515631	1.885802
8	1.640334	-2.330681	0.519483
7	4.179046	-0.213837	1.986082
8	0.800596	-1.691760	-1.688378
1	-3.821764	0.841214	-1.467621
1	-4.781795	2.140349	-0.706899
1	-2.456185	2.995155	0.253088
1	-2.750833	3.237027	-1.497158
1	-3.553875	-1.662699	-0.723655
1	-6.751896	0.229671	1.455489
1	-5.117482	-3.446705	-1.469852
1	-8.331022	-1.578238	0.702258
1	-7.496914	-3.403875	-0.758573
1	-0.887395	4.469784	-0.805968
1	1.514925	0.953490	-1.578520
1	1.145571	5.865224	-0.891567
1	3.528171	2.362293	-1.692327
1	3.355336	4.831132	-1.351302
1	-0.833829	2.233349	1.700537
1	1.566764	2.295580	1.216024
1	-0.640488	0.826673	2.799513
1	1.202463	-1.916658	-0.388301
1	1.685020	0.058101	3.295753
1	4.898825	-0.706171	2.493539
1	3.913937	0.929012	3.655685
1	3.833072	2.358587	0.954251

1	3.671534	3.144024	2.539198
1	5.186054	2.325110	2.098257
1	-1.809558	-2.872607	-3.188707
1	-1.210708	-1.307794	-3.761227
1	-0.133409	-2.728834	-3.824401
6	4.159270	-0.441508	0.633595
8	3.499516	0.199233	-0.171553
8	4.989208	-1.471165	0.350994
6	5.247415	-1.885990	-1.037279
6	3.964764	-2.391466	-1.696674
1	3.248653	-1.588147	-1.855193
1	4.209457	-2.842627	-2.664234
1	3.489170	-3.146741	-1.067425
6	5.879652	-0.725454	-1.812326
1	6.195508	-1.073855	-2.800672
1	5.165112	0.088266	-1.939350
1	6.760576	-0.348831	-1.282468
6	6.252822	-3.024463	-0.851647
1	6.546483	-3.427655	-1.825189
1	7.149698	-2.667903	-0.336021
1	5.809838	-3.830566	-0.259899
6	1.040857	-2.199607	1.652565
6	1.709074	-2.930739	2.790420
1	1.927400	-3.960975	2.499937
1	2.662970	-2.428672	2.983100
1	1.086990	-2.903559	3.684610

TS[2'-4] mode **m**

Number of imaginary frequencies : 1
The smallest frequency is : -1128.5189 cm(-1)

Electronic energy : = -2670.2282711
Zero-point correction= 0.633683 (Hartree/Particle)
Thermal correction to Energy= 0.678620
Thermal correction to Enthalpy= 0.679564
Thermal correction to Gibbs Free Energy= 0.553018
Sum of electronic and zero-point Energies= -2669.594588
Sum of electronic and thermal Energies= -2669.549651
Sum of electronic and thermal Enthalpies= -2669.548707
Sum of electronic and thermal Free Energies= -2669.675253

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Cartesian Coordinates

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6	1.662337	2.163249	-1.347258
6	0.412491	2.778112	-1.216884
6	0.282016	4.164121	-1.087665
6	1.438772	4.944772	-1.067866

6	2.696016	4.344164	-1.181507
6	2.807246	2.958959	-1.321329
16	-0.984215	1.640210	-1.232537
8	-1.374702	1.257475	-2.625408
6	-2.405345	2.628173	-0.603300
6	-3.620800	1.704250	-0.540660
16	-3.671824	0.744053	1.053646
8	-4.385872	1.642185	2.043254
6	-4.833426	-0.519663	0.462606
6	-6.140603	-0.494379	0.941169
6	-7.026019	-1.491992	0.526364
6	-6.592919	-2.492991	-0.346161
6	-5.271584	-2.506672	-0.805146
6	-4.371441	-1.521046	-0.397936
46	-0.576877	-0.032281	0.322997
6	-0.134079	1.364496	1.906064
6	1.274645	1.186463	1.919096
6	2.005924	0.342609	2.778437
6	3.541137	0.490004	2.906797
6	4.064549	1.915811	2.670128
8	-1.113354	-1.441397	-1.131541
6	-0.297484	-1.468057	-2.152911
6	-0.798621	-2.315988	-3.310243
8	-0.435133	-1.552512	1.756377
8	1.728632	-2.127731	1.894669
7	4.307721	-0.470086	2.096506
8	0.771047	-0.855119	-2.223548
1	-3.630310	1.014415	-1.388563
1	-4.547410	2.285823	-0.536063
1	-2.163640	3.075196	0.363964
1	-2.561394	3.414259	-1.347285
1	-3.338537	-1.535972	-0.742619
1	-6.437506	0.293158	1.627734
1	-4.936764	-3.291286	-1.477495
1	-8.050865	-1.488541	0.886374
1	-7.283413	-3.268958	-0.664070
1	-0.688329	4.638152	-0.996077
1	1.737107	1.083198	-1.432232
1	1.355165	6.021820	-0.959327
1	3.776189	2.475856	-1.380276
1	3.590145	4.960047	-1.154128
1	-0.459836	2.335340	1.535380
1	1.830882	1.693486	1.135911
1	-0.702187	1.001638	2.760567
1	1.824380	-0.849295	2.265669
1	1.500265	0.135839	3.726386
1	4.645482	-1.308233	2.544967
1	3.781632	0.218530	3.939373
1	3.945805	2.201595	1.623151
1	3.521130	2.631312	3.295268

1	5.128829	1.967942	2.917053
1	-1.342682	-3.194424	-2.955071
1	-1.489765	-1.700097	-3.895509
1	0.036434	-2.610430	-3.947723
6	4.157132	-0.560591	0.742645
8	3.501466	0.229577	0.071657
8	4.867448	-1.607592	0.277036
6	4.631817	-2.150837	-1.071553
6	3.193285	-2.659166	-1.151282
1	2.480590	-1.838492	-1.081893
1	3.031647	-3.162440	-2.109736
1	3.006121	-3.368652	-0.340827
6	4.942430	-1.105849	-2.147479
1	4.943564	-1.589696	-3.129490
1	4.197418	-0.312073	-2.147341
1	5.932460	-0.670702	-1.977084
6	5.633826	-3.305213	-1.134481
1	5.546401	-3.822766	-2.094226
1	6.657852	-2.934324	-1.029204
1	5.440797	-4.023008	-0.332058
6	0.525661	-2.374771	1.569657
6	0.198775	-3.710074	0.950929
1	-0.195150	-3.514436	-0.050644
1	1.069772	-4.363903	0.907452
1	-0.604053	-4.179007	1.527198

2' mode **n**

Number of imaginary frequencies : 0
Electronic energy : = -3399.8464681
Zero-point correction= 0.855447 (Hartree/Particle)
Thermal correction to Energy= 0.913170
Thermal correction to Enthalpy= 0.914114
Thermal correction to Gibbs Free Energy= 0.755644
Sum of electronic and zero-point Energies= -3398.991021
Sum of electronic and thermal Energies= -3398.933298
Sum of electronic and thermal Enthalpies= -3398.932354
Sum of electronic and thermal Free Energies= -3399.090824

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Cartesian Coordinates

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6	0.698417	-0.430073	-2.499433
6	-0.173972	0.658695	-2.391209
6	0.266482	1.980881	-2.526867
6	1.620313	2.200775	-2.774459
6	2.509224	1.128164	-2.848954
6	2.048285	-0.183696	-2.723200
16	-1.801924	0.244427	-1.794141

8	-2.356901	-0.975705	-2.459234
6	-2.873061	1.660980	-2.256729
6	-4.286733	1.427094	-1.732358
16	-4.404859	2.015514	0.028490
8	-4.175485	3.511052	-0.046094
6	-6.184152	1.698528	0.201702
6	-7.049104	2.790317	0.206039
6	-8.416252	2.561170	0.376767
6	-8.893759	1.258972	0.543074
6	-8.008092	0.176503	0.545231
6	-6.638438	0.388395	0.382003
46	-1.911160	-0.004779	0.494388
6	-0.526393	1.626319	0.906534
6	0.348913	0.541695	0.975349
6	0.720710	-0.148409	2.233504
6	0.783327	-1.694088	2.131440
6	1.407208	-2.271581	3.406390
8	-2.457255	-0.512816	2.460053
8	2.758490	1.546146	0.259469
8	3.757492	-0.564305	1.480252
7	1.575556	-2.093270	0.977274
8	-3.736942	-1.211709	0.812801
1	-4.585101	0.376093	-1.783496
1	-4.994692	2.038331	-2.298243
1	-2.455982	2.587297	-1.852058
1	-2.841735	1.686045	-3.349570
1	-5.936739	-0.441874	0.391717
1	-6.642161	3.789883	0.084517
1	-8.383549	-0.833934	0.677732
1	-9.106795	3.399264	0.382259
1	-9.957436	1.086165	0.677240
1	-0.407980	2.824410	-2.434061
1	0.347021	-1.442901	-2.358820
1	1.985279	3.218392	-2.863697
1	2.734177	-1.021472	-2.731341
1	3.572140	1.308481	-2.947398
1	-0.497836	2.273835	0.036324
1	0.883421	0.254101	0.078884
1	-0.929726	2.064273	1.817193
1	1.747912	0.197237	2.428709
1	0.075000	0.153941	3.062974
1	2.544899	-1.731899	0.993123
1	-0.228422	-2.081670	2.002516
1	2.441134	-1.924636	3.497292
1	0.848102	-1.953474	4.293030
1	1.407515	-3.364633	3.366228
6	1.141910	-2.658836	-0.164935
8	1.874836	-2.990440	-1.093392
8	-0.229244	-2.788283	-0.200059
6	-0.825137	-3.992390	-0.805355

6	-0.699969	-3.972530	-2.332030
1	0.348327	-3.984012	-2.629842
1	-1.199620	-4.855108	-2.745989
1	-1.189570	-3.085119	-2.739459
6	-0.153511	-5.227942	-0.199145
1	-0.659561	-6.134361	-0.544948
1	0.896470	-5.282281	-0.494580
1	-0.212964	-5.193755	0.893523
6	-2.290008	-3.892355	-0.383620
1	-2.853210	-4.742269	-0.781641
1	-2.376621	-3.896785	0.707430
1	-2.731515	-2.968396	-0.761812
15	3.919659	0.628100	0.559351
8	4.503115	0.115674	-0.901642
8	5.189146	1.482672	1.147095
6	5.126094	-1.174085	-1.007830
6	6.445037	-1.274835	-0.247014
1	5.299888	-1.319822	-2.081890
1	4.426247	-1.951224	-0.678672
6	7.126705	-2.630487	-0.459437
1	7.106315	-0.461028	-0.572779
1	6.244648	-1.118040	0.817504
6	8.448050	-2.752658	0.306277
1	6.444282	-3.431029	-0.143366
1	7.307715	-2.790320	-1.531961
1	8.919052	-3.728833	0.147472
1	9.159332	-1.981600	-0.012087
1	8.288267	-2.627502	1.383103
6	5.567637	2.674659	0.451623
6	6.766563	3.279566	1.166723
1	4.723510	3.376744	0.431342
1	5.825354	2.430234	-0.589484
6	7.260959	4.569408	0.502712
1	6.490545	3.474564	2.210725
1	7.572394	2.534899	1.190909
6	8.469639	5.179150	1.219638
1	7.521076	4.363961	-0.544965
1	6.442570	5.302036	0.474746
1	8.808483	6.098031	0.729405
1	8.226494	5.424314	2.259840
1	9.311434	4.477495	1.235526
6	-3.504359	-1.139605	2.064094
6	-4.448246	-1.746117	3.056691
1	-5.370806	-1.155444	3.066662
1	-4.704216	-2.761509	2.743708
1	-4.008417	-1.750709	4.054621

TS[2'-4] mode **n**

Number of imaginary frequencies : 1
The smallest frequency is : -601.7390 cm(-1)

Electronic energy : = -3399.8373672
Zero-point correction= 0.850807 (Hartree/Particle)
Thermal correction to Energy= 0.908164
Thermal correction to Enthalpy= 0.909108
Thermal correction to Gibbs Free Energy= 0.751151
Sum of electronic and zero-point Energies= -3398.986560
Sum of electronic and thermal Energies= -3398.929203
Sum of electronic and thermal Enthalpies= -3398.928259
Sum of electronic and thermal Free Energies= -3399.086216

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Cartesian Coordinates

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6	-0.752028	-1.051305	2.648054
6	0.040002	0.086624	2.482275
6	-0.454771	1.372535	2.725866
6	-1.772272	1.506866	3.157098
6	-2.577397	0.379514	3.326843
6	-2.070002	-0.894938	3.075121
16	1.653430	-0.204744	1.744966
8	2.187889	-1.538211	2.178700
6	2.722712	1.073629	2.516723
6	4.122493	1.006258	1.913648
16	4.178064	2.004269	0.344903
8	3.954126	3.434764	0.791900
6	5.951834	1.755567	0.044651
6	6.818148	2.818381	0.290070
6	8.179314	2.647614	0.027748
6	8.649463	1.431813	-0.474610
6	7.761837	0.380176	-0.724102
6	6.397692	0.536051	-0.473652
46	1.766262	-0.014283	-0.554297
6	0.140603	1.315790	-0.728051
6	-0.739692	0.203963	-0.856355
6	-1.240801	-0.312986	-2.071689
6	-1.514518	-1.827465	-2.177479
6	-2.369672	-2.149460	-3.406237
8	2.249225	-0.153097	-2.607994
8	-2.809092	1.461544	0.283261
8	-3.811814	0.187979	-1.733576
7	-2.166633	-2.329102	-0.970664
8	3.616052	-1.140948	-1.183651
1	4.439323	-0.019491	1.704062
1	4.839457	1.480266	2.589432
1	2.283752	2.064750	2.372566
1	2.724566	0.821036	3.580717
1	5.693284	-0.268048	-0.673792

1	6.416256	3.753038	0.670290
1	8.131120	-0.561976	-1.118668
1	8.870958	3.464217	0.213056
1	9.708540	1.304586	-0.678809
1	0.151635	2.257415	2.568793
1	-0.363901	-2.033759	2.419228
1	-2.178887	2.497785	3.325430
1	-2.694305	-1.776998	3.163757
1	-3.613751	0.501272	3.624409
1	0.050425	1.911904	0.174747
1	-1.090870	-0.248760	0.063621
1	0.373258	1.884308	-1.627866
1	-2.420140	0.102516	-1.962371
1	-0.797446	0.112975	-2.974194
1	-3.132967	-2.061767	-0.835044
1	-0.554573	-2.343115	-2.252125
1	-3.342149	-1.654576	-3.334562
1	-1.872558	-1.793725	-4.314310
1	-2.520656	-3.229296	-3.493346
6	-1.572211	-2.967291	0.070652
8	-2.179568	-3.414373	1.038386
8	-0.218787	-3.012184	-0.076187
6	0.522623	-4.249487	0.246242
6	0.587215	-4.485651	1.757272
1	-0.414700	-4.605253	2.170381
1	1.163728	-5.396278	1.952110
1	1.095387	-3.653946	2.249088
6	-0.156231	-5.415381	-0.477187
1	0.432758	-6.327848	-0.345929
1	-1.157351	-5.592033	-0.075382
1	-0.235320	-5.206831	-1.548852
6	1.909986	-3.961093	-0.324203
1	2.568617	-4.818478	-0.154105
1	1.851680	-3.773612	-1.400715
1	2.346283	-3.083829	0.157500
15	-4.025016	1.154398	-0.549299
8	-5.257158	0.587819	0.360311
8	-4.726947	2.481720	-1.152300
6	-5.113975	-0.722733	0.934440
6	-5.785478	-1.781984	0.066598
1	-5.582546	-0.681870	1.925275
1	-4.053780	-0.957966	1.091464
6	-5.654169	-3.191291	0.657444
1	-6.841541	-1.513610	-0.061591
1	-5.339843	-1.737332	-0.934886
6	-6.255261	-4.264190	-0.255922
1	-4.596320	-3.416270	0.840782
1	-6.150669	-3.221733	1.637595
1	-6.161465	-5.262835	0.183302
1	-7.318926	-4.077846	-0.444665

1	-5.746212	-4.277999	-1.226819
6	-4.944457	3.595767	-0.268043
6	-5.334332	4.799742	-1.110811
1	-4.028240	3.792990	0.302496
1	-5.742420	3.341301	0.442466
6	-5.609827	6.044295	-0.259301
1	-4.527955	5.002654	-1.826630
1	-6.221977	4.543419	-1.702450
6	-5.998878	7.262162	-1.103231
1	-6.410715	5.824610	0.459926
1	-4.719461	6.281576	0.339189
1	-6.189424	8.140636	-0.477960
1	-5.202348	7.520169	-1.810302
1	-6.905111	7.062663	-1.686230
6	3.316561	-0.825603	-2.379139
6	4.222636	-1.201678	-3.517534
1	5.111541	-0.562259	-3.480009
1	4.550565	-2.237380	-3.400364
1	3.720788	-1.062390	-4.475784

2' mode **o**

Number of imaginary frequencies : 0
Electronic energy : = -3399.855874
Zero-point correction= 0.855806 (Hartree/Particle)
Thermal correction to Energy= 0.913449
Thermal correction to Enthalpy= 0.914393
Thermal correction to Gibbs Free Energy= 0.757713
Sum of electronic and zero-point Energies= -3399.000068
Sum of electronic and thermal Energies= -3398.942425
Sum of electronic and thermal Enthalpies= -3398.941481
Sum of electronic and thermal Free Energies= -3399.098161

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Cartesian Coordinates

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6	0.460280	-3.029123	-0.440435
6	-0.827546	-2.621192	-0.085270
6	-1.971583	-3.366934	-0.389570
6	-1.808126	-4.597098	-1.022475
6	-0.526516	-5.047707	-1.359775
6	0.594448	-4.264603	-1.080948
16	-0.945545	-0.978017	0.640599
8	0.370598	-0.591767	1.207278
6	-2.171835	-1.177069	2.020371
6	-2.841962	0.153988	2.323235
16	-3.706962	0.807583	0.831879
6	-4.984249	-0.458581	0.638420
6	-5.004444	-1.261417	-0.502782

6	-5.990580	-2.247321	-0.608715
6	-6.941215	-2.403562	0.400452
6	-6.928510	-1.564066	1.520479
6	-5.951487	-0.579049	1.643199
46	-1.999449	0.471427	-0.848821
6	-0.738274	-0.123691	-2.628859
6	0.099976	0.759167	-1.973508
6	0.224432	2.213421	-2.269628
6	-0.013754	3.119352	-1.032811
6	0.230395	4.588534	-1.400451
8	-2.907737	1.837427	-2.054842
8	2.439616	-0.858538	-0.974081
8	3.141136	1.679858	-0.940514
7	0.840621	2.725964	0.071696
8	-3.972285	0.131405	-3.072182
1	-2.117144	0.941053	2.552380
1	-3.587167	0.055091	3.115983
1	-2.886161	-1.956467	1.747402
1	-1.560480	-1.511220	2.862811
1	-5.949021	0.096053	2.493736
1	-4.305574	-1.089539	-1.317621
1	-7.683437	-1.673089	2.292953
1	-6.021414	-2.874605	-1.494095
1	-7.706846	-3.168204	0.309645
1	-2.967232	-2.999634	-0.163527
1	1.318099	-2.368511	-0.297968
1	-2.680220	-5.198908	-1.258687
1	1.584852	-4.598713	-1.373241
1	-0.408198	-6.005182	-1.858255
1	-0.599427	-1.193293	-2.496119
1	0.832077	0.340192	-1.279061
1	-1.361896	0.184680	-3.461611
1	1.269581	2.351421	-2.583676
1	-0.449649	2.517158	-3.075084
1	1.833246	2.512126	-0.144347
1	-1.051579	3.009704	-0.707870
1	1.273944	4.741012	-1.695648
1	-0.415718	4.897041	-2.229517
1	0.020430	5.228815	-0.539357
6	0.378070	2.360523	1.283565
8	-0.818603	2.228771	1.592412
8	1.422777	2.175174	2.113601
6	1.311917	2.051471	3.559274
6	0.512896	3.225489	4.134883
1	-0.528598	3.187924	3.812422
1	0.551315	3.197559	5.228759
1	0.947351	4.172349	3.800198
6	0.706239	0.701162	3.951020
1	0.747147	0.583686	5.039167
1	-0.333770	0.640237	3.631848

1	1.259444	-0.112230	3.479176
6	2.780291	2.119634	3.990933
1	2.871527	1.958211	5.069665
1	3.356813	1.362370	3.454390
1	3.201359	3.097847	3.743164
15	3.431913	0.228198	-0.628409
8	3.810913	0.154274	0.978377
8	4.848570	-0.210799	-1.332565
6	3.618426	-1.082840	1.670548
6	4.561742	-2.196803	1.218503
1	2.578086	-1.406182	1.559563
1	3.788459	-0.856771	2.730917
6	4.304073	-3.503503	1.976311
1	4.425505	-2.357335	0.144349
1	5.600653	-1.871756	1.360679
6	5.233845	-4.638249	1.535224
1	4.415884	-3.336131	3.057106
1	3.258272	-3.806869	1.822791
1	5.028498	-5.566784	2.079273
1	5.119563	-4.842379	0.464426
1	6.283577	-4.374544	1.707285
6	5.972438	0.658203	-1.153756
6	7.190374	-0.010844	-1.773764
1	6.136994	0.837835	-0.081889
1	5.768701	1.628022	-1.626169
6	8.457096	0.843500	-1.655504
1	7.343967	-0.982198	-1.285600
1	6.975862	-0.222896	-2.829057
6	9.686708	0.171019	-2.274030
1	8.287315	1.815033	-2.139314
1	8.652248	1.062029	-0.596595
1	10.579935	0.797909	-2.180274
1	9.897710	-0.787470	-1.785702
1	9.529616	-0.030912	-3.339872
6	-3.746996	1.334638	-2.925787
6	-4.429925	2.402674	-3.763247
1	-3.678559	3.017828	-4.266308
1	-5.085760	1.933521	-4.496985
1	-5.007490	3.062844	-3.109720
8	-4.332588	2.119707	1.159120

TS[2'-4] mode **o**

Number of imaginary frequencies : 1
The smallest frequency is : -909.7960 cm(-1)

Electronic energy : = -3399.8400171
Zero-point correction= 0.851413 (Hartree/Particle)

Thermal correction to Energy= 0.908549
Thermal correction to Enthalpy= 0.909493
Thermal correction to Gibbs Free Energy= 0.753921
Sum of electronic and zero-point Energies= -3398.988604
Sum of electronic and thermal Energies= -3398.931468
Sum of electronic and thermal Enthalpies= -3398.930524
Sum of electronic and thermal Free Energies= -3399.086096

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Cartesian Coordinates

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6	-0.097807	-1.303406	2.953205
6	-1.329722	-0.776203	2.555281
6	-2.544279	-1.230741	3.076360
6	-2.514772	-2.205110	4.072341
6	-1.292933	-2.728633	4.507728
6	-0.094461	-2.288247	3.943582
16	-1.257748	0.349454	1.151720
8	0.099089	0.985538	1.140923
6	-2.519646	1.655181	1.497241
6	-3.002942	2.247932	0.179756
16	-3.818829	0.986698	-0.894234
6	-5.228830	0.581971	0.166366
6	-5.348056	-0.705706	0.691887
6	-6.432552	-0.985542	1.530338
6	-7.378329	0.000688	1.812807
6	-7.262155	1.275432	1.245839
6	-6.186879	1.571767	0.411405
46	-2.102668	-0.793422	-0.722145
6	-0.613313	-2.327477	-0.542453
6	0.304908	-1.382545	-1.067410
6	0.823645	-1.327049	-2.371656
6	1.091318	0.060828	-2.986367
6	2.057445	-0.041010	-4.170833
8	-2.815904	-1.815181	-2.347259
8	2.413940	-1.859390	0.843066
8	3.307841	-1.888828	-1.640025
7	1.599449	1.024903	-2.018095
8	-3.989536	-3.037498	-0.860695
1	-2.172025	2.599702	-0.439084
1	-3.723924	3.051789	0.347474
1	-3.332754	1.219566	2.081889
1	-1.985311	2.397618	2.095443
1	-6.099725	2.546598	-0.059431
1	-4.643529	-1.489194	0.416910
1	-8.012659	2.033263	1.449205
1	-6.541712	-1.984523	1.941245
1	-8.219755	-0.225286	2.461189
1	-3.494719	-0.862433	2.704758
1	0.825860	-1.000007	2.467311
1	-3.446645	-2.564124	4.497983

1	0.851677	-2.718955	4.254747
1	-1.279899	-3.496421	5.275392
1	-0.557303	-2.565546	0.516447
1	0.714613	-0.656752	-0.372608
1	-0.951746	-3.134716	-1.185353
1	2.014187	-1.722506	-2.023249
1	0.403465	-2.039698	-3.084727
1	2.552628	0.927773	-1.679042
1	0.127448	0.458560	-3.321456
1	3.031010	-0.407557	-3.830417
1	1.672072	-0.744795	-4.915510
1	2.186776	0.934452	-4.648216
6	0.848397	2.029312	-1.503312
8	-0.366720	2.160322	-1.659595
8	1.649098	2.885592	-0.815342
6	1.208246	4.233922	-0.458040
6	0.700270	4.974439	-1.699910
1	-0.203492	4.508827	-2.093472
1	0.481181	6.015619	-1.442257
1	1.468023	4.968180	-2.479732
6	0.160134	4.183896	0.656690
1	0.026042	5.183560	1.083193
1	-0.796224	3.842207	0.266860
1	0.483991	3.495326	1.440221
6	2.493448	4.882934	0.060763
1	2.308163	5.929510	0.320042
1	2.851368	4.362596	0.950936
1	3.275737	4.844057	-0.702106
15	3.486979	-1.535760	-0.149269
8	3.779639	0.088870	-0.188397
8	4.902639	-2.142002	0.361522
6	3.711901	0.792934	1.068978
6	4.665993	1.973448	1.007667
1	3.984795	0.118179	1.888792
1	2.678993	1.122017	1.228228
6	4.692372	2.766297	2.319028
1	5.672924	1.602860	0.776294
1	4.365936	2.621502	0.176353
6	5.608122	3.992146	2.251473
1	3.671460	3.080342	2.577786
1	5.017453	2.107504	3.135546
1	5.616421	4.542691	3.197987
1	6.639417	3.698193	2.025799
1	5.283558	4.681951	1.464376
6	6.075533	-1.926939	-0.445599
6	7.291284	-2.318909	0.379132
1	6.131383	-0.870999	-0.741009
1	6.001087	-2.529423	-1.358976
6	8.604657	-2.135607	-0.389593
1	7.303026	-1.714114	1.295019

1	7.181632	-3.363677	0.695532
6	9.833328	-2.518582	0.441332
1	8.578174	-2.739666	-1.306598
1	8.693526	-1.090439	-0.716383
1	10.760262	-2.383022	-0.125543
1	9.901735	-1.905341	1.347170
1	9.783414	-3.567103	0.756263
6	-3.651959	-2.761913	-2.017310
6	-4.196306	-3.521314	-3.217436
1	-3.369594	-3.946052	-3.793912
1	-4.867547	-4.313285	-2.884025
1	-4.730296	-2.829552	-3.875651
8	-4.295062	1.687905	-2.127789

2' mode **p**

Number of imaginary frequencies : 0

Electronic energy : = -4129.507388
Zero-point correction= 1.077416 (Hartree/Particle)
Thermal correction to Energy= 1.145805
Thermal correction to Enthalpy= 1.146749
Thermal correction to Gibbs Free Energy= 0.968486
Sum of electronic and zero-point Energies= -4128.429972
Sum of electronic and thermal Energies= -4128.361583
Sum of electronic and thermal Enthalpies= -4128.360639
Sum of electronic and thermal Free Energies= -4128.538902

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Cartesian Coordinates

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6	2.787556	-2.726375	1.205894
6	1.397279	-2.830795	1.237883
6	0.729060	-4.045425	1.059384
6	1.497005	-5.195223	0.872683
6	2.893555	-5.119278	0.846077
6	3.534983	-3.890605	1.010580
16	0.480323	-1.272962	1.339746
8	1.425404	-0.212482	1.836338
6	-0.733315	-1.634179	2.705887
6	-2.173225	-1.256248	2.397815
16	-2.886148	-2.480084	1.183195
8	-2.557116	-3.854124	1.755276
6	-4.635686	-2.141912	1.549995
6	-5.392536	-3.186272	2.079144
6	-6.756113	-2.982825	2.303594
6	-7.340733	-1.750655	2.002202
6	-6.564548	-0.715099	1.473132
6	-5.202828	-0.903772	1.232748

46	-0.553432	-0.736325	-0.651661
6	1.189200	-1.157823	-1.629388
6	2.060601	0.079140	-1.505123
6	1.671900	1.228255	-2.453675
6	0.957758	2.390571	-1.746784
6	0.518924	3.457954	-2.755069
8	-1.456735	-0.091951	-2.465885
8	3.439325	-0.364240	-1.768587
8	4.682191	1.906559	-1.324239
7	1.834084	2.949004	-0.714873
8	-2.666956	0.318551	-0.280075
1	-2.285259	-0.264559	1.955813
1	-2.761808	-1.330856	3.316192
1	-0.657841	-2.695125	2.955671
1	-0.328231	-1.032336	3.524352
1	-4.592197	-0.121418	0.792232
1	-4.907971	-4.131936	2.301938
1	-7.021774	0.240969	1.235559
1	-7.360465	-3.787443	2.711885
1	-8.401882	-1.597808	2.174967
1	-0.356720	-4.108853	1.077545
1	3.268656	-1.758787	1.300250
1	0.999381	-6.151603	0.745021
1	4.618522	-3.829100	0.978940
1	3.479987	-6.020159	0.691500
1	1.669230	-2.038212	-1.202597
1	2.041768	0.436488	-0.468979
1	0.846384	-1.352514	-2.648042
1	2.581693	1.609260	-2.926995
1	1.012526	0.856158	-3.242472
1	2.826616	3.030790	-0.915652
1	0.068958	2.012903	-1.238422
1	1.376086	3.818724	-3.334768
1	-0.228691	3.047098	-3.439642
1	0.074962	4.309341	-2.233835
6	1.457530	3.424004	0.501310
8	2.241041	3.909703	1.310736
8	0.120631	3.274145	0.705547
6	-0.458027	3.510705	2.034214
6	0.244056	2.651913	3.091490
1	1.267930	2.987238	3.252474
1	-0.306478	2.720624	4.035855
1	0.276012	1.609627	2.768081
6	-0.390727	5.003929	2.364192
1	-0.924390	5.202615	3.299700
1	0.645906	5.325410	2.466921
1	-0.865660	5.586347	1.568015
6	-1.906803	3.049091	1.854475
1	-2.419570	3.035649	2.821174
1	-2.449239	3.728847	1.194024

1	-1.940590	2.051572	1.407871
15	4.609836	0.456445	-1.021369
8	4.412103	0.091889	0.537049
8	5.894266	-0.393542	-1.456479
6	4.179331	1.130937	1.540666
6	5.447604	1.889655	1.892574
1	3.773114	0.587109	2.395398
1	3.410454	1.813755	1.184308
6	5.168729	2.946333	2.970659
1	6.217578	1.183312	2.231267
1	5.824052	2.378131	0.987049
6	6.415437	3.761641	3.326282
1	4.373433	3.610092	2.612625
1	4.781178	2.454039	3.874004
1	6.196068	4.513654	4.091480
1	7.217269	3.118673	3.708565
1	6.803478	4.285182	2.445293
6	5.982622	-1.785670	-1.061349
6	7.113179	-2.434491	-1.838586
1	5.028186	-2.283106	-1.269013
1	6.165301	-1.826960	0.019206
6	7.285202	-3.910839	-1.459364
1	6.903730	-2.341060	-2.910841
1	8.041614	-1.883154	-1.646807
6	8.411601	-4.592916	-2.241686
1	7.486904	-3.989306	-0.381849
1	6.340364	-4.443908	-1.634248
1	8.517909	-5.644337	-1.956068
1	8.218755	-4.555800	-3.319547
1	9.371739	-4.097332	-2.060121
15	-2.660084	0.595529	-1.790589
8	-4.061491	0.170361	-2.459988
8	-2.590870	2.152914	-2.150607
6	-3.504456	3.086045	-1.524997
6	-2.824075	4.443316	-1.479121
1	-3.745222	2.736308	-0.514919
1	-4.427439	3.112558	-2.115919
6	-3.707089	5.519070	-0.836876
1	-1.887115	4.337345	-0.920951
1	-2.552678	4.737438	-2.499954
6	-3.006892	6.879613	-0.768479
1	-4.644380	5.612645	-1.401905
1	-3.992726	5.203468	0.176140
1	-3.646227	7.637220	-0.304376
1	-2.082921	6.815516	-0.182866
1	-2.737883	7.233866	-1.769747
6	-4.535837	-1.185547	-2.259355
6	-6.051378	-1.159586	-2.154144
1	-4.098497	-1.595294	-1.343361
1	-4.197740	-1.794547	-3.105080

6	-6.627422	-2.532557	-1.788246
1	-6.327646	-0.429798	-1.384952
1	-6.475589	-0.802863	-3.100854
6	-8.153491	-2.512241	-1.663916
1	-6.326705	-3.272102	-2.542618
1	-6.191878	-2.862117	-0.836510
1	-8.544765	-3.499796	-1.399346
1	-8.468107	-1.809894	-0.884345
1	-8.625172	-2.204154	-2.603917

TS[2'-4] mode **p**

Number of imaginary frequencies : 1 The smallest frequency is : -735.7220 cm(-1)

Electronic energy : = -4129.4523174
Zero-point correction= 1.068908 (Hartree/Particle)
Thermal correction to Energy= 1.137943
Thermal correction to Enthalpy= 1.138887
Thermal correction to Gibbs Free Energy= 0.956124
Sum of electronic and zero-point Energies= -4128.383410
Sum of electronic and thermal Energies= -4128.314374
Sum of electronic and thermal Enthalpies= -4128.313430
Sum of electronic and thermal Free Energies= -4128.496194

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Cartesian Coordinates

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6	1.858326	0.008239	3.009610
6	1.148197	-1.151264	2.692942
6	1.779512	-2.395018	2.582350
6	3.154349	-2.464134	2.796587
6	3.879778	-1.312001	3.104421
6	3.234009	-0.081087	3.216489
16	-0.577122	-0.897710	2.249655
8	-1.161331	0.205416	3.083130
6	-1.387174	-2.455314	2.795739
6	-2.891161	-2.334593	2.576585
16	-3.334599	-2.791209	0.831075
8	-3.141854	-4.291899	0.755538
6	-5.107806	-2.442315	1.019549
6	-5.986270	-3.519018	1.121146
6	-7.355744	-3.260201	1.215069
6	-7.822228	-1.943191	1.204098
6	-6.924267	-0.876784	1.092382
6	-5.553157	-1.117348	0.989961
46	-0.950386	-0.570089	-0.005974
6	0.754684	-1.627528	-0.651792
6	1.481251	-0.400218	-0.616268
6	1.710655	0.453611	-1.712859
6	1.736527	1.974714	-1.458159

6	2.293594	2.726598	-2.669458
8	-1.442348	-0.067026	-2.005531
8	3.869443	-1.537473	-0.084546
8	4.339525	0.341874	-1.804395
7	2.523500	2.292045	-0.268719
8	-2.935502	0.591157	-0.099676
1	-3.255316	-1.326692	2.794769
1	-3.420310	-3.058573	3.202508
1	-0.967771	-3.301938	2.244971
1	-1.140783	-2.546232	3.857247
1	-4.844611	-0.301751	0.863372
1	-5.588214	-4.529537	1.111989
1	-7.292048	0.144843	1.072904
1	-8.057361	-4.085547	1.291562
1	-8.888054	-1.746925	1.272559
1	1.230463	-3.291880	2.318148
1	1.360295	0.965683	3.061735
1	3.662931	-3.415858	2.688901
1	3.786219	0.829107	3.421998
1	4.956146	-1.372877	3.226534
1	1.034276	-2.386609	0.071794
1	1.921757	-0.123285	0.334463
1	0.450105	-2.008025	-1.625430
1	2.957171	0.239230	-1.845252
1	1.187884	0.180274	-2.630216
1	3.521001	2.135573	-0.339115
1	0.712585	2.301272	-1.262011
1	3.325068	2.420607	-2.866778
1	1.693620	2.504295	-3.557347
1	2.267404	3.805948	-2.493544
6	2.061212	2.596140	0.970244
8	2.787248	2.881565	1.918675
8	0.704059	2.508622	1.042886
6	-0.060843	3.512693	1.812453
6	0.147240	3.353190	3.320435
1	1.192728	3.506918	3.587506
1	-0.467956	4.093518	3.843226
1	-0.177015	2.361313	3.642707
6	0.359358	4.902070	1.325362
1	-0.265279	5.667058	1.796149
1	1.402813	5.104542	1.580229
1	0.238867	4.976708	0.239652
6	-1.500589	3.191345	1.422874
1	-2.183888	3.912400	1.883190
1	-1.610123	3.234560	0.339350
1	-1.771360	2.185888	1.748042
15	4.876625	-0.826678	-0.946103
8	6.144880	-0.277529	-0.078003
8	5.654606	-1.819593	-1.959421
6	5.923032	0.837403	0.803199

6	6.324860	2.149705	0.138183
1	6.531882	0.654011	1.696788
1	4.875961	0.867469	1.129944
6	6.123136	3.359591	1.058828
1	7.372813	2.074934	-0.178236
1	5.738346	2.260098	-0.782227
6	6.443103	4.683648	0.357816
1	5.088051	3.375732	1.420801
1	6.760372	3.250080	1.947726
1	6.302081	5.537104	1.029307
1	7.478628	4.705690	-0.001468
1	5.790279	4.831007	-0.510472
6	6.173986	-3.054736	-1.434997
6	6.571390	-3.936798	-2.608099
1	5.407836	-3.539913	-0.817469
1	7.041821	-2.838638	-0.797257
6	7.156819	-5.279776	-2.157313
1	5.687833	-4.101631	-3.237404
1	7.299740	-3.395949	-3.225070
6	7.560739	-6.172563	-3.334870
1	8.031094	-5.100511	-1.516532
1	6.423129	-5.806409	-1.531605
1	7.977626	-7.125523	-2.992627
1	6.698593	-6.394062	-3.974146
1	8.315880	-5.681100	-3.958692
15	-2.659216	0.793876	-1.598317
8	-3.953587	0.492987	-2.497373
8	-2.348771	2.312880	-1.996499
6	-3.339804	3.344511	-1.754850
6	-2.670521	4.687740	-1.989251
1	-3.701800	3.258943	-0.723350
1	-4.182917	3.188200	-2.436883
6	-3.605729	5.864268	-1.687758
1	-1.778947	4.750028	-1.353875
1	-2.320528	4.733960	-3.027545
6	-2.920004	7.218895	-1.890923
1	-4.496513	5.800593	-2.327081
1	-3.964307	5.786013	-0.652404
1	-3.598897	8.048307	-1.669289
1	-2.045900	7.316385	-1.237219
1	-2.574899	7.334571	-2.924363
6	-4.552984	-0.828616	-2.445307
6	-6.062160	-0.676389	-2.506967
1	-4.254420	-1.333378	-1.521880
1	-4.166746	-1.404093	-3.293275
6	-6.782150	-2.028026	-2.438569
1	-6.378417	-0.045473	-1.668234
1	-6.330137	-0.144702	-3.428559
6	-8.305580	-1.880398	-2.476186
1	-6.451150	-2.662995	-3.271327

1	-6.491262	-2.545680	-1.517136
1	-8.800749	-2.855021	-2.419312
1	-8.657209	-1.278967	-1.630926
1	-8.635219	-1.388714	-3.398504

2' mode **q**

Number of imaginary frequencies : 0

Electronic energy : = -1563.0371752
Zero-point correction= 0.475744 (Hartree/Particle)
Thermal correction to Energy= 0.511201
Thermal correction to Enthalpy= 0.512145
Thermal correction to Gibbs Free Energy= 0.405952
Sum of electronic and zero-point Energies= -1562.561431
Sum of electronic and thermal Energies= -1562.525975
Sum of electronic and thermal Enthalpies= -1562.525030
Sum of electronic and thermal Free Energies= -1562.631223

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Cartesian Coordinates

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46	0.810072	-0.579812	0.842157
6	0.042307	-2.149947	2.101666
6	-0.988626	-1.177710	2.023095
6	-0.707644	0.137965	2.409214
6	-1.632688	1.315472	2.172962
6	-2.216909	1.802117	3.511316
8	2.008459	1.457891	2.232185
8	-1.144219	-3.910226	-0.273287
8	-3.184829	-3.298517	0.434751
7	-2.704069	1.018701	1.233872
8	1.508012	1.295713	0.053622
1	-0.118175	-3.124302	1.651274
1	-1.875253	-1.388633	1.431399
1	0.770886	-2.098985	2.910221
1	-2.894296	-3.874105	1.162295
1	0.083126	0.320667	3.133352
1	-3.398193	0.335381	1.502994
1	-1.036103	2.120371	1.739125
1	-2.840062	1.025945	3.970320
1	-1.416979	2.053796	4.213419
1	-2.833511	2.689167	3.345825
6	-2.671597	1.229500	-0.125110
8	-3.427419	0.648459	-0.893566
8	-1.755889	2.155353	-0.446626
6	-1.456263	2.478246	-1.856224
6	-0.909559	1.227320	-2.540426
1	-1.668727	0.449690	-2.620145

1	-0.556879	1.475656	-3.546303
1	-0.066101	0.855568	-1.957931
6	-2.700968	3.046594	-2.539924
1	-2.432655	3.399617	-3.540843
1	-3.481498	2.291126	-2.624999
1	-3.088748	3.896807	-1.969970
6	-0.361350	3.536245	-1.722313
1	-0.051702	3.876922	-2.714958
1	-0.728991	4.399582	-1.158980
1	0.499013	3.106229	-1.206200
6	2.596057	-1.670741	-0.029048
6	1.525942	-2.024483	-0.831744
1	2.903414	-2.273168	0.822034
1	0.910826	-2.902289	-0.653486
6	1.358155	-1.400473	-2.182487
8	0.463238	-1.760404	-2.939791
6	3.586067	-0.640929	-0.472784
8	4.570494	-0.377177	0.201700
6	2.334215	-0.366153	-2.587447
6	3.347337	0.004144	-1.788235
1	2.162096	0.083840	-3.559994
1	4.058861	0.775749	-2.064839
6	-2.182017	-3.309121	-0.484407
6	-2.525799	-2.511146	-1.704700
1	-3.331425	-3.019931	-2.244814
1	-2.902253	-1.524183	-1.416868
1	-1.643526	-2.421205	-2.335999
6	2.006765	1.918465	1.078400
6	2.588298	3.291804	0.783165
1	3.240431	3.608036	1.598022
1	3.137482	3.277637	-0.161392
1	1.771004	4.013704	0.679399

TS[2'-4] mode **q**

Number of imaginary frequencies : 1
The smallest frequency is : -729.2514 cm(-1)

Electronic energy : = -1562.9746499
Zero-point correction= 0.471410 (Hartree/Particle)
Thermal correction to Energy= 0.505365
Thermal correction to Enthalpy= 0.506309
Thermal correction to Gibbs Free Energy= 0.405000
Sum of electronic and zero-point Energies= -1562.503240
Sum of electronic and thermal Energies= -1562.469285
Sum of electronic and thermal Enthalpies= -1562.468341
Sum of electronic and thermal Free Energies= -1562.569650

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Cartesian Coordinates

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46	1.440697	-0.761354	0.190529
6	0.008051	-2.030736	-0.647927
6	-1.181967	-1.327168	-0.212930
6	-1.886261	-1.626751	0.980109
6	-2.575531	-0.474592	1.749768
6	-3.386817	-1.031562	2.920746
8	0.677059	-0.628172	2.162009
8	-2.478079	-2.085354	-1.884366
8	-4.038396	-2.420631	-0.314931
7	-3.453024	0.300139	0.875424
8	2.474267	0.568623	1.708173
1	0.131781	-2.064194	-1.728864
1	-1.424164	-0.420546	-0.751187
1	0.187133	-2.995102	-0.167461
1	-2.841611	-2.207732	0.466493
1	-1.378283	-2.346738	1.625141
1	-4.277834	-0.184471	0.541650
1	-1.804142	0.200078	2.122525
1	-4.168513	-1.708934	2.559569
1	-2.739013	-1.593208	3.600664
1	-3.859410	-0.219097	3.479258
6	-3.069985	1.330250	0.060973
8	-3.762954	1.759720	-0.851310
8	-1.842926	1.792532	0.411010
6	-1.169207	2.833433	-0.380225
6	-0.938192	2.325321	-1.805735
1	-1.886793	2.173507	-2.321050
1	-0.326868	3.040207	-2.361683
1	-0.386698	1.381104	-1.781155
6	-1.983358	4.129579	-0.353176
1	-1.409385	4.929888	-0.831107
1	-2.930023	4.004401	-0.877996
1	-2.187216	4.423247	0.681191
6	0.155407	3.007239	0.363955
1	0.786505	3.734706	-0.152739
1	-0.023809	3.354286	1.386234
1	0.703566	2.063898	0.413619
6	2.844062	-1.320363	-1.419462
6	2.202763	-0.143094	-1.793056
1	2.535223	-2.292482	-1.792450
1	1.359931	-0.136864	-2.477900
6	2.872418	1.186090	-1.590364
8	2.357446	2.215782	-2.000191
6	4.205154	-1.286304	-0.787746
8	4.790222	-2.322889	-0.512062
6	4.188880	1.185249	-0.908245
6	4.804022	0.047786	-0.540751
1	4.622250	2.164345	-0.730778

1	5.770095	0.042931	-0.045839
6	-3.672129	-2.016896	-1.476303
6	-4.707685	-1.332883	-2.344269
1	-5.709541	-1.706701	-2.121547
1	-4.673505	-0.258427	-2.120930
1	-4.470325	-1.470479	-3.401555
6	1.571351	0.227048	2.526653
6	1.480392	0.825122	3.900127
1	1.217774	0.055076	4.629117
1	2.420781	1.308196	4.167791
1	0.679867	1.572937	3.899175

2' mode **s**

Number of imaginary frequencies : 0 Electronic energy : = -2292.6421639
Zero-point correction= 0.695668 (Hartree/Particle)
Thermal correction to Energy= 0.741858
Thermal correction to Enthalpy= 0.742803
Thermal correction to Gibbs Free Energy= 0.611717
Sum of electronic and zero-point Energies= -2291.946496
Sum of electronic and thermal Energies= -2291.900305
Sum of electronic and thermal Enthalpies= -2291.899361
Sum of electronic and thermal Free Energies= -2292.030447

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Cartesian Coordinates

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46	1.708856	1.748051	-0.435724
6	0.207849	1.862823	-1.813159
6	-0.406741	0.474015	-1.925628
6	0.234325	-0.461495	-2.967274
6	1.147440	-1.518665	-2.323059
6	1.820608	-2.403153	-3.377833
8	3.162198	0.992394	-1.757169
8	-1.832201	0.669350	-2.206479
8	-2.571048	-1.836811	-1.918135
7	0.365780	-2.310063	-1.371832
8	3.822825	1.206910	0.346189
1	-0.541468	2.590050	-1.494668
1	-0.348522	-0.023084	-0.950680
1	0.720611	2.203659	-2.716296
1	-0.569873	-0.967211	-3.510412
1	0.814899	0.111187	-3.696421
1	-0.595563	-2.544913	-1.604952
1	1.928136	-1.008327	-1.758424
1	1.072918	-2.935642	-3.975817
1	2.439638	-1.800137	-4.050705
1	2.460415	-3.142176	-2.887302
6	0.829937	-2.871844	-0.221031

8	0.142898	-3.575053	0.511287
8	2.122524	-2.525664	0.004723
6	2.836643	-3.017188	1.191299
6	2.143309	-2.542406	2.470627
1	1.161675	-3.001736	2.579807
1	2.761109	-2.804125	3.336153
1	2.015852	-1.457945	2.452240
6	2.951468	-4.542299	1.122449
1	3.579497	-4.902604	1.943537
1	1.967609	-5.005938	1.197203
1	3.415518	-4.842186	0.177337
6	4.207855	-2.354231	1.047939
1	4.858966	-2.659075	1.872699
1	4.679274	-2.655125	0.107233
1	4.111676	-1.264973	1.062213
15	-2.801312	-0.428507	-1.514847
8	-2.587232	-0.117528	0.056069
8	-4.245814	0.130952	-1.887869
6	-2.274056	-1.206838	0.991931
6	-3.458961	-2.118358	1.259795
1	-1.934609	-0.693141	1.891434
1	-1.437926	-1.783603	0.596966
6	-3.058210	-3.245966	2.223221
1	-4.294928	-1.536737	1.670778
1	-3.792883	-2.552494	0.310764
6	-4.205295	-4.226613	2.482435
1	-2.195159	-3.775418	1.802124
1	-2.721003	-2.811675	3.174461
1	-3.901249	-5.023493	3.168896
1	-5.071697	-3.718317	2.922043
1	-4.535881	-4.696926	1.549541
6	-4.693768	1.429940	-1.415248
6	-5.531495	1.285924	-0.153196
1	-5.280293	1.848897	-2.237919
1	-3.829000	2.082162	-1.249788
6	-6.079303	2.633630	0.331793
1	-6.356337	0.592477	-0.357066
1	-4.912519	0.828674	0.626007
6	-6.919141	2.498138	1.605771
1	-5.243071	3.322463	0.515028
1	-6.684889	3.092348	-0.461626
1	-7.300144	3.468551	1.939300
1	-7.778592	1.838847	1.440949
1	-6.326853	2.070816	2.422638
6	0.744522	3.233638	0.862969
6	0.206345	1.988175	1.177991
1	-0.752686	1.650210	0.791116
1	0.228303	3.943823	0.223610
6	0.728113	1.218027	2.349874
6	1.866992	3.813974	1.672239

6	1.907680	1.767800	3.060992
6	2.432475	2.965891	2.750896
8	2.276666	4.944002	1.453462
8	0.182545	0.186245	2.719057
1	3.287774	3.380727	3.274650
1	2.307298	1.144673	3.854837
6	4.067686	0.860610	-0.842545
6	5.386821	0.261895	-1.244463
1	5.778314	0.783447	-2.121810
1	6.096915	0.314423	-0.418983
1	5.225122	-0.783682	-1.523653

TS[2'-4] mode **s**

Number of imaginary frequencies : 1
The smallest frequency is : -750.8340 cm(-1)

Electronic energy : = -2292.589647
Zero-point correction= 0.689225 (Hartree/Particle)
Thermal correction to Energy= 0.734855
Thermal correction to Enthalpy= 0.735799
Thermal correction to Gibbs Free Energy= 0.609428
Sum of electronic and zero-point Energies= -2291.900422
Sum of electronic and thermal Energies= -2291.854792
Sum of electronic and thermal Enthalpies= -2291.853848
Sum of electronic and thermal Free Energies= -2291.980219

Cartesian Coordinates

46	-1.153863	-0.859569	0.219847
6	-0.269864	-2.621527	-0.480468
6	1.019396	-2.011455	-0.746408
6	1.390316	-1.474507	-2.005226
6	2.260477	-0.194995	-2.028501
6	2.541619	0.232967	-3.468542
8	-1.048604	0.124641	-1.663495
8	2.221410	-3.898422	-0.520472
8	3.317552	-3.232450	-2.355707
7	3.520947	-0.399993	-1.315911
8	-1.609468	1.374743	0.439157
1	-0.266391	-3.373818	0.306158
1	1.636803	-1.793267	0.116928
1	-0.848525	-2.909234	-1.358821
1	2.178184	-2.358082	-2.346000
1	0.579145	-1.464528	-2.733821
1	4.138896	-1.095259	-1.719530
1	1.718695	0.604430	-1.523316
1	3.084058	-0.549983	-4.010260

1	1.601311	0.426827	-3.992538
1	3.142189	1.146553	-3.481219
6	3.734412	-0.225458	0.022058
8	4.688808	-0.708753	0.616908
8	2.768321	0.551595	0.581749
6	2.711765	0.734739	2.043885
6	2.491024	-0.625620	2.709879
1	3.337895	-1.287462	2.527294
1	2.352486	-0.496407	3.785976
1	1.578827	-1.084860	2.319505
6	3.978993	1.431554	2.546673
1	3.849123	1.700112	3.600101
1	4.851156	0.787874	2.442340
1	4.148424	2.352178	1.978882
6	1.494164	1.640807	2.228478
1	1.247829	1.724696	3.289528
1	1.699306	2.640239	1.836707
1	0.620698	1.241465	1.708948
15	-1.345082	1.526103	-1.068239
8	-2.572953	2.260103	-1.792867
8	-0.098311	2.440560	-1.449907
6	0.277742	3.616420	-0.686169
6	1.784921	3.766032	-0.810399
1	-0.024728	3.478229	0.356869
1	-0.256033	4.479826	-1.099072
6	2.324486	4.961621	-0.017316
1	2.251615	2.839090	-0.458489
1	2.042900	3.869232	-1.871611
6	3.848951	5.076269	-0.114393
1	1.858329	5.888081	-0.378835
1	2.031293	4.864427	1.037160
1	4.224579	5.927723	0.461563
1	4.334028	4.170804	0.267292
1	4.167919	5.206524	-1.154431
6	-3.929905	1.923598	-1.387025
6	-4.367493	0.546007	-1.868163
1	-4.549960	2.707885	-1.828950
1	-3.994544	1.998200	-0.295692
6	-5.823435	0.246344	-1.490202
1	-4.231298	0.489709	-2.954711
1	-3.716977	-0.220537	-1.432521
6	-6.262905	-1.148257	-1.944693
1	-5.934848	0.315231	-0.400852
1	-6.481978	1.009241	-1.927639
1	-7.310177	-1.337001	-1.688328
1	-6.155512	-1.263181	-3.029307
1	-5.656495	-1.916516	-1.455245
6	-2.423964	-2.013618	1.563338
6	-1.311855	-1.600131	2.299543
1	-0.474669	-2.264678	2.491870

1	-2.507512	-3.015559	1.152827
6	-1.411661	-0.416702	3.212752
6	-3.708806	-1.238802	1.609415
6	-2.674335	0.363507	3.180686
6	-3.734960	-0.019128	2.449279
8	-4.689093	-1.615588	0.980773
8	-0.504299	-0.133327	3.981099
1	-4.664187	0.541888	2.433279
1	-2.685306	1.255843	3.798275
6	3.290566	-3.730593	-1.172405
6	4.617585	-4.028445	-0.507942
1	5.365474	-4.315794	-1.250629
1	4.953615	-3.109716	-0.010033
1	4.501377	-4.810412	0.245636

2' mode **t**

Number of imaginary frequencies : 0

Electronic energy : = -3022.2463072
Zero-point correction= 0.909513 (Hartree/Particle)
Thermal correction to Energy= 0.969003
Thermal correction to Enthalpy= 0.969947
Thermal correction to Gibbs Free Energy= 0.808367
Sum of electronic and zero-point Energies= -3021.336795
Sum of electronic and thermal Energies= -3021.277305
Sum of electronic and thermal Enthalpies= -3021.276360
Sum of electronic and thermal Free Energies= -3021.437941

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Cartesian Coordinates

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46	-1.680996	-1.141041	-0.047623
6	-0.083719	-1.968824	-1.063779
6	0.523905	-0.646426	-1.134767
6	0.055695	0.308898	-1.986929
6	0.430792	1.768766	-1.992864
6	0.528000	2.311014	-3.427288
8	-2.866310	-0.215303	-1.860571
8	3.262675	-1.218958	0.303381
8	3.563860	-0.234574	-2.111070
7	1.653063	2.091610	-1.269953
8	-3.281045	0.337858	0.578987
1	0.460244	-2.715126	-0.486386
1	1.277423	-0.408093	-0.390039
1	-0.546742	-2.362536	-1.970449
1	2.640025	-0.493009	-2.266030
1	-0.729551	0.040430	-2.689912
1	2.529996	1.922501	-1.744490

1	-0.406933	2.276691	-1.500989
1	1.346756	1.831041	-3.976349
1	-0.403164	2.123119	-3.968097
1	0.710975	3.388011	-3.406278
6	1.800715	2.180417	0.088950
8	2.898718	2.264257	0.622886
8	0.608621	2.183442	0.716695
6	0.538265	1.985426	2.184834
6	1.138714	0.619067	2.516639
1	2.194135	0.570158	2.248773
1	1.019089	0.411565	3.582202
1	0.603603	-0.162830	1.973694
6	1.240453	3.133391	2.913553
1	1.022664	3.061190	3.984012
1	2.318210	3.101056	2.762214
1	0.860381	4.094889	2.553091
6	-0.964687	2.013287	2.457845
1	-1.157851	1.706865	3.489012
1	-1.363720	3.021267	2.309775
1	-1.500644	1.333429	1.793513
15	4.170028	-1.077199	-0.866593
8	5.576405	-0.375791	-0.608589
8	4.576004	-2.452296	-1.586376
6	5.677440	0.786763	0.272761
6	5.789150	2.060872	-0.546141
1	6.577130	0.612395	0.870346
1	4.807115	0.819865	0.931382
6	5.952052	3.296843	0.345874
1	6.631979	1.971128	-1.242956
1	4.878195	2.165120	-1.143213
6	5.982639	4.595665	-0.464968
1	5.116658	3.328721	1.053064
1	6.874443	3.206657	0.936418
1	6.111535	5.469004	0.182692
1	6.802822	4.593543	-1.192377
1	5.045943	4.726353	-1.018609
6	4.873352	-3.612309	-0.765241
6	6.315147	-3.602906	-0.272980
1	4.686943	-4.472006	-1.415404
1	4.166660	-3.648000	0.071535
6	6.658028	-4.871374	0.517660
1	6.981184	-3.500801	-1.138182
1	6.477210	-2.716728	0.351347
6	8.103977	-4.872737	1.023632
1	5.970881	-4.967218	1.369228
1	6.488577	-5.754160	-0.113973
1	8.330166	-5.784275	1.585884
1	8.812177	-4.807973	0.190061
1	8.289749	-4.017318	1.682675
15	-3.525833	0.756188	-0.884954

8	-5.104375	0.971504	-1.132540
8	-2.946208	2.230885	-1.190211
6	-3.237837	3.312323	-0.270859
6	-2.070640	4.285206	-0.302705
1	-3.370948	2.905595	0.737520
1	-4.174345	3.788615	-0.583618
6	-2.265159	5.473749	0.645314
1	-1.162440	3.740901	-0.022133
1	-1.930153	4.642315	-1.331088
6	-1.044608	6.398994	0.668671
1	-3.158372	6.041916	0.352767
1	-2.459911	5.101268	1.660481
1	-1.190957	7.240866	1.352769
1	-0.149325	5.854783	0.990701
1	-0.840829	6.807497	-0.327606
6	-6.027549	-0.031872	-0.639013
6	-6.018811	-1.301231	-1.482440
1	-7.008860	0.451064	-0.668224
1	-5.780835	-0.252881	0.406399
6	-7.059143	-2.317336	-0.997468
1	-6.206595	-1.029646	-2.528369
1	-5.022315	-1.753523	-1.449893
6	-7.025701	-3.613603	-1.811507
1	-6.863542	-2.557633	0.054907
1	-8.062124	-1.870121	-1.042008
1	-7.789083	-4.319791	-1.468375
1	-7.203529	-3.417544	-2.875279
1	-6.049603	-4.097413	-1.710493
6	-2.209723	-3.021196	0.909577
6	-1.377551	-2.299983	1.782138
1	-0.318668	-2.523824	1.879992
1	-1.824367	-3.820726	0.283100
6	-1.974485	-1.549274	2.932140
6	-3.693743	-3.017208	1.080274
6	-3.454979	-1.522747	3.034833
6	-4.245970	-2.203488	2.189624
8	-4.418012	-3.675206	0.342281
8	-1.271498	-1.014113	3.779359
1	-5.328513	-2.194577	2.271206
1	-3.852342	-0.922944	3.847513

TS[2'-4] mode **t**

Number of imaginary frequencies : 1
The smallest frequency is : -418.0298 cm(-1)

Electronic energy : = -3022.2014305
Zero-point correction= 0.906153 (Hartree/Particle)

Thermal correction to Energy= 0.964271
Thermal correction to Enthalpy= 0.965215
Thermal correction to Gibbs Free Energy= 0.807817
Sum of electronic and zero-point Energies= -3021.295278
Sum of electronic and thermal Energies= -3021.237159
Sum of electronic and thermal Enthalpies= -3021.236215
Sum of electronic and thermal Free Energies= -3021.393613

Cartesian Coordinates

46	-1.678908	-1.125414	0.342024
6	0.216655	-1.917694	-0.089460
6	0.828466	-0.635868	-0.361661
6	0.887281	-0.048152	-1.648916
6	0.739448	1.491502	-1.760442
6	0.916094	1.931784	-3.213751
8	-2.003670	-0.414901	-1.631623
8	2.973579	-1.400000	0.172055
8	3.525069	-0.071151	-1.970443
7	1.713980	2.172856	-0.913829
8	-3.528818	0.227518	0.253796
1	0.607432	-2.435150	0.783499
1	1.131118	-0.047662	0.495557
1	0.057621	-2.563635	-0.953596
1	2.071430	-0.180335	-1.896652
1	0.328391	-0.592692	-2.410093
1	2.685345	2.021944	-1.162298
1	-0.258313	1.768181	-1.418101
1	1.910803	1.656462	-3.580333
1	0.167362	1.447567	-3.847337
1	0.796110	3.015326	-3.297563
6	1.546400	2.541639	0.387796
8	2.476820	2.856840	1.120469
8	0.238173	2.521950	0.753612
6	-0.135448	2.700940	2.170443
6	0.497081	1.578829	2.997616
1	1.583388	1.668450	3.010531
1	0.113055	1.605570	4.019858
1	0.221094	0.610047	2.572564
6	0.272592	4.091604	2.663390
1	-0.154158	4.260210	3.657480
1	1.355742	4.190959	2.713507
1	-0.123019	4.857385	1.988367
6	-1.658283	2.570744	2.141902
1	-2.047642	2.517094	3.161187
1	-2.106021	3.432880	1.641668
1	-1.969019	1.668424	1.611929
15	4.019665	-1.022766	-0.867882
8	5.338392	-0.402776	-0.168008
8	4.637827	-2.324906	-1.590606

6	5.239059	0.901309	0.456969
6	5.729039	1.985533	-0.495163
1	5.869104	0.851312	1.351023
1	4.212344	1.097626	0.785291
6	5.718124	3.377106	0.148635
1	6.741041	1.724574	-0.830432
1	5.096382	1.970601	-1.391270
6	6.181000	4.470243	-0.819549
1	4.706632	3.596941	0.507028
1	6.368423	3.372632	1.034746
1	6.171134	5.456825	-0.344270
1	7.199712	4.280740	-1.177801
1	5.527219	4.517477	-1.698351
6	4.868357	-3.531654	-0.833267
6	6.225310	-3.520087	-0.137533
1	4.816328	-4.345611	-1.564103
1	4.056163	-3.666143	-0.109250
6	6.510945	-4.839491	0.589055
1	7.001710	-3.322822	-0.886904
1	6.256466	-2.684358	0.570002
6	7.865888	-4.834999	1.304080
1	5.712593	-5.034621	1.318470
1	6.477415	-5.670322	-0.129416
1	8.052824	-5.783480	1.818399
1	8.684135	-4.671521	0.593735
1	7.912217	-4.033561	2.049956
15	-3.233166	0.446496	-1.239815
8	-4.523577	0.124795	-2.133770
8	-2.868528	1.940114	-1.650839
6	-3.477470	3.103728	-1.032859
6	-2.449916	4.222386	-1.082063
1	-3.753097	2.859554	-0.001779
1	-4.385434	3.355492	-1.592343
6	-2.945425	5.505884	-0.406104
1	-1.534540	3.868060	-0.594364
1	-2.194379	4.421389	-2.130053
6	-1.885108	6.611243	-0.420192
1	-3.857875	5.859708	-0.904612
1	-3.230825	5.286203	0.631909
1	-2.246207	7.519292	0.072561
1	-0.975216	6.286284	0.097011
1	-1.604278	6.874250	-1.446028
6	-5.348868	-1.025937	-1.793820
6	-4.685667	-2.355357	-2.132208
1	-6.263791	-0.886339	-2.375378
1	-5.599022	-0.971277	-0.728319
6	-5.611356	-3.542452	-1.838501
1	-4.391471	-2.347226	-3.188456
1	-3.762871	-2.467374	-1.552215
6	-4.937307	-4.886060	-2.131053

1	-5.905765	-3.517459	-0.781833
1	-6.532273	-3.446690	-2.429749
1	-5.618077	-5.721450	-1.939221
1	-4.614234	-4.948052	-3.176471
1	-4.059578	-5.017509	-1.490848
6	-2.052312	-2.764957	1.733257
6	-1.590527	-1.685542	2.488046
1	-0.557928	-1.618558	2.818482
1	-1.406126	-3.588043	1.442898
6	-2.561291	-0.822094	3.234928
6	-3.522377	-3.033106	1.589766
6	-4.007426	-1.075660	3.015620
6	-4.451004	-2.098709	2.265601
8	-3.921330	-3.993341	0.944028
8	-2.175004	0.026521	4.025168
1	-5.507807	-2.294325	2.113099
1	-4.680546	-0.385379	3.513767

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4 [L1=AcO^{-}, L′=BQ]

Number of imaginary frequencies : 0

Electronic energy : = -1333.9115475
Zero-point correction= 0.412023 (Hartree/Particle)
Thermal correction to Energy= 0.441407
Thermal correction to Enthalpy= 0.442351
Thermal correction to Gibbs Free Energy= 0.350177
Sum of electronic and zero-point Energies= -1333.499525
Sum of electronic and thermal Energies= -1333.470141
Sum of electronic and thermal Enthalpies= -1333.469196
Sum of electronic and thermal Free Energies= -1333.561371

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Cartesian Coordinates

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46	1.295706	-0.360188	-0.660513
6	0.700724	-2.228719	-1.375920
6	-0.737973	-2.271464	-1.130669
6	-1.314185	-2.932026	-0.104633
6	-2.773703	-2.789314	0.297745
6	-3.772774	-3.091849	-0.827049
8	1.824922	1.869381	-0.937690
7	-3.011888	-1.465378	0.916784
8	1.478391	0.455854	-2.606940
1	0.993088	-2.074388	-2.416100
1	-1.359949	-1.653192	-1.770928
1	1.293363	-3.004372	-0.888071
1	-0.690989	-3.551168	0.542039
1	-2.802551	-1.384157	1.901892

1	-2.968577	-3.500379	1.107344
1	-3.639280	-2.411096	-1.666536
1	-3.631459	-4.120305	-1.172206
1	-4.795150	-2.981573	-0.453773
6	-2.909128	-0.287108	0.216454
8	-2.997866	-0.187719	-0.998219
8	-2.700660	0.730350	1.081978
6	-2.723807	2.136006	0.615486
6	-1.557294	2.390163	-0.343524
1	-1.657865	1.791714	-1.249299
1	-1.546939	3.449528	-0.620614
1	-0.603517	2.165537	0.136438
6	-4.081643	2.442139	-0.021971
1	-4.147902	3.514515	-0.230649
1	-4.213715	1.892721	-0.954217
1	-4.890708	2.177481	0.666226
6	-2.540057	2.913474	1.918675
1	-2.527718	3.987192	1.708937
1	-3.362419	2.703368	2.609446
1	-1.594260	2.639310	2.389354
1	1.141427	-2.364103	1.272442
1	-0.292369	-0.283647	1.549839
6	3.053029	-1.341626	1.559224
6	1.419189	1.038020	1.957748
8	0.735963	1.995011	2.290972
8	3.726966	-2.361568	1.495012
6	3.654775	-0.022216	1.883435
6	2.900234	1.075915	2.061691
6	0.792099	-0.241713	1.486540
6	1.579607	-1.375110	1.328608
1	3.323270	2.042281	2.316723
1	4.735964	-0.009577	1.983128
6	1.750829	1.639559	-2.178913
6	1.939335	2.740419	-3.188320
1	0.954888	3.052057	-3.553491
1	2.434208	3.596186	-2.727220
1	2.512630	2.374570	-4.043151

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4 [L1=DBPO^{-}, L′=BQ]

Number of imaginary frequencies : 0

Electronic energy : = -2063.5259273
Zero-point correction= 0.629842 (Hartree/Particle)
Thermal correction to Energy= 0.670776
Thermal correction to Enthalpy= 0.671720
Thermal correction to Gibbs Free Energy= 0.553710
Sum of electronic and zero-point Energies= -2062.896086

Sum of electronic and thermal Energies= -2062.855151
Sum of electronic and thermal Enthalpies= -2062.854207
Sum of electronic and thermal Free Energies= -2062.972218

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Cartesian Coordinates

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46	-0.257828	-0.881124	-0.733392
6	-1.210383	-0.775211	-2.588311
6	-2.459260	-0.096681	-2.255677
6	-3.650804	-0.726655	-2.153437
6	-4.869382	-0.153855	-1.441211
6	-5.577713	0.964272	-2.217668
8	1.266141	-0.414447	1.005258
7	-4.497129	0.217775	-0.059616
8	0.997454	0.796275	-1.191727
1	-0.456154	-0.183949	-3.109219
1	-2.387527	0.949900	-1.963636
1	-1.319959	-1.782409	-2.997892
1	-3.724524	-1.760809	-2.494936
1	-4.216391	-0.579831	0.506866
1	-5.588031	-0.972080	-1.320743
1	-4.903920	1.795835	-2.417055
1	-5.947874	0.562479	-3.166231
1	-6.424155	1.341689	-1.637615
6	-3.727147	1.330296	0.201941
8	-3.794999	2.394529	-0.394418
8	-2.878834	1.052741	1.219390
6	-2.110041	2.115881	1.885949
6	-1.242694	2.888618	0.887945
1	-1.843397	3.546623	0.262513
1	-0.511311	3.480714	1.445650
1	-0.693537	2.199069	0.243887
6	-3.090930	3.032047	2.620729
1	-2.540613	3.794569	3.180950
1	-3.751860	3.531822	1.909253
1	-3.696494	2.454553	3.325964
6	-1.236855	1.322325	2.860078
1	-0.662981	2.008266	3.489996
1	-1.863965	0.695573	3.501427
1	-0.530390	0.685825	2.319907
15	1.853708	0.668714	0.103342
8	3.395391	0.409236	-0.286959
8	1.949249	2.064564	0.875338
6	2.172662	3.299697	0.144029
6	3.655960	3.612899	0.002413
1	1.664634	4.070546	0.730199
1	1.677563	3.235696	-0.831141
6	3.888085	4.960219	-0.693135
1	4.110893	3.618428	1.000476
1	4.140110	2.807770	-0.560250

6	5.376285	5.289143	-0.847657
1	3.409986	4.947255	-1.681987
1	3.392044	5.758602	-0.124278
1	5.524409	6.253430	-1.344265
1	5.871782	5.334575	0.128685
1	5.887384	4.523393	-1.441904
6	3.760809	-0.841888	-0.925060
6	4.172147	-1.880103	0.108106
1	4.588623	-0.593902	-1.596477
1	2.928291	-1.201652	-1.542800
6	4.608753	-3.199086	-0.538495
1	4.985275	-1.464340	0.716268
1	3.324620	-2.056115	0.776934
6	4.970291	-4.261519	0.503392
1	3.791386	-3.578244	-1.163974
1	5.464445	-3.019220	-1.204404
1	5.298186	-5.191630	0.027560
1	5.779353	-3.916642	1.158007
1	4.098848	-4.489655	1.124359
1	-0.226284	-3.513536	-1.424371
1	-2.461182	-2.505865	-0.755210
6	0.633052	-3.388392	0.588693
6	-1.951477	-2.280062	1.352554
8	-3.080000	-1.935822	1.688942
8	1.659184	-3.985331	0.292590
6	0.311545	-3.031212	1.993349
6	-0.883444	-2.527657	2.347628
6	-1.613066	-2.504774	-0.082656
6	-0.382371	-3.043762	-0.457246
1	-1.127765	-2.276321	3.374627
1	1.102045	-3.215043	2.713234

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4 [L1=DBPO^{-}, L′=BS]

Number of imaginary frequencies : 0
Electronic energy : = -3170.7624058
Zero-point correction= 0.792370 (Hartree/Particle)
Thermal correction to Energy= 0.844216
Thermal correction to Enthalpy= 0.845160
Thermal correction to Gibbs Free Energy= 0.702442
Sum of electronic and zero-point Energies= -3169.970035
Sum of electronic and thermal Energies= -3169.918190
Sum of electronic and thermal Enthalpies= -3169.917245
Sum of electronic and thermal Free Energies= -3170.059964

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Cartesian Coordinates

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46	-0.146118	-0.854813	-0.546109

6	-0.571541	-1.241513	-2.559633
6	-1.578444	-0.212407	-2.801542
6	-2.891447	-0.381334	-2.554656
6	-3.916260	0.728490	-2.529712
6	-3.478337	2.029224	-3.210821
7	-4.351386	0.970147	-1.140110
8	1.332438	0.461287	-1.256103
1	0.399922	-1.075281	-3.022706
1	-1.194335	0.774317	-3.046287
1	-0.915754	-2.272728	-2.657046
1	-3.249814	-1.347763	-2.202840
1	-5.301722	1.275520	-0.989551
1	-4.818395	0.358644	-3.036095
1	-2.625732	2.462956	-2.687505
1	-3.197057	1.848151	-4.252752
1	-4.294135	2.758217	-3.190759
6	-3.491291	1.194028	-0.100380
8	-2.287475	0.983410	-0.121635
8	-4.175828	1.684340	0.959961
6	-3.558588	1.659412	2.304168
6	-3.267008	0.203100	2.670095
1	-2.522459	-0.200367	1.986815
1	-2.855786	0.146478	3.680822
1	-4.181444	-0.395936	2.610439
6	-2.305873	2.538563	2.369086
1	-1.994025	2.627410	3.414508
1	-1.471199	2.126972	1.803862
1	-2.538048	3.540932	1.996212
6	-4.673175	2.234935	3.178816
1	-4.357592	2.242431	4.226143
1	-4.903042	3.261361	2.877758
1	-5.583842	1.634876	3.090710
16	0.532622	-0.663575	1.936216
16	-1.461042	-2.643828	0.127191
6	0.355446	-2.490427	2.255024
6	-1.076211	-2.890365	1.932119
1	1.085686	-3.031805	1.647030
1	0.573837	-2.642190	3.315710
1	-1.287136	-3.938677	2.154726
1	-1.797739	-2.254340	2.452281
8	-0.113122	-0.009552	3.126816
6	2.330806	-0.556496	2.087317
6	3.145424	-1.037019	1.061088
6	2.853687	0.062970	3.217918
6	4.528222	-0.924953	1.197490
1	2.707194	-1.441243	0.154221
6	4.239585	0.175792	3.337353
1	2.175013	0.459941	3.965798
6	5.074273	-0.322422	2.334276
1	5.177696	-1.285279	0.405242

1	4.666694	0.661033	4.209837
1	6.151994	-0.226823	2.429529
8	-2.953366	-2.701945	-0.033122
6	-0.773880	-4.197209	-0.515029
6	-1.626368	-5.298328	-0.598039
6	0.560636	-4.265966	-0.916335
6	-1.115554	-6.507163	-1.071760
1	-2.668612	-5.189621	-0.313792
6	1.061374	-5.483695	-1.379913
1	1.180118	-3.373075	-0.890331
6	0.225629	-6.600843	-1.454991
1	-1.765533	-7.373568	-1.148294
1	2.097611	-5.553861	-1.696309
1	0.616614	-7.543428	-1.826283
15	1.519941	1.778884	-0.458169
8	0.875796	1.918273	0.883640
8	1.091451	2.965716	-1.491224
8	3.128065	1.982941	-0.285543
6	4.010544	1.660533	-1.366841
6	5.428124	1.986838	-0.922049
1	3.738061	2.237272	-2.261681
1	3.911642	0.594949	-1.611381
6	6.479217	1.591390	-1.964204
1	5.494398	3.060187	-0.704729
1	5.618134	1.464515	0.023362
6	7.907706	1.907521	-1.510299
1	6.391792	0.517042	-2.179428
1	6.271375	2.107632	-2.911313
1	8.645484	1.614844	-2.264707
1	8.030844	2.979545	-1.319309
1	8.150338	1.378662	-0.581159
6	0.482875	4.155289	-0.939852
6	-1.030992	4.058786	-1.063676
1	0.881358	5.000248	-1.512803
1	0.772365	4.274942	0.109157
6	-1.778266	5.227136	-0.414469
1	-1.286955	3.999129	-2.129354
1	-1.342877	3.117955	-0.600233
6	-3.299339	5.083055	-0.546160
1	-1.505680	5.281974	0.647879
1	-1.457398	6.177560	-0.863544
1	-3.826291	5.918623	-0.072801
1	-3.599476	5.053408	-1.600374
1	-3.648881	4.156513	-0.077523

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4 [L1=AcO^{-}, L′=BS]

Number of imaginary frequencies : 0 Electronic energy : = -2441.1570019

Zero-point correction= 0.575289 (Hartree/Particle)
Thermal correction to Energy= 0.615033
Thermal correction to Enthalpy= 0.615977
Thermal correction to Gibbs Free Energy= 0.502122
Sum of electronic and zero-point Energies= -2440.581713
Sum of electronic and thermal Energies= -2440.541969
Sum of electronic and thermal Enthalpies= -2440.541025
Sum of electronic and thermal Free Energies= -2440.654879

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Cartesian Coordinates

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46	-0.671775	-0.860463	1.066715
6	0.565704	-1.429817	2.644909
6	1.663739	-0.464302	2.561178
6	2.844010	-0.692533	1.956585
6	3.940651	0.339876	1.786547
6	4.034813	1.373663	2.916812
8	-1.568422	2.055269	0.422032
7	3.857167	1.010658	0.472315
8	-1.069747	0.804192	2.244583
1	-0.102550	-1.286461	3.494654
1	1.453040	0.519789	2.966208
1	0.843270	-2.477310	2.508608
1	3.025497	-1.659324	1.486796
1	4.434638	0.664932	-0.278144
1	4.896202	-0.196712	1.749163
1	3.144983	2.003183	2.942903
1	4.141584	0.867707	3.880475
1	4.904191	2.017910	2.755747
6	2.795498	1.786917	0.097937
8	1.886313	2.133079	0.836943
8	2.934700	2.125021	-1.211251
6	2.003538	3.068995	-1.859878
6	0.626625	2.425404	-1.994395
1	0.186233	2.199436	-1.024405
1	-0.053235	3.108193	-2.513589
1	0.678504	1.508315	-2.586753
6	1.954413	4.388791	-1.083871
1	1.407293	5.131757	-1.672648
1	1.453226	4.259770	-0.125665
1	2.967858	4.765437	-0.910722
6	2.655879	3.274694	-3.228721
1	2.047955	3.954680	-3.832455
1	3.658221	3.700495	-3.122401
1	2.737674	2.322958	-3.763251
6	-1.232341	1.930840	1.605921
6	-0.921730	3.155742	2.449986
1	0.159928	3.312932	2.380852
1	-1.433862	4.031774	2.048280
1	-1.183860	2.997116	3.498315

16	-2.133573	-0.323001	-0.898995
16	-0.121031	-2.784465	-0.122709
6	-2.570123	-2.090935	-1.279219
6	-1.271680	-2.817889	-1.595546
1	-3.089725	-2.510596	-0.412503
1	-3.235590	-2.085264	-2.146929
1	-1.414276	-3.883594	-1.792062
1	-0.757215	-2.342008	-2.433410
8	-0.079680	-4.151324	0.498049
6	1.459992	-2.471879	-0.942536
6	1.691426	-1.224976	-1.526932
6	2.441607	-3.456925	-0.869672
6	2.945413	-0.974694	-2.082769
1	0.917252	-0.462763	-1.543664
6	3.694626	-3.188555	-1.426296
1	2.218747	-4.399885	-0.380724
6	3.942758	-1.954155	-2.032125
1	3.143197	-0.001167	-2.517576
1	4.474803	-3.942596	-1.383649
1	4.919876	-1.751214	-2.461429
8	-1.624493	0.211702	-2.214576
6	-3.794685	0.279580	-0.559767
6	-4.225398	0.356700	0.764368
6	-4.600737	0.657866	-1.631159
6	-5.527719	0.790986	1.012471
1	-3.543426	0.119549	1.576016
6	-5.897681	1.099204	-1.365802
1	-4.202367	0.628274	-2.640832
6	-6.361078	1.157171	-0.048567
1	-5.884082	0.862524	2.035593
1	-6.542745	1.402922	-2.184874
1	-7.370570	1.503273	0.153227

4' mode **u**

Number of imaginary frequencies : 0

Electronic energy : = -2670.2773574
Zero-point correction= 0.639011 (Hartree/Particle)
Thermal correction to Energy= 0.684241
Thermal correction to Enthalpy= 0.685186
Thermal correction to Gibbs Free Energy= 0.556526
Sum of electronic and zero-point Energies= -2669.638347
Sum of electronic and thermal Energies= -2669.593116
Sum of electronic and thermal Enthalpies= -2669.592172
Sum of electronic and thermal Free Energies= -2669.720831

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Cartesian Coordinates

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6	1.497620	4.154675	0.398752
6	2.282618	3.015679	0.209471
6	3.270832	2.958307	-0.779201
6	3.471364	4.081507	-1.584235
6	2.695630	5.229649	-1.407355
6	1.713592	5.267222	-0.415172
16	1.826625	1.582380	1.218047
8	1.183722	2.096117	2.480762
6	3.496275	0.877137	1.666659
6	3.683835	-0.559430	1.199576
16	3.761260	-0.634287	-0.652293
8	5.108716	-0.021485	-1.004665
6	3.874405	-2.438565	-0.764984
6	5.133430	-3.020502	-0.899369
6	5.221939	-4.409662	-1.002860
6	4.061902	-5.188589	-0.975512
6	2.806859	-4.584204	-0.856286
6	2.699052	-3.195662	-0.758577
46	0.555346	-0.056198	0.129105
6	0.397120	0.928905	-1.672292
6	-0.832281	1.701712	-1.465779
6	-2.048187	1.280627	-1.862776
6	-3.381884	1.877419	-1.488906
6	-3.306380	3.134185	-0.622730
8	0.661807	-1.030607	2.228741
6	-0.196504	-0.668865	3.056374
6	0.184391	-0.375018	4.480330
8	-0.499582	-1.626040	-0.802573
8	-2.282671	-1.216169	0.515657
7	-4.174637	0.851361	-0.780360
8	-1.450651	-0.469853	2.767328
1	2.878076	-1.204893	1.554111
1	4.651262	-0.938739	1.544389
1	4.274814	1.539215	1.282165
1	3.474368	0.938825	2.757952
1	1.721783	-2.722745	-0.690855
1	6.011098	-2.381529	-0.934832
1	1.906927	-5.191850	-0.849905
1	6.193807	-4.882942	-1.108453
1	4.134828	-6.269093	-1.058580
1	3.891986	2.079793	-0.930192
1	0.746927	4.163156	1.182094
1	4.239829	4.052751	-2.350384
1	1.114659	6.161389	-0.272013
1	2.858859	6.095638	-2.041665
1	1.305338	1.514782	-1.813935
1	-0.734035	2.623706	-0.894371
1	0.312118	0.118796	-2.397591
1	-2.124754	0.365081	-2.446532

1	-3.730068	0.495554	0.059374
1	-3.940608	2.093611	-2.405665
1	-2.794156	2.928724	0.323986
1	-2.760003	3.929278	-1.138781
1	-4.313359	3.492955	-0.395504
1	1.004783	-1.025909	4.786944
1	0.538907	0.661515	4.494935
1	-0.668219	-0.475181	5.152639
6	-4.786408	-0.135520	-1.526333
8	-4.787256	-0.167690	-2.744185
8	-5.382732	-1.133047	-0.821989
6	-6.188114	-0.949411	0.394727
6	-7.190848	0.186157	0.177864
1	-6.674714	1.141506	0.056217
1	-7.794752	-0.005200	-0.713846
1	-7.857693	0.262097	1.042440
6	-5.317357	-0.719047	1.637281
1	-4.456246	-1.389850	1.625951
1	-4.956561	0.310650	1.700772
1	-5.910158	-0.909797	2.537556
6	-6.903282	-2.299157	0.502366
1	-6.173957	-3.103483	0.636058
1	-7.586632	-2.301368	1.356987
1	-7.472920	-2.498299	-0.408911
1	-1.679325	-0.730724	1.790375
6	-1.718470	-1.792927	-0.453923
6	-2.540970	-2.717259	-1.328027
1	-1.911253	-3.493756	-1.765864
1	-3.366426	-3.145823	-0.759798
1	-2.976069	-2.127758	-2.142779

TS[4'-6] mode **u**

Number of imaginary frequencies : 1
The smallest frequency is : -291.8366 cm(-1)

Electronic energy : = -2670.2190675
Zero-point correction= 0.636795 (Hartree/Particle)
Thermal correction to Energy= 0.682480
Thermal correction to Enthalpy= 0.683424
Thermal correction to Gibbs Free Energy= 0.553344
Sum of electronic and zero-point Energies= -2669.582272
Sum of electronic and thermal Energies= -2669.536587
Sum of electronic and thermal Enthalpies= -2669.535643
Sum of electronic and thermal Free Energies= -2669.665723

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Cartesian Coordinates

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6	1.291025	4.370097	0.720397
6	1.903752	3.222567	0.226534
6	2.728918	3.249684	-0.902493
6	2.949272	4.471945	-1.535392
6	2.338829	5.637774	-1.056281
6	1.514458	5.586794	0.068688
16	1.466656	1.629909	0.983194
8	0.717673	1.949590	2.269498
6	3.175461	1.088588	1.502081
6	3.417196	-0.396230	1.287657
16	3.543733	-0.747646	-0.539336
8	4.579520	0.239522	-1.065239
6	4.356299	-2.363342	-0.343584
6	5.694819	-2.481853	-0.710477
6	6.313295	-3.729641	-0.604167
6	5.591592	-4.831985	-0.139918
6	4.246542	-4.693849	0.217592
6	3.611328	-3.455556	0.111369
46	0.512920	0.300369	-0.545738
6	-0.812108	2.306925	-1.594881
6	-1.785531	2.581604	-0.670793
6	-2.580915	1.505803	-0.159672
6	-3.395392	1.642163	1.107812
6	-2.573405	1.423777	2.374436
8	0.717461	-2.238884	1.312735
6	-0.112920	-1.756371	2.073425
6	0.227725	-1.249752	3.455895
8	-0.712671	-0.852282	-1.971577
8	-2.266823	-1.743159	-0.591863
7	-4.425089	0.592982	0.918313
8	-1.387551	-1.565718	1.763500
1	2.619228	-1.037896	1.669373
1	4.376573	-0.676261	1.731876
1	3.910800	1.671702	0.943012
1	3.216371	1.358886	2.561150
1	2.567939	-3.333921	0.389480
1	6.222052	-1.603920	-1.072237
1	3.687620	-5.553557	0.576137
1	7.356745	-3.841068	-0.885587
1	6.075394	-5.801495	-0.061025
1	3.191983	2.336988	-1.273132
1	0.657177	4.295158	1.598003
1	3.594996	4.513627	-2.407559
1	1.044039	6.492396	0.441246
1	2.508152	6.583833	-1.562291
1	-0.112968	3.079052	-1.901570
1	-1.865950	3.563910	-0.212866
1	-0.863938	1.420525	-2.217854
1	-2.078496	0.539949	-0.205253
1	-4.695919	-0.031087	1.660164

1	-3.897691	2.618721	1.128591
1	-2.182667	0.404528	2.395762
1	-1.714180	2.098361	2.389049
1	-3.186227	1.606144	3.263625
1	1.142756	-1.723014	3.814829
1	0.384040	-0.166515	3.375668
1	-0.593308	-1.425276	4.154817
6	-4.589799	0.305008	-0.380379
8	-3.908775	1.021061	-1.187991
8	-5.386372	-0.593719	-0.886750
6	-6.097617	-1.668941	-0.126812
6	-7.255328	-1.036835	0.644064
1	-6.912021	-0.340167	1.413233
1	-7.920234	-0.496833	-0.035324
1	-7.830117	-1.824801	1.139273
6	-5.111468	-2.446347	0.750003
1	-4.162858	-2.579077	0.222587
1	-4.906192	-1.964842	1.711076
1	-5.544257	-3.424112	0.979241
6	-6.601654	-2.549175	-1.269315
1	-5.756463	-2.970959	-1.818818
1	-7.206261	-3.366467	-0.866864
1	-7.213708	-1.965375	-1.961529
1	-1.582512	-1.690586	0.759450
6	-1.774194	-1.495400	-1.737303
6	-2.589206	-1.965433	-2.934574
1	-2.012778	-1.899016	-3.857924
1	-2.933398	-2.990688	-2.772634
1	-3.474172	-1.324322	-3.013140

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forward intermediate of IRC run in mode **u**

Number of imaginary frequencies : 0 Electronic energy : = -2670.2404267
Zero-point correction= 0.638206 (Hartree/Particle)
Thermal correction to Energy= 0.684156
Thermal correction to Enthalpy= 0.685101
Thermal correction to Gibbs Free Energy= 0.553823
Sum of electronic and zero-point Energies= -2669.602220
Sum of electronic and thermal Energies= -2669.556270
Sum of electronic and thermal Enthalpies= -2669.555326
Sum of electronic and thermal Free Energies= -2669.686604

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Cartesian Coordinates

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6	1.032259	4.396424	1.432201
6	1.339826	3.497595	0.414104
6	1.557185	3.922897	-0.898764
6	1.481319	5.284496	-1.188323

6	1.171525	6.201562	-0.176924
6	0.946030	5.758175	1.127557
16	1.361333	1.717287	0.798087
8	0.985054	1.606346	2.269955
6	3.192674	1.481107	0.765337
6	3.565910	0.007611	0.856299
16	3.427356	-0.791347	-0.822884
8	4.331415	0.033557	-1.724350
6	4.359129	-2.290127	-0.356545
6	5.640792	-2.448833	-0.879819
6	6.357866	-3.607418	-0.573468
6	5.789032	-4.588007	0.242807
6	4.498574	-4.415472	0.753122
6	3.767021	-3.265508	0.450840
46	0.367771	0.520599	-0.759601
6	-2.161515	3.574666	-1.554646
6	-3.185798	2.846395	-1.105526
6	-2.971152	1.497510	-0.528186
6	-3.279157	1.336951	0.964687
6	-2.138993	1.693157	1.896287
8	0.941572	-1.940382	1.492943
6	-0.028823	-1.587355	2.139714
6	0.030521	-1.197234	3.594515
8	-0.719355	-0.554828	-2.276365
8	-1.828317	-1.849486	-0.795096
7	-3.675751	-0.099086	1.008913
8	-1.251878	-1.458629	1.610327
1	2.931457	-0.555412	1.546212
1	4.615135	-0.086611	1.149390
1	3.582869	1.923389	-0.156887
1	3.561970	2.040290	1.630776
1	2.764216	-3.119661	0.840546
1	6.047150	-1.668208	-1.516480
1	4.057274	-5.181092	1.385321
1	7.358596	-3.745409	-0.973730
1	6.348288	-5.489498	0.477426
1	1.759560	3.190782	-1.677136
1	0.860212	4.016314	2.434310
1	1.654086	5.629449	-2.203635
1	0.702507	6.471376	1.910116
1	1.102072	7.260288	-0.409732
1	-2.299937	4.592841	-1.904931
1	-4.200503	3.241183	-1.076161
1	-1.150468	3.174504	-1.568109
1	-1.964715	1.111639	-0.756335
1	-3.119125	-0.746604	1.567813
1	-4.177212	1.918802	1.215701
1	-1.265570	1.070538	1.718016
1	-1.848149	2.732830	1.725696
1	-2.442703	1.590076	2.942141

1	0.831651	-1.747793	4.089714
1	0.272057	-0.129228	3.618650
1	-0.923068	-1.365478	4.099663
6	-4.078192	-0.445475	-0.219078
8	-3.940107	0.499043	-1.114058
8	-4.678279	-1.508761	-0.617217
6	-5.132401	-2.653529	0.256651
6	-6.152077	-2.117100	1.257467
1	-5.697102	-1.420980	1.964651
1	-6.975427	-1.614605	0.742143
1	-6.562038	-2.958246	1.823793
6	-3.928816	-3.327870	0.907460
1	-3.133194	-3.465974	0.174453
1	-3.520014	-2.757611	1.743693
1	-4.251151	-4.297233	1.299069
6	-5.778039	-3.566082	-0.782324
1	-5.033435	-3.893949	-1.511803
1	-6.195606	-4.445735	-0.285306
1	-6.581994	-3.045707	-1.309330
1	-1.256989	-1.595497	0.585907
6	-1.518881	-1.479438	-1.973384
6	-2.229705	-2.202559	-3.108270
1	-1.862580	-1.872663	-4.080346
1	-2.088122	-3.282034	-2.999411
1	-3.303775	-2.002197	-3.031685

4' mode **v**

Number of imaginary frequencies : 0

Electronic energy : = -1333.8949244
Zero-point correction= 0.411684 (Hartree/Particle)
Thermal correction to Energy= 0.440933
Thermal correction to Enthalpy= 0.441877
Thermal correction to Gibbs Free Energy= 0.348905
Sum of electronic and zero-point Energies= -1333.483241
Sum of electronic and thermal Energies= -1333.453991
Sum of electronic and thermal Enthalpies= -1333.453047
Sum of electronic and thermal Free Energies= -1333.546019

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Cartesian Coordinates

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46	1.732966	-0.064002	-0.827615
6	0.144970	-1.063538	-1.924908
6	-0.416921	0.033159	-1.259891
6	-1.062590	-0.148650	0.049133
6	-1.069034	1.059590	1.014591
6	-0.108440	0.918766	2.188490

8	2.133569	1.932893	-0.071468
7	-2.486947	1.094090	1.449836
1	0.372647	-0.993951	-2.985281
1	-0.568927	0.992309	-1.745087
1	0.067752	-2.072316	-1.523673
1	-0.791305	-1.087808	0.536056
1	-0.835116	1.966804	0.443677
1	-0.250789	-0.029807	2.716612
1	0.915007	0.985617	1.812802
1	-0.255812	1.741429	2.896392
6	-3.259854	0.358091	0.671362
8	-2.636839	-0.382867	-0.181647
8	-4.553417	0.407665	0.793650
6	-5.492107	-0.432444	-0.042212
6	-5.320742	-0.051082	-1.510341
1	-4.345210	-0.350442	-1.894706
1	-6.093648	-0.556623	-2.096481
1	-5.442978	1.027525	-1.642346
6	-5.214883	-1.907471	0.237247
1	-5.981680	-2.509709	-0.258546
1	-4.239601	-2.214233	-0.142343
1	-5.264585	-2.109765	1.310933
6	-6.850358	0.000979	0.500095
1	-7.640374	-0.540775	-0.026615
1	-6.930285	-0.218477	1.567980
1	-7.003253	1.072703	0.348725
1	-2.873215	1.801168	2.058780
6	3.786421	-0.810667	-0.441293
6	2.956408	-1.870442	-0.855961
1	4.486293	-0.337869	-1.123784
1	3.007847	-2.273738	-1.863190
6	4.022835	-0.546571	0.992829
6	2.235785	-2.708589	0.131885
6	3.244610	-1.375090	1.964495
1	3.407226	-1.135398	3.011966
6	2.437336	-2.374924	1.570361
8	1.487662	-3.632221	-0.196255
8	4.833413	0.279406	1.400299
1	1.895367	-3.001552	2.274188
6	1.459180	2.990335	-0.361500
8	0.292394	3.039763	-0.800152
6	2.225752	4.291215	-0.113243
1	2.690482	4.270639	0.876538
1	3.036743	4.371576	-0.844649
1	1.565183	5.155037	-0.208754

TS[4'-6] mode **v**

Number of imaginary frequencies : 1
The smallest frequency is : -173.7359 cm(-1)

Electronic energy : = -1333.894429
Zero-point correction= 0.411056 (Hartree/Particle)
Thermal correction to Energy= 0.439834
Thermal correction to Enthalpy= 0.440779
Thermal correction to Gibbs Free Energy= 0.349263
Sum of electronic and zero-point Energies= -1333.483373
Sum of electronic and thermal Energies= -1333.454595
Sum of electronic and thermal Enthalpies= -1333.453650
Sum of electronic and thermal Free Energies= -1333.545166

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Cartesian Coordinates

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46	1.741176	-0.082156	-0.808345
6	0.203151	-1.130774	-1.896505
6	-0.397456	-0.005225	-1.299623
6	-1.010519	-0.119585	0.003340
6	-1.120133	1.122848	0.902155
6	-0.185124	1.065980	2.109456
8	2.195221	1.888879	-0.029150
7	-2.537538	1.138866	1.318593
1	0.445061	-1.111720	-2.955953
1	-0.528240	0.932171	-1.830569
1	0.105602	-2.121198	-1.455620
1	-0.801927	-1.047923	0.534753
1	-0.893363	2.008758	0.299077
1	-0.326412	0.141490	2.678951
1	0.849220	1.139587	1.767521
1	-0.380444	1.916891	2.770972
6	-3.317801	0.355365	0.581529
8	-2.734242	-0.428006	-0.236292
8	-4.613174	0.438319	0.754245
6	-5.584089	-0.426732	0.002040
6	-5.465204	-0.126122	-1.490880
1	-4.502580	-0.448409	-1.889136
1	-6.258222	-0.658468	-2.024232
1	-5.588422	0.944835	-1.675189
6	-5.317128	-1.891480	0.343439
1	-6.105013	-2.507861	-0.099176
1	-4.356008	-2.226185	-0.048318
1	-5.335690	-2.040164	1.426960
6	-6.920955	0.046961	0.565900
1	-7.734015	-0.511945	0.094979
1	-6.965939	-0.116583	1.645909
1	-7.069122	1.111492	0.366069
1	-2.930447	1.868332	1.895644
6	3.810259	-0.809768	-0.446527

6	2.988142	-1.885793	-0.822234
1	4.490035	-0.340129	-1.151125
1	3.022920	-2.308399	-1.822074
6	4.066314	-0.509772	0.979869
6	2.293571	-2.710878	0.197672
6	3.309960	-1.320210	1.982248
1	3.482811	-1.051723	3.020873
6	2.508660	-2.338378	1.624019
8	1.558746	-3.653109	-0.101450
8	4.878224	0.330555	1.349803
1	1.982538	-2.952350	2.350365
6	1.540777	2.944156	-0.379812
8	0.430062	2.981382	-0.941281
6	2.261224	4.248069	-0.032726
1	2.596501	4.226743	1.008164
1	3.158047	4.336539	-0.654430
1	1.611190	5.107212	-0.207844

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forward intermediate of IRC run in mode **v**

Number of imaginary frequencies : 0

Electronic energy : = -1333.9196059
Zero-point correction= 0.410628 (Hartree/Particle)
Thermal correction to Energy= 0.440396
Thermal correction to Enthalpy= 0.441340
Thermal correction to Gibbs Free Energy= 0.347077
Sum of electronic and zero-point Energies= -1333.508977
Sum of electronic and thermal Energies= -1333.479210
Sum of electronic and thermal Enthalpies= -1333.478265
Sum of electronic and thermal Free Energies= -1333.572529

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Cartesian Coordinates

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46	1.384365	-0.447059	-0.269799
6	0.194458	-2.234566	-0.698910
6	-0.688079	-1.148900	-0.508926
6	-0.630753	-0.441495	0.706809
6	-1.370261	0.869735	0.919983
6	-0.788724	1.655058	2.094716
8	2.098696	1.412268	0.524080
7	-2.785891	0.595935	1.178387
1	0.282448	-2.679848	-1.685717
1	-1.208412	-0.694514	-1.347636
1	0.491251	-2.869340	0.134318
1	-0.350181	-0.983978	1.612526
1	-1.298994	1.458138	0.001738
1	-0.916560	1.098550	3.032617

1	0.279449	1.815629	1.943292
1	-1.292413	2.620310	2.194945
6	-3.665367	0.293457	0.179003
8	-3.364670	0.243549	-1.006239
8	-4.890709	0.069324	0.706930
6	-6.027999	-0.284385	-0.156138
6	-6.318675	0.857799	-1.133813
1	-5.499440	0.982656	-1.841838
1	-7.238238	0.641002	-1.686732
1	-6.460301	1.794532	-0.586036
6	-5.746903	-1.607786	-0.874399
1	-6.643225	-1.928946	-1.414369
1	-4.926322	-1.499310	-1.583618
1	-5.489414	-2.383580	-0.146346
6	-7.168271	-0.443994	0.851059
1	-8.092206	-0.714254	0.331616
1	-6.933133	-1.228738	1.575914
1	-7.333632	0.490825	1.394212
1	-3.119620	0.549218	2.129742
6	3.490892	-0.458370	-1.279938
6	3.245235	-1.712504	-0.763559
1	3.296337	-0.208088	-2.318911
1	2.881417	-2.530858	-1.376186
6	4.340941	0.519953	-0.530063
6	3.715090	-2.091128	0.605966
6	4.734831	0.147767	0.853993
1	5.281258	0.907752	1.403009
6	4.458571	-1.061615	1.371681
8	3.490570	-3.207026	1.060340
8	4.754026	1.535781	-1.068733
1	4.760673	-1.350106	2.373933
6	1.673104	2.342194	-0.286961
8	0.870503	2.136368	-1.206592
6	2.276888	3.712093	-0.037356
1	2.256755	3.955290	1.028452
1	3.326216	3.675973	-0.350042
1	1.749540	4.472888	-0.614003

4' mode **w**

Number of imaginary frequencies : 0
Electronic energy : = -3399.8947316
Zero-point correction= 0.855229 (Hartree/Particle)
Thermal correction to Energy= 0.912880
Thermal correction to Enthalpy= 0.913824
Thermal correction to Gibbs Free Energy= 0.756913
Sum of electronic and zero-point Energies= -3399.039503
Sum of electronic and thermal Energies= -3398.981852

Sum of electronic and thermal Enthalpies= -3398.980908
Sum of electronic and thermal Free Energies= -3399.137818

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Cartesian Coordinates

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6	3.111540	4.956521	0.380314
6	3.087280	3.806333	-0.404584
6	3.237041	3.853872	-1.793894
6	3.433361	5.092322	-2.403382
6	3.465528	6.257805	-1.630748
6	3.304559	6.190434	-0.245663
16	2.789413	2.232790	0.438552
8	2.834261	2.482685	1.923502
6	4.370443	1.391984	-0.018469
6	4.399041	-0.078850	0.368410
16	3.495452	-1.090705	-0.904807
8	4.291071	-0.911525	-2.184283
6	3.942280	-2.701126	-0.183626
6	4.828135	-3.509732	-0.892170
6	5.135639	-4.775956	-0.387725
6	4.560733	-5.214315	0.807202
6	3.667536	-4.392106	1.501437
6	3.341502	-3.130238	1.004261
46	0.967837	0.984773	-0.267942
6	0.090202	2.429568	-1.458868
6	-0.894255	2.951070	-0.510748
6	-2.173546	2.524804	-0.460661
6	-3.203046	2.876139	0.586755
6	-2.612453	3.468037	1.869243
8	1.557243	-0.463893	1.560226
6	1.237904	-0.171026	2.731642
6	2.275763	-0.149788	3.822845
8	-0.548766	-0.304362	-1.018085
15	-1.493726	-0.896785	0.035640
8	-1.693351	-0.157818	1.348368
7	-3.994771	1.684944	0.929662
8	0.038885	0.155145	3.103078
8	-1.025452	-2.415600	0.350161
6	-0.061974	-3.064797	-0.513067
6	0.179922	-4.465160	0.022122
6	1.129726	-5.268960	-0.874457
6	1.387801	-6.679546	-0.338058
8	-2.969432	-1.009240	-0.601400
6	-3.157694	-1.498917	-1.948843
6	-4.582231	-1.178267	-2.368626
6	-4.898997	-1.680603	-3.781493
6	-6.336823	-1.355378	-4.198386
1	3.945375	-0.270915	1.340685
1	5.432211	-0.436995	0.353455
1	4.528320	1.513518	-1.094237

1	5.128360	1.963364	0.526287
1	2.625643	-2.491460	1.511465
1	5.252275	-3.140025	-1.821111
1	3.211271	-4.739888	2.423584
1	5.821738	-5.420194	-0.929784
1	4.798577	-6.201137	1.192839
1	3.191419	2.946468	-2.389956
1	2.987156	4.870784	1.454846
1	3.554165	5.146950	-3.480748
1	3.328329	7.097213	0.350891
1	3.612482	7.219651	-2.112473
1	0.861708	-2.478699	-0.531079
1	-0.449477	-3.104135	-1.538537
1	0.594131	-4.389931	1.035026
1	-0.783937	-4.981610	0.111355
1	0.708002	-5.332279	-1.886796
1	2.083227	-4.736662	-0.969037
1	2.074907	-7.232876	-0.986438
1	1.834680	-6.639173	0.661084
1	0.456760	-7.253169	-0.264994
1	-2.975377	-2.582536	-1.960242
1	-2.427472	-1.018778	-2.610911
1	-5.272574	-1.620542	-1.641788
1	-4.737706	-0.095910	-2.307115
1	-4.198050	-1.229499	-4.497662
1	-4.735332	-2.766224	-3.836868
1	-6.515942	-0.275257	-4.169324
1	-6.551639	-1.708818	-5.212362
1	-7.056376	-1.824756	-3.518194
1	0.855606	3.133932	-1.778621
1	-0.530324	3.664178	0.226827
1	-0.320166	1.845268	-2.282648
1	-2.521204	1.819059	-1.211319
1	-3.439796	0.925354	1.316154
1	-3.914401	3.583608	0.145056
1	-1.894356	2.773190	2.317113
1	-2.096961	4.411980	1.668644
1	-3.410107	3.661676	2.590897
1	2.973734	-0.979564	3.686654
1	2.830234	0.787922	3.712143
1	1.818827	-0.190241	4.811761
6	-5.013088	1.320356	0.078870
8	-5.318477	1.953002	-0.920139
8	-5.704097	0.192401	0.375799
6	-5.944344	-0.383427	1.703936
6	-6.349893	0.704058	2.703298
1	-5.524065	1.386934	2.907726
1	-7.192373	1.281654	2.310728
1	-6.658155	0.238068	3.644580
6	-4.741347	-1.200321	2.186640

1	-4.394317	-1.861189	1.390169
1	-3.897311	-0.582250	2.494837
1	-5.039257	-1.806799	3.048446
6	-7.127099	-1.317489	1.423764
1	-6.844121	-2.071449	0.683481
1	-7.438606	-1.826754	2.340912
1	-7.972780	-0.748646	1.028314
1	-0.655966	0.041688	2.328042

TS[4'-6] mode **u**

Number of imaginary frequencies : 1
The smallest frequency is : -254.5267 cm(-1)

Electronic energy : = -3399.8462476
Zero-point correction= 0.854560 (Hartree/Particle)
Thermal correction to Energy= 0.912237
Thermal correction to Enthalpy= 0.913182
Thermal correction to Gibbs Free Energy= 0.755641
Sum of electronic and zero-point Energies= -3398.991687
Sum of electronic and thermal Energies= -3398.934010
Sum of electronic and thermal Enthalpies= -3398.933066
Sum of electronic and thermal Free Energies= -3399.090607

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Cartesian Coordinates

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6	2.459791	5.209771	-0.024928
6	2.591457	3.941696	-0.581922
6	2.853283	3.756386	-1.942723
6	3.004824	4.878336	-2.755836
6	2.877023	6.162586	-2.212629
6	2.604854	6.326819	-0.853481
16	2.308019	2.491776	0.474777
8	2.079098	3.008661	1.885537
6	4.041147	1.830268	0.435756
6	4.106070	0.353489	0.788944
16	3.499376	-0.666069	-0.650645
8	4.293703	-0.187368	-1.856845
6	4.249967	-2.229230	-0.086815
6	5.259823	-2.785903	-0.869356
6	5.785272	-4.029871	-0.510858
6	5.300294	-4.698092	0.615548
6	4.284316	-4.126439	1.388099
6	3.742325	-2.889295	1.037542
46	0.812462	1.052717	-0.363867
6	-0.560098	2.657786	-1.789270
6	-1.492301	3.157647	-0.914580
6	-2.270507	2.205772	-0.181938

6	-2.560905	2.373229	1.288505
6	-1.345489	2.189998	2.186835
8	1.366410	-0.930288	1.985425
6	1.010250	-0.500521	3.081870
6	1.941502	0.246993	4.004490
8	-0.817822	-0.471251	-0.696202
15	-1.573883	-1.406420	0.240277
8	-1.930227	-0.972795	1.655565
7	-3.621825	1.361684	1.527447
8	-0.225386	-0.590433	3.541143
8	-0.853777	-2.851300	0.278337
6	0.314748	-3.098073	-0.541417
6	0.767022	-4.526568	-0.289088
6	1.881964	-4.960333	-1.248753
6	2.385593	-6.376961	-0.959201
8	-3.037411	-1.682173	-0.433693
6	-3.133138	-1.943778	-1.844534
6	-4.595590	-1.812720	-2.240342
6	-4.832427	-2.043785	-3.736415
6	-6.309027	-1.904634	-4.119471
1	3.479060	0.079983	1.638755
1	5.144615	0.064533	0.970258
1	4.449496	1.993233	-0.565503
1	4.582682	2.444544	1.161852
1	2.934396	-2.446635	1.611909
1	5.608836	-2.242046	-1.742202
1	3.903121	-4.650573	2.259858
1	6.570816	-4.477590	-1.113038
1	5.706913	-5.667786	0.887572
1	2.930562	2.750778	-2.350709
1	2.249063	5.301118	1.036020
1	3.216634	4.751721	-3.813440
1	2.505242	7.324272	-0.435015
1	2.986963	7.033035	-2.852726
1	1.096281	-2.380647	-0.280855
1	0.058017	-2.949824	-1.597642
1	1.109937	-4.610920	0.749360
1	-0.097864	-5.194079	-0.393373
1	1.513071	-4.903469	-2.282023
1	2.721300	-4.260034	-1.181052
1	3.177995	-6.668348	-1.656335
1	2.796703	-6.440311	0.053839
1	1.576174	-7.111919	-1.040359
1	-2.756303	-2.954851	-2.053337
1	-2.511073	-1.226296	-2.392493
1	-5.183219	-2.532264	-1.654230
1	-4.942155	-0.813474	-1.952206
1	-4.233571	-1.326894	-4.313979
1	-4.470481	-3.042017	-4.017549
1	-6.684558	-0.905347	-3.871568

1	-6.464044	-2.065220	-5.191181
1	-6.925276	-2.632939	-3.579523
1	0.170146	3.310346	-2.257176
1	-1.456404	4.194605	-0.589830
1	-0.682552	1.668163	-2.223696
1	-2.005192	1.184668	-0.438996
1	-3.277643	0.462829	1.891341
1	-3.007926	3.362073	1.456438
1	-0.891578	1.218013	2.014944
1	-0.593065	2.953053	1.976698
1	-1.637992	2.257854	3.238481
1	2.923758	-0.231292	4.012121
1	2.053692	1.257891	3.592205
1	1.541901	0.310890	5.017259
6	-4.365104	1.289828	0.394227
8	-3.996175	2.020281	-0.586230
8	-5.422896	0.547748	0.230205
6	-6.170281	-0.175079	1.314954
6	-6.651129	0.847148	2.342263
1	-5.813466	1.311449	2.865326
1	-7.248101	1.626687	1.860025
1	-7.278891	0.338955	3.080195
6	-5.307579	-1.281823	1.919024
1	-4.789374	-1.837233	1.136390
1	-4.560040	-0.906684	2.619383
1	-5.960649	-1.963347	2.472773
6	-7.333770	-0.765206	0.519944
1	-6.963215	-1.463014	-0.235072
1	-8.005308	-1.301927	1.195692
1	-7.897649	0.025340	0.017981
1	-0.849556	-0.896120	2.801334

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forward intermediate of IRC run in mode **w**

Number of imaginary frequencies : 0

Electronic energy : = -3399.8678556
Zero-point correction= 0.856252 (Hartree/Particle)
Thermal correction to Energy= 0.913672
Thermal correction to Enthalpy= 0.914616
Thermal correction to Gibbs Free Energy= 0.759098
Sum of electronic and zero-point Energies= -3399.011604
Sum of electronic and thermal Energies= -3398.954184
Sum of electronic and thermal Enthalpies= -3398.953240
Sum of electronic and thermal Free Energies= -3399.108758

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Cartesian Coordinates

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6	0.916167	5.297111	-0.412135
6	0.923448	4.044056	-1.020847
6	0.538647	3.872931	-2.352180
6	0.156198	4.991597	-3.093178
6	0.144715	6.257915	-2.497328
6	0.521600	6.409144	-1.160745
16	1.381077	2.591790	-0.019133
8	1.488769	3.091195	1.413919
6	3.129188	2.489832	-0.603570
6	3.879905	1.360580	0.084025
16	3.554862	-0.265909	-0.763590
8	3.921685	-0.042725	-2.223094
6	4.987718	-1.099552	0.006458
6	6.112306	-1.314719	-0.787680
6	7.209646	-1.983676	-0.241908
6	7.170658	-2.432155	1.080681
6	6.031561	-2.215186	1.861982
6	4.926348	-1.549525	1.327984
46	0.182755	0.802658	-0.476443
6	-2.631682	4.702583	-0.355425
6	-3.312468	3.815999	0.371251
6	-2.919735	2.385812	0.465401
6	-2.713002	1.832918	1.888053
6	-1.308355	1.963693	2.437003
8	1.867614	-0.693419	1.887928
6	1.414843	-0.263131	2.939760
6	2.131147	0.761631	3.784115
8	-1.160161	-0.880554	-0.704988
15	-1.217714	-2.006295	0.318625
8	-1.568773	-1.658868	1.767826
7	-3.176516	0.432717	1.712929
8	0.225292	-0.602843	3.431942
8	0.138423	-2.866512	0.360024
6	0.999574	-2.951858	-0.798521
6	2.284611	-3.634169	-0.367967
6	3.265162	-3.821876	-1.532379
6	4.538345	-4.559154	-1.105893
8	-2.366703	-3.051116	-0.175423
6	-2.458989	-3.386629	-1.575093
6	-3.915364	-3.299136	-2.003741
6	-4.127632	-3.660362	-3.477392
6	-5.598531	-3.563512	-3.894772
1	3.598244	1.243198	1.133416
1	4.956046	1.535619	0.006482
1	3.122880	2.355277	-1.690157
1	3.570248	3.459583	-0.352352
1	4.025494	-1.387381	1.911235
1	6.100314	-0.967208	-1.816660
1	5.999031	-2.572649	2.887351
1	8.091452	-2.161619	-0.851046

1	8.023260	-2.958415	1.500369
1	0.516847	2.874436	-2.782736
1	1.198524	5.375384	0.633113
1	-0.145019	4.873884	-4.129934
1	0.503742	7.391944	-0.698251
1	-0.166490	7.123858	-3.074411
1	1.193149	-1.947159	-1.184341
1	0.496955	-3.533698	-1.583592
1	2.738937	-3.033019	0.425965
1	2.036337	-4.608137	0.072716
1	2.769882	-4.381415	-2.338551
1	3.529403	-2.847637	-1.962492
1	5.236608	-4.665230	-1.942510
1	5.055762	-4.019671	-0.307349
1	4.302887	-5.563592	-0.734406
1	-2.067579	-4.403353	-1.707718
1	-1.851684	-2.695782	-2.168648
1	-4.509405	-3.969060	-1.367371
1	-4.262762	-2.277429	-1.809974
1	-3.522036	-2.993512	-4.105299
1	-3.757367	-4.677560	-3.663541
1	-5.982260	-2.548203	-3.743124
1	-5.735415	-3.818845	-4.950428
1	-6.221043	-4.244834	-3.302954
1	-2.908171	5.752110	-0.371715
1	-4.174517	4.117402	0.965273
1	-1.771850	4.414055	-0.950577
1	-2.058297	2.137827	-0.171811
1	-2.568914	-0.424703	1.909250
1	-3.430041	2.318586	2.566591
1	-0.598765	1.432321	1.798472
1	-1.006739	3.013155	2.447629
1	-1.243180	1.555912	3.447287
1	3.203979	0.555654	3.781013
1	1.969291	1.734116	3.303777
1	1.749718	0.788959	4.805856
6	-3.988601	0.405928	0.674272
8	-4.052015	1.522431	-0.018111
8	-4.753657	-0.563281	0.282735
6	-5.585298	-1.379752	1.266662
6	-6.206725	-0.417256	2.276877
1	-5.456510	0.006559	2.947747
1	-6.738428	0.392572	1.768195
1	-6.927237	-0.969745	2.886356
6	-4.725608	-2.451438	1.918477
1	-4.224232	-3.060976	1.167434
1	-3.957081	-2.029672	2.566543
1	-5.377601	-3.086985	2.526731
6	-6.642207	-1.974100	0.341768
1	-6.177908	-2.604282	-0.417928

1	-7.331538	-2.586902	0.929318
1	-7.210884	-1.184219	-0.155765
1	-0.295784	-1.142216	2.771437

4' mode **x**

Number of imaginary frequencies : 0

Electronic energy : = -2063.5161246
Zero-point correction= 0.629889 (Hartree/Particle)
Thermal correction to Energy= 0.670780
Thermal correction to Enthalpy= 0.671724
Thermal correction to Gibbs Free Energy= 0.552537
Sum of electronic and zero-point Energies= -2062.886235
Sum of electronic and thermal Energies= -2062.845344
Sum of electronic and thermal Enthalpies= -2062.844400
Sum of electronic and thermal Free Energies= -2062.963587

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Cartesian Coordinates

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46	1.466521	-1.120450	-0.425654
6	0.100145	-2.388397	-1.533666
6	-0.621526	-1.281843	-1.070887
6	-1.444187	-1.367059	0.155636
6	-1.571250	-0.064078	0.985473
6	-0.917272	-0.125530	2.355320
8	1.436323	0.924170	0.407734
7	-3.038755	0.127839	1.049760
8	-0.361312	1.929528	-1.230237
1	0.443935	-2.420372	-2.563981
1	-0.782504	-0.399655	-1.687172
1	0.059455	-3.344995	-1.015477
1	-1.214843	-2.244647	0.763640
1	-1.162070	0.755027	0.396660
1	-1.307835	-0.958071	2.950100
1	0.160526	-0.230016	2.217009
1	-1.080692	0.812712	2.892484
6	-3.672878	-0.710464	0.253762
8	-2.937320	-1.639679	-0.269749
8	-4.947155	-0.585477	0.039680
6	-5.714168	-1.458426	-0.928277
6	-5.124334	-1.278256	-2.324894
1	-4.116797	-1.689427	-2.396576
1	-5.761566	-1.800487	-3.044436
1	-5.099122	-0.219351	-2.596602
6	-5.671656	-2.901396	-0.432295
1	-6.334370	-3.507099	-1.057182
1	-4.666284	-3.319564	-0.492267

1	-6.026446	-2.962623	0.600338
6	-7.115201	-0.864580	-0.824438
1	-7.789607	-1.409614	-1.490124
1	-7.495150	-0.943423	0.197446
1	-7.111723	0.188270	-1.117917
1	-3.465037	0.995893	1.347683
15	0.785799	2.128421	-0.277486
8	0.285001	3.043445	1.002773
8	1.936831	3.031443	-0.984445
6	-0.710388	4.048234	0.776884
1	-0.539306	4.828218	1.528064
6	3.321723	2.814502	-0.631393
1	3.399745	2.399279	0.377698
1	-0.596825	4.501439	-0.215453
1	3.797683	3.801380	-0.645429
6	3.581647	-1.559270	0.126871
6	2.866642	-2.749251	-0.089175
1	4.261854	-1.167729	-0.622336
1	3.000756	-3.341891	-0.989261
6	3.725365	-0.984384	1.478949
6	2.160066	-3.424050	1.030433
6	2.987460	-1.669611	2.581801
1	3.081085	-1.208761	3.561123
6	2.276556	-2.792100	2.376583
8	1.495326	-4.448565	0.872776
8	4.430654	-0.007725	1.719074
1	1.751401	-3.304858	3.178113
6	3.981242	1.876039	-1.635018
1	3.393455	0.950674	-1.664340
1	3.923327	2.322133	-2.636519
6	5.433610	1.552514	-1.267505
1	5.449739	1.081270	-0.277534
1	6.009450	2.484831	-1.181733
6	6.106874	0.636054	-2.294462
1	7.136716	0.397261	-2.008492
1	5.562582	-0.311401	-2.396244
1	6.132067	1.101279	-3.286861
6	-2.112031	3.455872	0.924080
1	-2.220632	2.703681	0.135953
1	-2.157252	2.945646	1.898624
6	-3.252733	4.470096	0.821852
1	-3.140049	5.244736	1.591809
1	-3.197654	4.984505	-0.146043
6	-4.622195	3.795501	0.966420
1	-4.719141	3.310412	1.946973
1	-5.446555	4.509763	0.874220
1	-4.763808	3.027272	0.194931

TS[4'-6] mode **x**

Number of imaginary frequencies : 1
The smallest frequency is : -217.6826 cm(-1)

Electronic energy : = -2063.513968
Zero-point correction= 0.628515 (Hartree/Particle)
Thermal correction to Energy= 0.669257
Thermal correction to Enthalpy= 0.670202
Thermal correction to Gibbs Free Energy= 0.551293
Sum of electronic and zero-point Energies= -2062.885453
Sum of electronic and thermal Energies= -2062.844711
Sum of electronic and thermal Enthalpies= -2062.843766
Sum of electronic and thermal Free Energies= -2062.962675

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Cartesian Coordinates

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46	-1.399110	-1.119142	0.417925
6	-0.068500	-2.342600	1.573342
6	0.674051	-1.225389	1.133212
6	1.386711	-1.265698	-0.113949
6	1.652067	0.045100	-0.869432
6	1.063555	0.036322	-2.277740
8	-1.551565	0.848813	-0.528855
7	3.114373	0.217491	-0.879358
8	0.097107	1.932536	1.211674
1	-0.412705	-2.385054	2.603335
1	0.791442	-0.336228	1.748044
1	0.014559	-3.301221	1.063903
1	1.221252	-2.144623	-0.733847
1	1.222442	0.855740	-0.280644
1	1.466416	-0.793542	-2.868277
1	-0.023484	-0.035547	-2.206892
1	1.289973	0.979406	-2.782067
6	3.788907	-0.695818	-0.185509
8	3.138824	-1.682529	0.278090
8	5.081557	-0.505312	-0.045373
6	5.943764	-1.430864	0.755013
6	5.465105	-1.429475	2.206345
1	4.475421	-1.877542	2.300978
1	6.167954	-2.006865	2.814149
1	5.434392	-0.408043	2.596431
6	5.921597	-2.820018	0.118931
1	6.658186	-3.453621	0.621836
1	4.940556	-3.286915	0.212268
1	6.190119	-2.758132	-0.939662
6	7.315702	-0.775340	0.617494
1	8.056451	-1.356990	1.172793

1	7.620436	-0.733532	-0.431688
1	7.299443	0.241770	1.017838
1	3.537135	1.102320	-1.124184
15	-0.962261	2.089869	0.156375
8	-0.362806	2.954439	-1.110060
8	-2.174880	3.013795	0.720173
6	0.504062	4.061912	-0.825210
1	0.351187	4.787068	-1.632949
6	-3.546453	2.670501	0.426234
1	-3.615443	2.156661	-0.537035
1	0.224587	4.545790	0.118604
1	-4.087734	3.620803	0.360868
6	-3.523118	-1.648418	-0.053859
6	-2.774862	-2.809235	0.175615
1	-4.184145	-1.241927	0.704486
1	-2.854793	-3.368455	1.102823
6	-3.726197	-1.126654	-1.424691
6	-2.090974	-3.509243	-0.945934
6	-3.002516	-1.826427	-2.525588
1	-3.133772	-1.397968	-3.514940
6	-2.260783	-2.926241	-2.306751
8	-1.404297	-4.513746	-0.768406
8	-4.474289	-0.185950	-1.669755
1	-1.746495	-3.452081	-3.106469
6	-4.121864	1.793174	1.532267
1	-3.488905	0.901247	1.618261
1	-4.047448	2.325916	2.489031
6	-5.570132	1.374624	1.255959
1	-5.607990	0.849164	0.294482
1	-6.197426	2.270394	1.148043
6	-6.144446	0.484512	2.363078
1	-7.174581	0.183425	2.145328
1	-5.550227	-0.430314	2.484010
1	-6.141664	1.000451	3.330233
6	1.963801	3.612824	-0.774367
1	2.056896	2.901101	0.052736
1	2.186168	3.080158	-1.711435
6	2.962315	4.757209	-0.585218
1	2.853123	5.488338	-1.397485
1	2.730016	5.291986	0.344811
6	4.408944	4.252952	-0.537866
1	4.679927	3.747681	-1.474031
1	5.122453	5.069595	-0.388242
1	4.547017	3.537027	0.281725

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forward intermediate of IRC run in mode **x**

Number of imaginary frequencies : 0

Electronic energy : = -2063.5161246
Zero-point correction= 0.629889 (Hartree/Particle)
Thermal correction to Energy= 0.670780
Thermal correction to Enthalpy= 0.671724
Thermal correction to Gibbs Free Energy= 0.552531
Sum of electronic and zero-point Energies= -2062.886236
Sum of electronic and thermal Energies= -2062.845345
Sum of electronic and thermal Enthalpies= -2062.844401
Sum of electronic and thermal Free Energies= -2062.963593

Cartesian Coordinates

46	1.466583	-1.120150	-0.425605
6	0.100237	-2.387789	-1.534131
6	-0.621448	-1.281419	-1.071001
6	-1.443978	-1.367056	0.155620
6	-1.571074	-0.064212	0.985729
6	-0.917450	-0.126027	2.355723
8	1.436238	0.924337	0.408804
7	-3.038560	0.127863	1.049680
8	-0.360601	1.929614	-1.230052
1	0.444002	-2.419460	-2.564463
1	-0.782447	-0.399029	-1.686986
1	0.059646	-3.344508	-1.016159
1	-1.214440	-2.244742	0.763411
1	-1.161614	0.754966	0.397223
1	-1.308026	-0.958822	2.950140
1	0.160403	-0.230313	2.217665
1	-1.081168	0.812005	2.893178
6	-3.672658	-0.710493	0.253745
8	-2.937096	-1.639781	-0.269660
8	-4.946916	-0.585546	0.039622
6	-5.713762	-1.458201	-0.928732
6	-5.123642	-1.277605	-2.325172
1	-4.116107	-1.688792	-2.396790
1	-5.760765	-1.799562	-3.045010
1	-5.098328	-0.218609	-2.596518
6	-5.671348	-2.901307	-0.433141
1	-6.334108	-3.506806	-1.058174
1	-4.665996	-3.319518	-0.493188
1	-6.026152	-2.962759	0.599475
6	-7.114814	-0.864373	-0.825001
1	-7.789064	-1.409146	-1.491059
1	-7.495017	-0.943589	0.196759
1	-7.111241	0.188588	-1.118081
1	-3.464870	0.995921	1.347548
15	0.786265	2.128566	-0.276998
8	0.285191	3.044193	1.002712
8	1.937759	3.031105	-0.983828

6	-0.710550	4.048499	0.776304
1	-0.539765	4.828941	1.527078
6	3.322640	2.813144	-0.631391
1	3.400775	2.397543	0.377532
1	-0.597186	4.501205	-0.216278
1	3.799231	3.799721	-0.645298
6	3.581578	-1.559361	0.127463
6	2.866173	-2.749157	-0.088229
1	4.262208	-1.168505	-0.621716
1	3.000369	-3.342338	-0.987946
6	3.725153	-0.983869	1.479289
6	2.158765	-3.422969	1.031471
6	2.986622	-1.668223	2.582264
1	3.080170	-1.206945	3.561390
6	2.275219	-2.790454	2.377365
8	1.493374	-4.447112	0.874081
8	4.430838	-0.007424	1.719122
1	1.749550	-3.302546	3.178983
6	3.981199	1.874613	-1.635570
1	3.393081	0.949446	-1.664765
1	3.922900	2.320904	-2.636958
6	5.433664	1.550505	-1.268928
1	5.450235	1.079447	-0.278869
1	6.009952	2.482587	-1.183657
6	6.105877	0.633596	-2.296171
1	7.135835	0.394481	-2.010884
1	5.561158	-0.313675	-2.397394
1	6.130543	1.098627	-3.288675
6	-2.111961	3.455665	0.923787
1	-2.220325	2.703222	0.135869
1	-2.156898	2.945693	1.898475
6	-3.253077	4.469414	0.821349
1	-3.140665	5.244295	1.591101
1	-3.198247	4.983589	-0.146685
6	-4.622257	3.794301	0.966158
1	-4.718964	3.309443	1.946850
1	-5.446920	4.508189	0.873799
1	-4.763596	3.025799	0.194885

Pd reoxidation

Intermediate **A**

Normal termination of Gaussian 09 at Sun Mar 24 12:21:17 2019.

Number of imaginary frequencies : 0
The smallest frequencies are : 23.9861 31.8067 33.7901 cm(-1)

Electronic energy : HF=-2455.2248344
Zero-point correction= 0.464641 (Hartree/Particle)
Thermal correction to Energy= 0.501892
Thermal correction to Enthalpy= 0.502836
Thermal correction to Gibbs Free Energy= 0.393267
Sum of electronic and zero-point Energies= -2454.760194
Sum of electronic and thermal Energies= -2454.722942
Sum of electronic and thermal Enthalpies= -2454.721998
Sum of electronic and thermal Free Energies= -2454.831567

Cartesian Coordinates

8	0.357432	2.338651	-1.746018
16	0.646684	0.931414	-1.275946
46	-0.235289	-0.114457	0.731081
6	-1.599448	-0.126615	-2.379694
6	-0.087421	-0.208165	-2.531585
16	-2.124723	-0.741289	-0.687302
8	-2.769848	-2.092463	-0.881198
1	-2.121344	-0.788690	-3.075331
1	0.242080	0.148806	-3.511038
1	0.286699	-1.213942	-2.324791
1	-1.956216	0.898935	-2.499059
6	0.872095	0.186387	2.563320
6	0.033012	-0.935036	2.745130
6	0.529896	-2.279729	2.424930
6	1.950502	-2.408784	1.995841
1	2.287520	-3.420337	1.792147
6	2.758780	-1.342781	1.872466
1	3.793267	-1.421691	1.554630
6	2.253326	0.036901	2.091726
1	-0.886267	-0.879833	3.319622
1	0.591973	1.168714	2.928628
8	-0.185050	-3.290017	2.511377
8	2.986783	1.009536	1.850495
1	-0.301611	-4.225954	1.090823
8	-0.564488	-4.653707	0.232452
6	-0.243983	-3.879231	-0.793312
8	0.432071	-2.857077	-0.697453
6	-0.820319	-4.370160	-2.095100
1	-0.899002	-5.458578	-2.109784
1	-1.824897	-3.942434	-2.173734
1	-0.212682	-4.014661	-2.928847
8	-0.100014	2.982557	1.469427
6	0.740708	3.660780	0.897439
8	2.045220	3.372332	0.869692
1	2.252679	2.530120	1.353922
6	0.424037	4.909912	0.115073
1	1.183238	5.677813	0.280146
1	0.423456	4.639793	-0.944506

1	-0.563653	5.277125	0.394807
6	-5.428726	2.289835	0.223236
6	-4.089197	2.684087	0.303799
6	-3.068926	1.776262	0.020908
6	-3.425605	0.475761	-0.350772
6	-4.751710	0.058256	-0.425304
6	-5.759394	0.981669	-0.137261
1	-6.215761	3.002629	0.451406
1	-3.831887	3.696934	0.597872
1	-2.028177	2.082016	0.105842
1	-4.972366	-0.970381	-0.692861
1	-6.800281	0.676574	-0.189606
6	5.134118	0.169713	-1.632014
6	4.270128	-0.915087	-1.450944
6	2.892832	-0.714213	-1.366097
6	2.405810	0.590181	-1.491247
6	3.248708	1.687061	-1.656021
6	4.625231	1.465553	-1.729603
1	6.205946	0.003609	-1.686580
1	4.668527	-1.922136	-1.368064
1	2.221976	-1.548597	-1.188343
1	2.827242	2.684622	-1.702024
1	5.297895	2.308714	-1.852717

TS A-B

Normal termination of Gaussian 09 at Wed Mar 27 04:26:38 2019.

Number of imaginary frequencies : 1
The smallest frequencies are : -988.7844 19.5302 23.4132 cm(-1)

Electronic energy : HF=-2455.1855117
Zero-point correction= 0.459758 (Hartree/Particle)
Thermal correction to Energy= 0.496224
Thermal correction to Enthalpy= 0.497168
Thermal correction to Gibbs Free Energy= 0.389174
Sum of electronic and zero-point Energies= -2454.725753
Sum of electronic and thermal Energies= -2454.689288
Sum of electronic and thermal Enthalpies= -2454.688344
Sum of electronic and thermal Free Energies= -2454.796338

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Cartesian Coordinates

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8	-2.387777	3.392897	1.341441
1	-2.224285	3.931072	0.207827
8	1.767549	-0.968241	-3.035270
16	1.268956	-1.211692	-1.638755
46	-0.143803	0.339650	-0.606411
6	-1.170005	-2.614090	-1.418846
6	0.322527	-2.828549	-1.628738

16	-1.417257	-1.752930	0.203958
8	-0.921194	-2.723413	1.254967
1	-1.695453	-3.571865	-1.359252
1	0.542462	-3.252768	-2.611689
1	0.736519	-3.467565	-0.847386
1	-1.622613	-1.986309	-2.191882
6	0.729902	2.005649	-1.966212
6	-0.380350	2.854125	-2.069421
8	-1.851432	1.539940	0.224578
6	-1.942110	1.411221	2.617436
6	-0.706818	3.706400	-1.001206
1	-2.213811	2.042302	3.464208
6	0.280532	3.905114	0.062379
1	-2.579979	0.522102	2.591182
1	0.030478	4.639039	0.821973
1	-0.905922	1.068968	2.712068
6	1.423451	3.186672	0.128688
1	3.285620	1.225193	0.619693
1	2.154621	3.333720	0.916004
8	3.523880	1.037903	1.581520
6	1.738446	2.195923	-0.901996
6	2.457900	0.667053	2.279792
1	-1.102890	2.726113	-2.867503
8	1.320383	0.592293	1.831834
1	1.043998	1.391788	-2.807025
6	2.805022	0.344006	3.713761
8	-1.879860	4.248198	-0.867466
1	3.568974	-0.438354	3.730854
8	2.821937	1.560375	-0.896648
1	3.230528	1.226734	4.200433
1	1.913875	0.014118	4.246891
6	-2.070917	2.153441	1.307435
6	-5.983506	-1.711212	0.304363
6	-5.278676	-2.738331	0.938885
6	-3.884098	-2.752792	0.906244
6	-3.223040	-1.729458	0.225932
6	-3.905132	-0.680342	-0.394714
6	-5.300531	-0.686601	-0.356687
1	-7.068973	-1.701828	0.337279
1	-5.813904	-3.524152	1.463458
1	-3.305875	-3.523521	1.406678
1	-3.360152	0.137679	-0.853463
1	-5.851413	0.120917	-0.828976
6	4.846071	-2.181066	1.026995
6	5.038988	-1.652148	-0.249951
6	3.942007	-1.379554	-1.069049
6	2.666048	-1.651029	-0.582252
6	2.445046	-2.156550	0.702454
6	3.554344	-2.434260	1.499723
1	5.702928	-2.389586	1.660686

1	6.041946	-1.444389	-0.609410
1	4.056918	-0.956949	-2.060669
1	1.439559	-2.314091	1.083888
1	3.406108	-2.839674	2.496038

Intermediate **B**

Normal termination of Gaussian 09 at Sun Mar 24 12:15:19 2019.

Number of imaginary frequencies : 0
The smallest frequencies are : 22.1208 25.2206 29.1839 cm(-1)

Electronic energy : HF=-2455.1969839
Zero-point correction= 0.464890 (Hartree/Particle)
Thermal correction to Energy= 0.501529
Thermal correction to Enthalpy= 0.502473
Thermal correction to Gibbs Free Energy= 0.394003
Sum of electronic and zero-point Energies= -2454.732094
Sum of electronic and thermal Energies= -2454.695455
Sum of electronic and thermal Enthalpies= -2454.694511
Sum of electronic and thermal Free Energies= -2454.802981

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Cartesian Coordinates

.....

8	0.791240	-2.205823	-2.029776
16	1.309600	-1.531910	-0.784837
46	-0.051541	0.239663	-0.099475
6	-0.360951	-3.031328	0.761921
6	1.122436	-2.730916	0.604359
16	-1.321440	-1.465308	1.089459
8	-1.645836	-1.377445	2.551922
1	-0.557960	-3.662685	1.632031
1	1.679321	-3.625662	0.313267
1	1.552567	-2.256189	1.489091
1	-0.773305	-3.489790	-0.139411
6	1.157905	1.738192	-1.198799
6	0.149342	2.284450	-2.064457
6	-0.548157	3.398652	-1.682187
6	-0.151952	4.127223	-0.513020
1	-0.717744	5.023694	-0.274823
6	0.865602	3.705536	0.292693
1	1.160851	4.262089	1.175899
6	1.606718	2.503381	-0.017575
1	-0.135503	1.742646	-2.959863
1	1.930338	1.115632	-1.644517
8	-1.682225	3.820160	-2.322600
8	2.585694	2.114900	0.681659
1	-2.196399	3.015941	-2.520375
8	-2.624687	1.226514	-1.431945
6	-2.541422	1.696811	-0.287956

8	-1.543691	1.533025	0.530279
6	-3.628483	2.616635	0.248739
1	-4.607770	2.229595	-0.042165
1	-3.565911	2.735040	1.331014
1	-3.493862	3.592996	-0.229269
1	2.148211	1.954308	2.195818
8	1.680944	1.813871	3.084828
6	1.328836	0.549360	3.222819
8	1.641171	-0.337479	2.425956
6	0.473547	0.280736	4.433200
1	0.513699	1.104713	5.146062
1	-0.552860	0.136292	4.081937
1	0.789775	-0.654390	4.900089
6	5.823728	-1.103748	-1.155109
6	5.169246	-0.531807	-0.060745
6	3.786443	-0.652793	0.079381
6	3.095641	-1.368484	-0.900151
6	3.720967	-1.939631	-2.009929
6	5.104082	-1.803646	-2.128207
1	6.899696	-0.995492	-1.256409
1	5.730550	0.025611	0.682331
1	3.254195	-0.192603	0.903326
1	3.128776	-2.463721	-2.752809
1	5.616695	-2.237971	-2.981039
6	-5.174996	-2.171755	-1.235982
6	-3.958549	-2.098815	-1.922488
6	-2.769866	-1.903745	-1.223701
6	-2.831307	-1.808405	0.168482
6	-4.030060	-1.865251	0.873477
6	-5.212702	-2.053221	0.154831
1	-6.098258	-2.310692	-1.790588
1	-3.936546	-2.172463	-3.005019
1	-1.821845	-1.813357	-1.747747
1	-4.022842	-1.756762	1.953080
1	-6.160698	-2.102149	0.681856

Intermediate **C**

Normal termination of Gaussian 09 at Sat Mar 30 07:19:27 2019.

Number of imaginary frequencies : 0
The smallest frequencies are : 6.9183 20.2166 24.0929 cm(-1)

Electronic energy : HF=-2455.1987786
Zero-point correction= 0.464369 (Hartree/Particle)
Thermal correction to Energy= 0.501500
Thermal correction to Enthalpy= 0.502445
Thermal correction to Gibbs Free Energy= 0.389475
Sum of electronic and zero-point Energies= -2454.734410
Sum of electronic and thermal Energies= -2454.697278

Sum of electronic and thermal Enthalpies= -2454.696334
Sum of electronic and thermal Free Energies= -2454.809303

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Cartesian Coordinates

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46	-0.056726	0.058859	0.002936
16	-0.607820	2.207706	0.811920
8	-1.189774	2.430500	2.172568
16	1.937128	1.028785	-0.756953
8	2.045241	1.840755	-2.013919
6	0.985974	3.170468	0.638348
6	2.179476	2.225900	0.635834
1	0.988657	3.839136	1.502495
1	0.929338	3.746722	-0.287474
1	3.108069	2.764087	0.427867
1	2.251862	1.651580	1.562033
8	0.356900	-1.841279	-0.589596
6	0.927624	-2.026350	-1.749670
8	-1.030805	-0.596848	3.376146
8	1.403562	-1.141810	-2.464201
6	0.180714	-0.132446	3.601238
8	0.998605	0.161303	2.729712
6	0.473162	0.031095	5.074580
1	1.540391	0.189619	5.229867
1	-0.081153	0.901442	5.441150
1	0.125374	-0.840466	5.634225
6	0.958267	-3.494583	-2.148809
1	1.544516	-4.059041	-1.417335
1	-0.059222	-3.895265	-2.133691
6	-2.301219	-1.775924	0.409788
1	1.397144	-3.602866	-3.141120
6	-2.099037	-2.991501	1.083055
1	-1.487216	-2.996858	1.979041
6	-3.075056	-1.770232	-0.765491
8	-1.778288	-0.626956	0.885211
6	-2.679140	-4.165341	0.610070
8	-4.036119	-5.270099	-1.079323
6	-3.641762	-2.941730	-1.248624
1	-3.824194	-6.025058	-0.515774
1	-3.209453	-0.828180	-1.288514
1	-4.239284	-2.949269	-2.154359
6	-3.448476	-4.147247	-0.559407
1	-1.277851	-0.605918	2.390203
1	-2.524670	-5.101577	1.143376
6	-3.310362	4.195294	-2.281266
6	-3.633364	4.260304	-0.924450
6	-2.795713	3.669867	0.024604
6	-1.641583	3.029813	-0.418124
6	-1.302034	2.939621	-1.772065
6	-2.149291	3.538457	-2.703304

1	-3.967393	4.652305	-3.015215
1	-4.538703	4.765487	-0.602138
1	-3.022978	3.690657	1.085423
1	-0.401477	2.422099	-2.095454
1	-1.904216	3.484807	-3.759413
6	5.540731	-1.702986	-0.260333
6	4.566860	-1.660511	0.742000
6	3.458012	-0.823837	0.612285
6	3.368348	-0.031983	-0.534254
6	4.315288	-0.065820	-1.553682
6	5.415585	-0.910255	-1.404192
1	6.396122	-2.363515	-0.152815
1	4.663930	-2.285886	1.624195
1	2.684527	-0.793584	1.374207
1	4.168443	0.540604	-2.440782
1	6.167287	-0.957359	-2.186139

Intermediate **D**

Normal termination of Gaussian 09 at Sun Mar 24 12:37:02 2019.

Number of imaginary frequencies : 0
The smallest frequencies are : 20.9702 23.5556 31.7681 cm(-1)

Electronic energy : HF=-2455.1982549
Zero-point correction= 0.465155 (Hartree/Particle)
Thermal correction to Energy= 0.502115
Thermal correction to Enthalpy= 0.503059
Thermal correction to Gibbs Free Energy= 0.392766
Sum of electronic and zero-point Energies= -2454.733100
Sum of electronic and thermal Energies= -2454.696140
Sum of electronic and thermal Enthalpies= -2454.695196
Sum of electronic and thermal Free Energies= -2454.805489

.....

Cartesian Coordinates

.....

46	0.273513	-0.326321	0.806459
16	1.578180	-1.267940	-0.882430
8	1.558642	-2.764400	-1.032315
16	-1.558945	-0.622423	-0.681873
8	-2.583478	0.423888	-0.944174
6	0.763332	-0.517300	-2.346259
6	-0.689757	-0.974044	-2.326211
1	1.285037	-0.880102	-3.236152
1	0.868180	0.564483	-2.232461
1	-1.289778	-0.409180	-3.042814
1	-0.774462	-2.045324	-2.516053
8	-0.729883	0.636810	2.273193
6	-1.987190	0.346007	2.479920
8	-2.636693	-0.504296	1.873995

6	-0.268558	2.801070	-0.906917
6	-1.041505	3.051079	0.229895
6	-0.811386	3.016480	-2.177647
6	-2.354641	3.495981	0.087243
6	-2.124797	3.457120	-2.316220
1	-0.189994	2.842206	-3.051812
6	-2.906214	3.690297	-1.181672
1	-2.959072	3.676148	0.974249
6	-2.609450	1.214273	3.564004
1	-1.957673	1.262630	4.439391
1	-2.718390	2.232373	3.175812
1	-3.589928	0.821668	3.835093
1	-0.628484	2.855650	1.213067
8	1.009314	2.310478	-0.829944
8	-4.196972	4.115880	-1.377318
1	-4.640204	4.164341	-0.521228
1	-2.561688	3.621857	-3.295644
1	1.328554	2.236254	0.111472
8	2.198588	1.994074	1.483884
6	2.515870	0.956824	2.087570
8	1.940237	-0.199878	1.989917
6	3.731811	0.956858	2.998385
1	3.867334	1.950763	3.427975
1	3.642767	0.202620	3.781403
1	4.610160	0.721817	2.386561
6	5.951490	0.019741	-0.870432
6	5.597872	-1.324195	-0.729588
6	4.255501	-1.701770	-0.765155
6	3.289728	-0.710695	-0.948791
6	3.617390	0.639485	-1.092461
6	4.966227	0.993476	-1.055400
1	6.997355	0.309876	-0.835413
1	6.363680	-2.080333	-0.587802
1	3.952359	-2.737114	-0.655598
1	2.855134	1.396723	-1.221908
1	5.241825	2.037605	-1.163644
6	-3.662136	-4.620860	-0.028409
6	-4.402974	-3.460099	-0.262737
6	-3.753775	-2.241285	-0.461632
6	-2.363436	-2.222504	-0.432865
6	-1.598408	-3.363090	-0.190664
6	-2.265782	-4.571999	0.008969
1	-4.173564	-5.565331	0.132359
1	-5.487872	-3.499288	-0.279830
1	-4.298605	-1.316493	-0.614876
1	-0.513777	-3.319038	-0.163774
1	-1.691556	-5.473808	0.197929

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