Supporting Information

Prediction on chemoselectivity for selected organocatalytic reactions by the DFT version of the Hückel-defined free valence index

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Table of Contents

Part 1: Computational methods

All the geometries of the stationary points and frequencies (1 atm, 298 K) were optimized and calculated using B3LYP-D3[1] functional with 6-31G(d, p) basis set for main group atoms and Lan2LDZ basis set for Cs atom in tetrahydrofuran (THF) solvent using the SMD[2] for implicit solvation model in case study 1. The solvents are different among the several reaction models, *o*-dichlorobenzene solvent was selected in case study 2, toluene solvent was selected in case study 3, acetonitrile solvent was selected in case study 4, whereas the mixed solvent of acetonitrile and 1,2-dichloroethane (DCE) with the ratio of 1:1 was selected in case study 5 by using a dielectric constant value of 22.9, and other calculation settings are the same. Frequency calculations verify that all the reactants, products, catalysts, and intermediates have no imaginary frequency and each transition state that connects the two expected intermediates has only one imaginary frequency. All the energies discussed in the main text are the relative Gibbs free energies (GFE), which are obtained by the addition of the thermal Gibbs free energy corrections (GFEC) at the B3LYP-D3/6-31G(d, p)(Lan2LDZ for Cs)/$SMD_{solvent}$ level and the single-point energies (SPE) at a higher computational level of B3LYP-D3/6-311++G(2df, 2pd)(SDD for Cs)/$SMD_{solvent}$ (L1).

Herein, the different computational methods including B3LYP,[3,4] M06-2X,[5,6] and ωB97X-D[7] were employed to check whether the selected method (L1) is reliable, the additional calculations by employing other different DFT methods and basis sets, i.e., B3LYP-D3/6-311++G(2df, 2pd)/SMD_{THF}//B3LYP/6-31G(d, p)/SMD_{THF}(L2), M06-2X/6-311++G(2df, 2pd)/SMD_{THF}//M06-2X/6-31G(d, p)/SMD_{THF} (L3), and ωB97X-D/6-311++G(2df, 2pd)/SMD_{THF}//ωB97X-D/6-31G(d, p)/SMD_{THF} (L4) have been performed for the key transition state ε-TS4 involved in the chemoselectivity-determining step of case study 1, and the computed and tested results can be found in the Table S1. There are small differences between the calculated results obtained by L1~L4, but the trend and conclusions should be the same, indicating the computational method is reliable.

Table S1. Comparison of relative Gibbs free energies of the key step calculated by using different levels L1~L4. (Unit: kcal/mol).

	L1	**L2**	**L3**	**L4**
M3	0.0	0.0	0.0	0.0
ε-TS4	13.1	13.1	14.6	14.7

Part 2: Additionally computational results

2.1 Different bases assisted [1,2]-proton transfer processes

Fig. S1 depicts the energy profiles of the [1,2]-proton transfer processes for the formation of the Breslow intermediate **M2** assisted by different bases. As shown in Fig. S1, the energy barrier for [Cs]HCO_3 assisted [1,2]-proton transfer process via transition state **TS2** is 10.6 kcal/mol. Moreover, we investigated the THF-coordinated [Cs]HCO_3 assised [1,2]-proton transfer processes. The calculated results show that the [1,2]-proton transfer process assisted by [Cs]HCO_3-THF occurs via the transition state **TS2'** with an energy barrier of 12.1 kcal/mol. While the [Cs]HCO_3-2THF assisted [1,2]-proton transfer process occurs via the transition state **TS2''** with an energy barrier of 11.6 kcal/mol. The result indicates that the coordination of more THF molecules would not lower the energy barrier of the [1,2]-proton transfer process. The energy barrier for HCO_3^- assisted [1,2]-proton transfer process via transition state **TS2'''** is 16.4 kcal/mol, which is much higher than that of transition state **TS2**, so we can exclude this pathway safely.

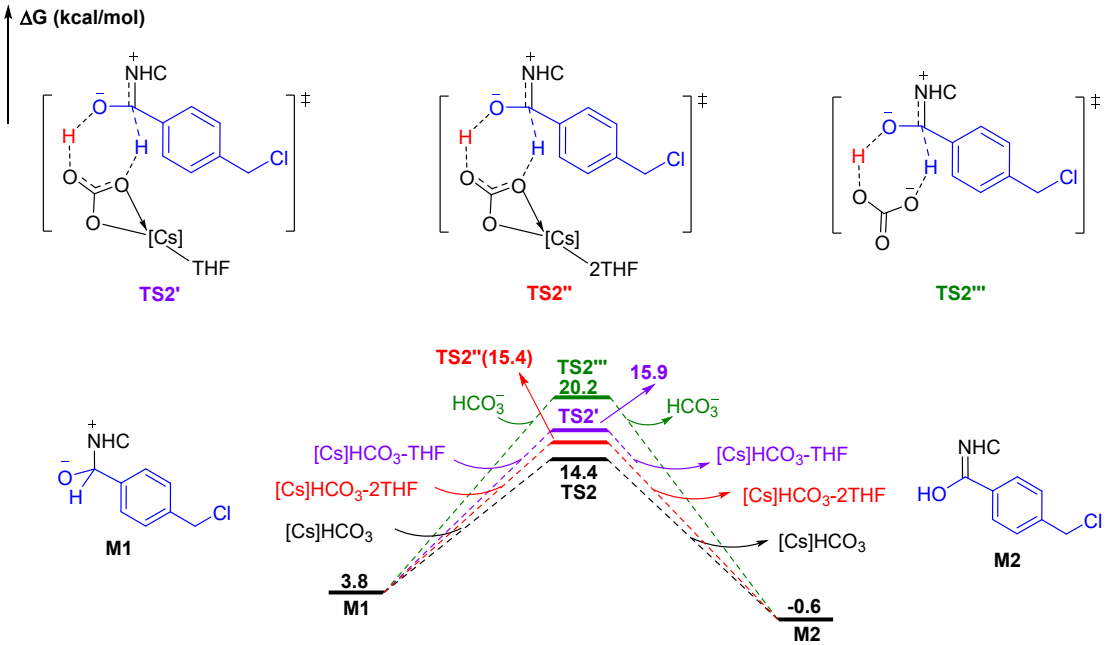


Fig. S1. Different bases assisted [1,2]-proton transfer processes

2.2 Other possible pathway to generate intermediate M4

Fig. S2 depicts that the C–Cl bond of Breslow intermediate **M2** is cleaved to afford intermediate **M3'** via transition state **TS3'** ($\Delta G^{\ddagger}$ = 3.3 kcal/mol). In the next step, the nucleophilic attack of the Cε to the C1 of **2a** form Cε–C1 bond accompanied by the breakage of O–H bond via transition state **TS4'**, then releasing HCl to form intermediate **M4**. The free energy barrier for this step is 24.0 kcal/mol, which is too high to overcome in experiment conditions.

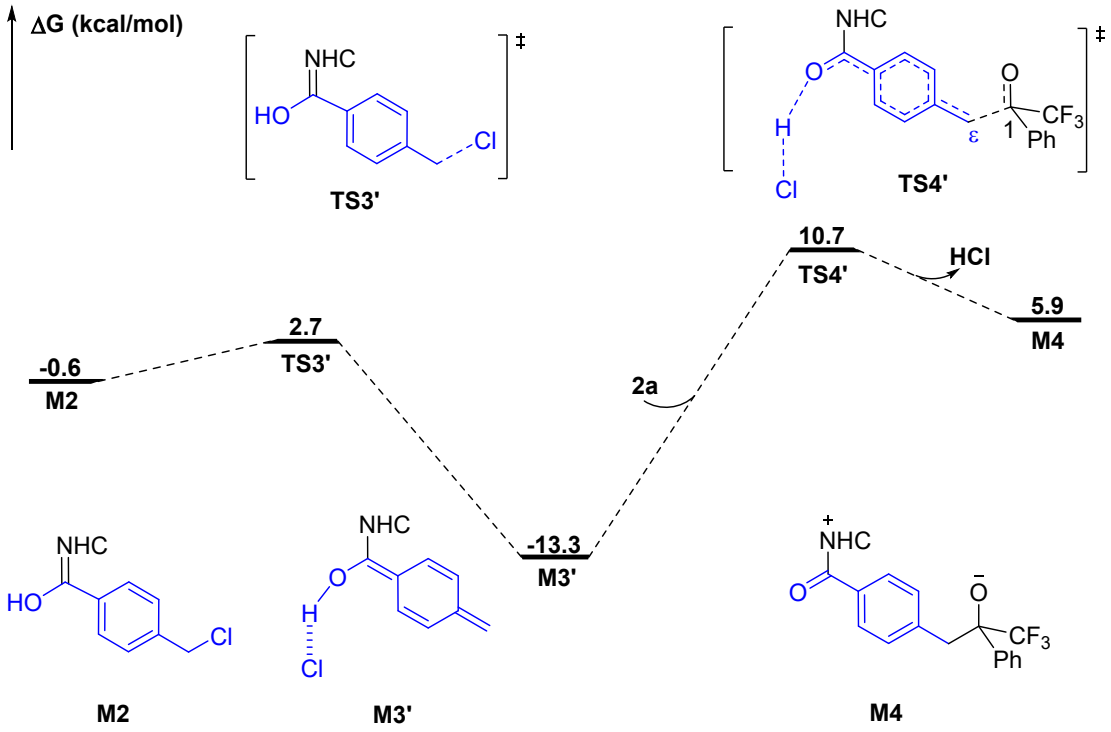
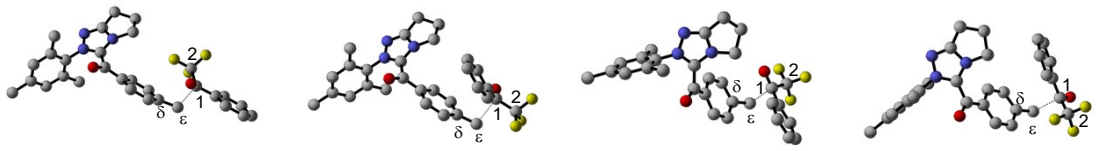


Fig. S2. Other possible pathway to generate intermediate **M4**.

2.3 Different conformers and configurations of ε-TS4

To ensure the selected and discussed configuration of the transition state **ε-TS4** with the lowest energy in the main text, we have searched multiple possible conformations for the fourth step. By rotating the dihedral angle Φ(Cδ−Cε−C1−C2) with 60° per time in transition state **ε-TS4** of case study 1, we have totally constructed four conformations as the initial structures, which have been subsequently optimized the structures and refined the single-point energies at the B3LYP-D3/6-31G(d, p)/SMD_{THF} and B3LYP-D3/6-311++G(2df, 2pd)/SMD_{THF} level, respectively. After the optimization, the corresponding dihedral angles Φ(Cδ−Cε−C1−C2) change to -60°/171°/-161°/78°. As revealed by Fig. S3, the most stable conformation with the lowest energy of the chemoselective transition state is associated with the dihedral angle Φ(Cδ−Cε−C1−C2) of -60°.



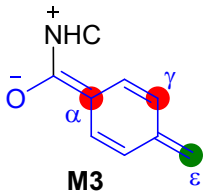
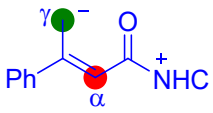
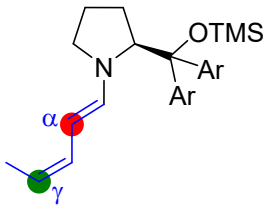
ε-TS4$_{Φ = -60°}$ 0.0 **ε-TS4$_{Φ = 171°}$** 1.5 **ε-TS4$_{Φ = -161°}$** 1.4 **ε-TS4$_{Φ = 78°}$** 2.4

Fig. S3. Different configurations and relative energies of the transition state **ε-TS4** with different dihedral angles Φ (Cδ−Cε−C1−C2) (energy in kcal/mol).

2.4 Comparison of the active sites predicted by HFV, Mulliken charge and Parr function

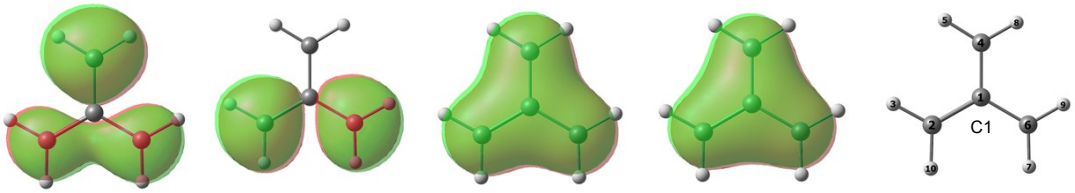
We have additionally calculated Mulliken charge and local reactivity indexes Parr function[8,9] of the key atoms in the active intermediates of the three non-radical reactions, and then added a comparison of HFV index with them in Table S2. As summarized in Table S2, the actual sites of nucleophiles **M3** and **M1b** should have the more negative Mulliken charge values, which can also be used for explaining and predicting the experiments. However, the Mulliken charge values of the atoms in **M1c** cannot be used for predicting the real active site, which is due to the tiny difference between the Mulliken charge values of the two active sites. In addition, the nucleophilic Parr function values (P_k^-) also have the same trends with the HFV indexes in the three cases. Noteworthy, we did not additionally consider the radical reactions, in which the nucleophilie and electrophilie were not clearly identified before.

Table S2. Comparison of the active sites predicted by HFV, Mulliken charge and nucleophilic Parr function (P_k^-). Green circles represent the high active sites and red circles represent the low active sites.

Reactants or intermediates	Active sites	HFV	Mulliken charge(e)	Parr function P_k^-
 **M3**	α	0.68	0.015	0.221
	γ	0.94	-0.205	0.222
	ε	1.17	-0.426	0.682
 **dienolate M1b**	α	1.01	-0.263	0.458
	γ	1.09	-0.371	0.570
 ***Z*-dienamine M1c**	α	0.91	-0.144	0.362
	γ	0.97	-0.121	0.470

Part 3: The occupied π-type molecular orbitals and computational details of HFV

3.1 The occupied π-type molecular orbitals of benchmark trimethylenemethane



HOMO$^{\alpha}$ (16$^{\alpha}$) HOMO$^{\alpha}$-1 (15$^{\alpha}$) HOMO$^{\alpha}$-2 (14$^{\alpha}$) HOMO$^{\beta}$ (14$^{\beta}$)

Fig. S4. The occupied π-type molecular orbitals of benchmark trimethylenemethane.

3.1.1 Molecular orbital coefficients of benchmark trimethylenemethane

		14^{α}	15^{α}	16^{α}	14^{β}
1C	1S	-0.00003	-0.00001	-0.00002	-0.00003
	2S	0.00006	0.00001	0.00005	0.00006
	2PX	-0.00045	-0.00001	-0.00003	-0.00017
	2PY	-0.00032	0.00001	-0.00011	-0.00017
	2PZ	0.34768	0.00001	0	0.44339
	3S	0.00005	0	-0.00001	0.00005
	3PX	-0.00007	-0.00011	-0.00011	-0.00005
	3PY	-0.00001	-0.00002	0.00001	0.00001
	3PZ	0.17758	0	0	0.27561
	4XX	0.00001	0	0.00001	0.00001
	4YY	-0.00001	0	-0.00001	-0.00001
	4ZZ	-0.00001	0	0	-0.00001
	4XY	-0.00004	0	-0.00003	-0.00002
	4XZ	0	-0.02888	0.0044	0
	4YZ	0	-0.0044	-0.02887	0
2C	1S	-0.00003	0.00002	-0.00003	-0.00001
	2S	0.00008	-0.00005	0.00009	0.00003
	2PX	0.00031	-0.00004	0.00009	0.00008
	2PY	-0.00015	-0.00005	-0.00004	-0.0001
	2PZ	0.25573	0.44775	-0.23596	0.18993
	3S	0.00017	-0.00015	0.00011	0.00007
	3PX	0.00011	-0.00005	-0.00002	0
	3PY	-0.00011	-0.00001	0.00004	-0.00006
	3PZ	0.16925	0.38413	-0.20244	0.12713
	4XX	0	0	0	0
	4YY	-0.00001	0	-0.00001	0
	4ZZ	0	0	0	0.00001
	4XY	-0.00002	0	0	0
	4XZ	0.01272	0.00057	-0.00187	0.01465
	4YZ	-0.00441	-0.00229	-0.00332	-0.00508
3C	1S	0.00007	-0.00001	0.00003	0.00004
	2S	-0.00015	0.00001	-0.00007	-0.00008
	2PX	0.00029	-0.00001	0.00006	0.0001
	2PY	0.00044	0.00001	0.00013	0.00018
	2PZ	0.25573	-0.42821	-0.2698	0.18992
	3S	-0.00031	0.00009	-0.00011	-0.00016
	3PX	0.00015	-0.00002	0.00003	0.00006
	3PY	0.00018	-0.00001	0	0.00005
	3PZ	0.16925	-0.36738	-0.23148	0.12713
	4XX	0	0	0	0
	4YY	0.00002	0	0.00002	0.00001
	4ZZ	0	0	0	0

	4XY	-0.00002	0	0	0
	4XZ	-0.01018	-0.00054	0.00293	-0.01173
	4YZ	-0.00881	0.00252	-0.0022	-0.01015
4C	1S	0.00003	0.00001	0.00007	0.00004
	2S	-0.00007	0	-0.00016	-0.00007
	2PX	0.0008	-0.00001	0.00046	0.00045
	2PY	0.00038	0	0.00022	0.0002
	2PZ	0.25575	-0.01954	0.50572	0.18995
	3S	-0.00004	-0.00012	-0.00032	-0.00003
	3PX	0.0003	0.00009	0.0004	0.00018
	3PY	0.0002	0.00007	0.00024	0.00013
	3PZ	0.16927	-0.01677	0.43389	0.12715
	4XX	0.00001	0	0.00001	0
	4YY	-0.00001	0	0.00001	-0.00001
	4ZZ	0	0	0	0.00001
	4XY	-0.00005	0	0	-0.00002
	4XZ	-0.00254	-0.00415	-0.00044	-0.00293
	4YZ	0.01322	-0.00085	0.0014	0.01523
5H	1S	-0.00006	0.00002	-0.00005	-0.00004
	2S	-0.00006	0.00001	-0.00011	-0.00006
	3PX	0.00001	0	0	0
	3PY	0	0	0	0
	3PZ	0.00515	0.01078	-0.00649	0.00484
6H	1S	-0.00009	0.00002	0	-0.00001
	2S	-0.00017	0.00004	-0.00007	-0.00007
	3PX	0	0	0	0
	3PY	0	0	0	0
	3PZ	0.00515	0.01144	-0.00523	0.00484
7H	1S	0.00021	0	0.00006	0.00009
	2S	0.00024	-0.00001	0.00014	0.00013
	3PX	0.00001	0	0	0
	3PY	0	0	0	0
	3PZ	0.00515	-0.01025	-0.0073	0.00484
8H	1S	0.00004	0	-0.00002	-0.00001
	2S	0.00008	-0.00001	0.00001	0.00001
	3PX	0	0	0	0
	3PY	0.00001	0	0	0
	3PZ	0.00515	-0.01101	-0.00609	0.00485
9H	1S	0.00037	0	0.00009	0.0002
	2S	0.00039	0	0.00011	0.00023
	3PX	0	0	0.00001	0
	3PY	0.00001	0	0.00001	0.00001
	3PZ	0.00515	-0.0012	0.01252	0.00485
10H	1S	-0.00042	0.00001	0.00008	-0.00025

2S	-0.00046	0.00016	0.0001	-0.0003
3PX	0	0	0.00002	0
3PY	0	0	0.00001	0
3PZ	0.00515	0.00023	0.01258	0.00485

3.1.2 Combined coefficients and computational details of P_{max}

$|c_{ki}|$ and $|c_{kj}|$ are absolute values of the normalized combination coefficients of the i and j atoms, respectively, and they were calculated as the arithmetic square root of the values obtained by the squares of all the orbital coefficients of i or j atoms dividing the sum of the squares of all the atomic orbital coefficients in the k_{th} occupied π-type molecular orbital.

Table S3. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of benchmark trimethylenemethane

i/j \ k ; $\lvert c_{ki}\rvert/\lvert c_{kj}\rvert$	14^{α}	15^{α}	16^{α}	14^{β}
1	0.5917	0.0357	0.0357	0.7960
2	0.4653	0.7216	0.3803	0.3493
3	0.4653	0.6901	0.4348	0.3493
4	0.4653	0.4500	0.6803	0.3493

In common structural chemistry and related literature reports, it is believed that the theoretically existing central carbon atom of trimethylenemethane[10] has the largest π bond order of 1.73,[11] which is obtained in the HMO method. Herein, we used the maximum π bond order P_{max} = 1.76 of the center carbon atom of the trimethylenemethane at the B3LYP-D3/6-31G(d, p) level depicted in Scheme 1, and this value is slightly higher than that one (1.73) in the corresponding HMO calculation.

Table S4. The computational details of P_{max}

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	ΣP	P_{max}
C1 (1)	1-2	14^{α} (1), 15^{α} (1), 16^{α} (1), 14^{β} (1)	0.59 [a]	1.76	1.76
	1-3	14^{α} (1), 15^{α} (1), 16^{α} (1), 14^{β} (1)	0.59 [b]		
	1-4	14^{α} (1), 16^{α} (1), 14^{β} (1)	0.58 [c]		

a : $P_{1\text{-}2}$=0.5917*0.4653+0.0357*0.7216+0.0357*0.3803+0.7960*0.3493=0.59
b : $P_{1\text{-}3}$=0.5917*0.4653+0.0357*0.6901+0.0357*0.4348+0.7960*0.3493=0.59
c : $P_{1\text{-}4}$=0.5917*0.4653+0.0357*0.6803+0.0357*0.3493=0.58

Reference

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3.2 The occupied π-type molecular orbitals associated with the active sites of M3

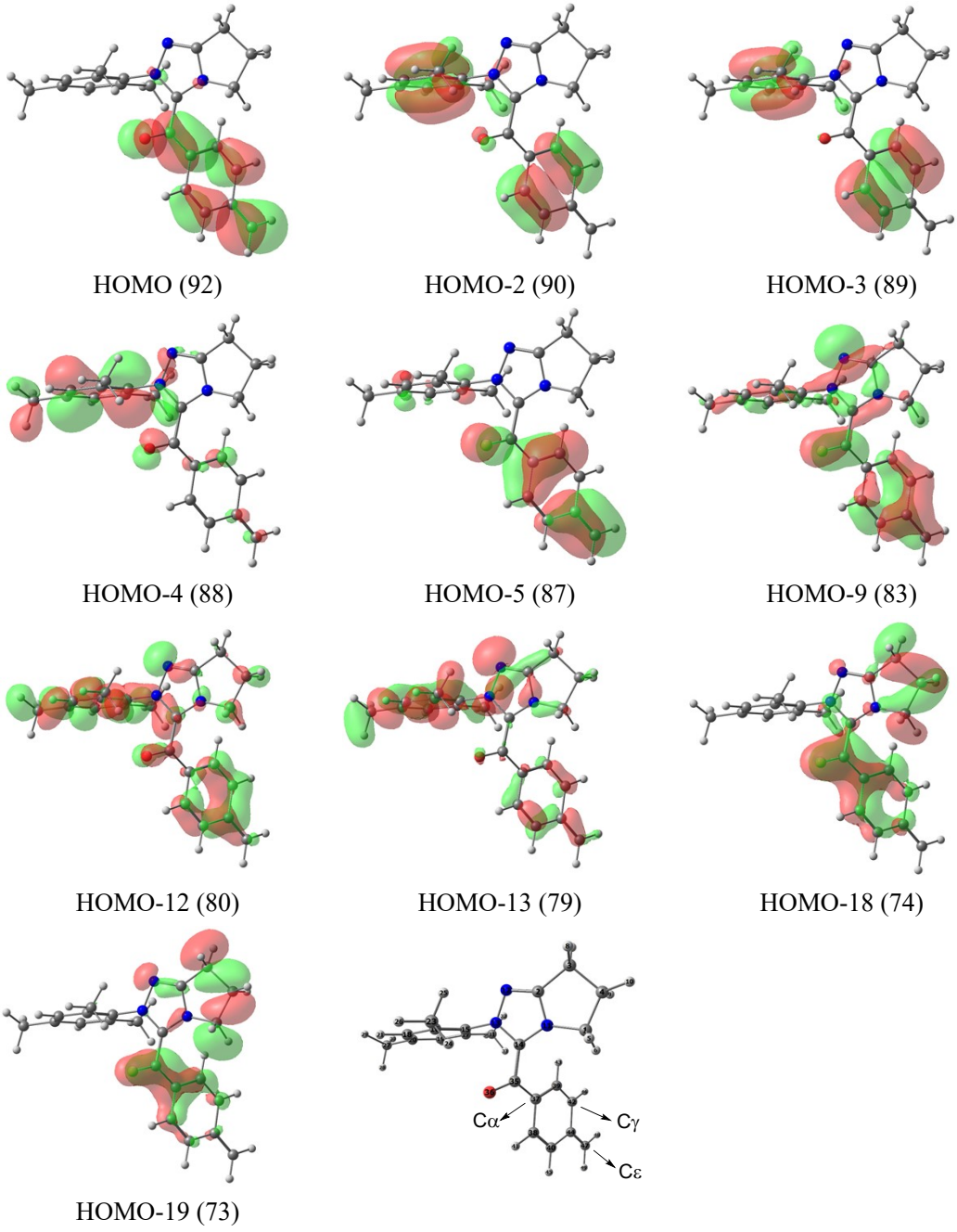


Fig. S5. The occupied π-type molecular orbitals associated with the active sites of **M3**.

3.2.1 Molecular orbital coefficients of M3

			73	74	79	80	83	87	88	89	90	92
1	C	1S	0.0137	-0.0046	-0.0016	0.0039	0.0011	-0.0046	-0.0009	-0.0028	0.0028	0.0014
		2S	-0.0333	0.0165	0.0040	-0.0095	-0.0046	0.0089	0.0022	0.0042	-0.0045	-0.0050
		2PX	0.0698	-0.0731	-0.0445	-0.0094	0.0556	0.0133	-0.0173	0.0138	-0.0055	-0.0013
		2PY	-0.2365	0.1427	-0.0253	0.0197	-0.0284	-0.0261	-0.0022	-0.0136	0.0120	0.0060
		2PZ	0.0826	-0.1145	-0.0322	0.0732	-0.0155	-0.0051	0.0017	-0.0081	0.0057	-0.0021
		3S	-0.0443	-0.0045	0.0304	-0.0229	-0.0179	0.0321	0.0036	0.0287	-0.0263	-0.0065
		3PX	0.0171	-0.0251	-0.0211	-0.0121	0.0354	0.0241	-0.0174	0.0255	-0.0161	0.0043
		3PY	-0.1275	0.0601	-0.0176	0.0174	-0.0154	-0.0016	-0.0028	-0.0117	0.0092	-0.0389
		3PZ	0.0442	-0.0458	-0.0220	0.0384	-0.0066	-0.0148	0.0013	-0.0065	0.0063	0.0157
		4XX	0.0055	-0.0015	0.0014	-0.0020	0.0034	0.0004	0.0003	0.0003	0.0000	-0.0012
		4YY	-0.0008	0.0056	0.0028	-0.0037	-0.0026	-0.0008	-0.0006	-0.0004	0.0004	0.0000
		4ZZ	-0.0019	-0.0045	-0.0034	0.0061	-0.0019	-0.0005	0.0004	-0.0009	0.0007	0.0008
		4XY	-0.0061	0.0057	0.0040	0.0013	-0.0045	-0.0006	0.0002	-0.0007	0.0004	-0.0001
		4XZ	-0.0008	0.0029	0.0000	0.0012	-0.0015	0.0000	0.0006	-0.0005	0.0002	0.0015
		4YZ	0.0074	-0.0030	0.0001	0.0008	-0.0001	0.0007	0.0002	0.0001	-0.0002	0.0004
2	C	1S	-0.0176	-0.0012	-0.0213	0.0149	0.0231	-0.0020	-0.0057	0.0001	0.0007	-0.0011
		2S	0.0429	0.0028	0.0545	-0.0381	-0.0582	0.0063	0.0143	-0.0001	-0.0021	0.0011
		2PX	0.0032	-0.0047	-0.0671	0.0694	0.1148	-0.0067	-0.0228	0.0036	0.0106	0.0066
		2PY	-0.0346	-0.0060	0.0176	0.0252	-0.0108	-0.0045	-0.0252	0.0017	-0.0017	-0.0038
		2PZ	-0.0212	-0.0624	-0.0411	0.0149	-0.0062	-0.0052	-0.0306	-0.0030	0.0009	0.0224
		3S	0.0541	0.0001	0.0312	-0.0361	-0.0561	0.0026	0.0438	-0.0063	-0.0046	0.0232
		3PX	0.0430	-0.0029	0.0254	0.0006	-0.0032	-0.0077	-0.0247	0.0067	0.0075	0.0038
		3PY	-0.0005	-0.0024	0.0183	0.0030	-0.0109	-0.0084	-0.0154	0.0050	-0.0012	0.0101
		3PZ	-0.0019	-0.0366	-0.0076	0.0012	-0.0301	-0.0069	-0.0213	-0.0009	0.0047	0.0183
		4XX	0.0015	-0.0026	-0.0093	0.0042	0.0069	0.0008	0.0016	-0.0006	-0.0003	0.0028
		4YY	-0.0026	0.0016	0.0047	0.0005	-0.0045	-0.0008	-0.0030	0.0003	0.0003	-0.0014
		4ZZ	-0.0031	0.0001	-0.0020	0.0001	0.0050	-0.0003	-0.0001	0.0002	0.0000	-0.0018
		4XY	0.0104	-0.0044	0.0102	-0.0065	-0.0096	-0.0004	-0.0013	0.0004	0.0002	-0.0016
		4XZ	-0.0005	0.0004	-0.0044	0.0010	0.0111	-0.0004	0.0018	0.0001	0.0001	-0.0017
		4YZ	0.0058	-0.0020	0.0017	0.0009	0.0007	0.0004	0.0011	0.0000	0.0001	0.0001
3	C	1S	-0.0097	0.0089	-0.0014	0.0023	0.0019	-0.0001	0.0038	-0.0011	0.0002	0.0021
		2S	0.0258	-0.0210	0.0014	-0.0051	-0.0038	-0.0005	-0.0073	0.0022	-0.0004	-0.0021
		2PX	0.2402	-0.1566	-0.0341	-0.0355	0.0191	0.0109	0.0080	0.0031	-0.0057	0.0005
		2PY	-0.0867	0.0510	-0.0464	0.0126	0.0419	0.0033	0.0222	-0.0038	-0.0001	0.0076
		2PZ	0.1121	-0.1176	-0.0066	0.0293	0.0183	0.0031	0.0069	0.0015	-0.0009	-0.0039
		3S	0.0172	-0.0306	0.0110	-0.0080	-0.0085	0.0078	-0.0193	0.0030	-0.0002	-0.0314
		3PX	0.1182	-0.0778	-0.0152	-0.0190	0.0118	0.0067	0.0075	0.0023	-0.0034	-0.0016
		3PY	-0.0227	0.0246	-0.0180	0.0009	0.0180	-0.0008	0.0144	-0.0016	-0.0006	0.0159
		3PZ	0.0454	-0.0548	-0.0070	0.0163	0.0211	0.0052	0.0018	0.0019	-0.0040	-0.0074
		4XX	0.0093	-0.0069	0.0001	-0.0016	-0.0014	0.0005	0.0007	0.0000	-0.0005	-0.0002
		4YY	-0.0013	0.0015	0.0007	0.0012	0.0007	0.0000	0.0000	0.0001	0.0002	0.0000
		4ZZ	-0.0093	0.0064	-0.0013	0.0005	0.0007	-0.0004	0.0002	-0.0004	0.0003	0.0004

		4XY	0.0017	0.0011	0.0034	-0.0010	-0.0024	0.0004	-0.0004	0.0002	-0.0003	-0.0004
		4XZ	-0.0012	0.0062	0.0011	-0.0034	-0.0003	-0.0001	0.0001	0.0000	0.0000	-0.0003
		4YZ	0.0036	-0.0023	0.0003	0.0013	0.0014	0.0005	0.0016	0.0002	-0.0001	-0.0009
4	C	1S	-0.0035	0.0014	-0.0015	0.0037	0.0045	0.0019	-0.0003	0.0005	0.0000	-0.0011
		2S	0.0066	-0.0040	0.0065	-0.0105	-0.0124	-0.0016	0.0002	-0.0011	-0.0002	-0.0038
		2PX	-0.2044	0.1355	0.0225	0.0404	-0.0003	-0.0075	-0.0061	-0.0019	0.0054	0.0016
		2PY	0.1940	-0.0616	0.0178	-0.0090	0.0216	0.0156	0.0024	0.0050	-0.0051	-0.0026
		2PZ	-0.0896	0.1835	0.0327	-0.0644	-0.0105	-0.0053	-0.0053	0.0001	0.0011	0.0018
		3S	0.0210	0.0084	-0.0074	-0.0104	-0.0071	-0.0233	0.0020	-0.0023	0.0016	0.0445
		3PX	-0.0836	0.0565	0.0183	0.0147	-0.0029	-0.0051	-0.0067	-0.0021	0.0048	-0.0048
		3PY	0.0788	-0.0283	0.0173	-0.0100	0.0030	0.0153	-0.0001	0.0027	-0.0039	-0.0192
		3PZ	-0.0288	0.0862	0.0192	-0.0359	-0.0082	-0.0104	-0.0025	-0.0010	0.0024	0.0106
		4XX	0.0123	-0.0088	-0.0008	-0.0009	0.0010	0.0006	-0.0005	0.0003	-0.0002	-0.0008
		4YY	-0.0071	0.0098	0.0019	-0.0029	0.0004	0.0002	0.0001	0.0002	-0.0002	0.0002
		4ZZ	-0.0059	-0.0012	-0.0008	0.0040	-0.0013	-0.0004	0.0000	-0.0005	0.0004	-0.0005
		4XY	-0.0006	0.0042	0.0026	-0.0001	-0.0012	-0.0003	-0.0003	-0.0001	0.0001	0.0003
		4XZ	0.0008	0.0049	0.0008	-0.0033	0.0000	0.0002	-0.0005	0.0002	-0.0002	0.0003
		4YZ	0.0073	-0.0034	0.0014	0.0005	0.0009	0.0008	0.0000	0.0002	-0.0001	-0.0005
5	H	1S	0.0142	-0.0569	-0.0267	0.0517	-0.0147	-0.0014	0.0023	-0.0054	0.0031	0.0023
		2S	0.0156	-0.0443	-0.0244	0.0472	-0.0079	-0.0002	0.0013	-0.0078	0.0047	0.0096
		3PX	0.0014	-0.0010	-0.0007	-0.0001	0.0008	0.0001	-0.0002	0.0000	0.0001	0.0001
		3PY	-0.0042	0.0036	-0.0001	-0.0002	-0.0007	-0.0007	0.0000	-0.0002	0.0002	0.0005
		3PZ	0.0003	0.0010	0.0008	-0.0011	0.0002	-0.0001	0.0000	0.0001	0.0000	0.0001
6	H	1S	0.1012	-0.0623	-0.0093	-0.0295	0.0443	0.0136	-0.0043	0.0096	-0.0059	-0.0083
		2S	0.0969	-0.0425	-0.0217	-0.0076	0.0326	-0.0250	0.0086	-0.0314	0.0253	-0.0245
		3PX	-0.0031	0.0013	-0.0002	0.0008	-0.0007	-0.0002	-0.0002	0.0001	0.0000	0.0001
		3PY	-0.0020	0.0000	-0.0006	-0.0007	0.0013	0.0013	-0.0006	0.0009	-0.0005	-0.0003
		3PZ	0.0032	-0.0031	-0.0006	0.0007	0.0004	0.0003	-0.0001	0.0002	-0.0001	0.0000
7	H	1S	-0.1170	0.0995	-0.0047	-0.0124	-0.0032	-0.0039	-0.0048	-0.0019	0.0018	0.0051
		2S	-0.1062	0.0864	-0.0132	-0.0065	0.0106	-0.0039	-0.0043	-0.0024	0.0008	0.0066
		3PX	0.0033	-0.0024	-0.0007	-0.0005	0.0002	0.0002	-0.0001	0.0001	-0.0001	0.0001
		3PY	0.0010	-0.0016	-0.0008	0.0006	0.0007	0.0001	0.0004	-0.0001	0.0000	0.0001
		3PZ	-0.0038	0.0028	-0.0004	0.0001	0.0004	-0.0001	0.0000	0.0000	0.0000	0.0001
8	H	1S	-0.0286	-0.0089	-0.0141	0.0291	0.0214	0.0000	0.0095	-0.0007	0.0013	-0.0011
		2S	-0.0273	-0.0090	-0.0185	0.0318	0.0214	-0.0001	0.0137	-0.0016	0.0034	0.0004
		3PX	0.0040	-0.0025	-0.0007	-0.0003	0.0008	0.0002	0.0003	0.0001	0.0000	-0.0001
		3PY	-0.0005	0.0014	-0.0004	-0.0007	0.0005	0.0002	0.0003	0.0000	-0.0001	0.0000
		3PZ	0.0037	-0.0020	0.0005	-0.0006	-0.0007	0.0000	-0.0001	0.0000	-0.0001	0.0000
9	H	1S	-0.0184	-0.0693	-0.0135	0.0517	-0.0015	-0.0030	0.0024	-0.0030	0.0023	-0.0014
		2S	-0.0156	-0.0604	-0.0125	0.0501	-0.0022	-0.0039	0.0039	-0.0043	0.0032	-0.0032
		3PX	-0.0032	0.0037	0.0005	-0.0003	0.0003	0.0000	-0.0002	0.0001	0.0000	0.0000
		3PY	0.0032	-0.0014	0.0001	0.0003	0.0004	0.0001	0.0001	0.0001	-0.0001	0.0002
		3PZ	-0.0024	0.0001	0.0000	0.0011	-0.0001	-0.0002	0.0000	-0.0001	0.0001	0.0000
10	H	1S	0.0138	0.0670	0.0314	-0.0185	0.0024	0.0036	-0.0027	0.0021	-0.0009	0.0004

		2S	0.0101	0.0592	0.0249	-0.0114	0.0063	0.0053	-0.0013	0.0024	-0.0010	0.0028
		3PX	-0.0042	0.0010	-0.0002	0.0011	-0.0003	-0.0003	-0.0002	-0.0001	0.0001	0.0001
		3PY	0.0033	-0.0038	-0.0008	0.0003	0.0004	0.0002	0.0002	0.0000	-0.0001	0.0001
		3PZ	-0.0022	0.0017	-0.0002	-0.0007	-0.0004	-0.0001	-0.0001	-0.0001	0.0001	-0.0001
11	N	1S	0.0156	-0.0004	0.0127	-0.0064	-0.0066	0.0012	0.0046	-0.0011	0.0010	0.0058
		2S	-0.0355	0.0020	-0.0328	0.0149	0.0198	-0.0012	-0.0100	0.0013	-0.0016	-0.0118
		2PX	0.0381	0.0443	0.0929	-0.0178	-0.0886	0.0087	0.0075	-0.0020	-0.0016	0.0090
		2PY	0.0059	0.0391	-0.0142	0.0093	0.0876	0.0070	0.0264	-0.0031	0.0037	0.0159
		2PZ	0.0015	-0.0347	0.0485	-0.0656	0.0084	-0.0087	-0.0074	0.0076	-0.0016	-0.0436
		3S	-0.1037	-0.0092	-0.0595	0.0440	0.0213	-0.0183	-0.0285	0.0194	-0.0122	-0.0574
		3PX	0.0210	0.0293	0.0277	-0.0043	-0.0367	0.0141	-0.0018	-0.0033	0.0001	0.0041
		3PY	-0.0081	0.0341	-0.0282	0.0045	0.0903	0.0224	0.0210	-0.0042	0.0008	0.0152
		3PZ	-0.0008	-0.0269	0.0279	-0.0481	0.0136	-0.0010	-0.0123	0.0108	-0.0047	-0.0486
		4XX	0.0051	-0.0008	0.0036	-0.0044	-0.0006	0.0014	0.0018	0.0003	-0.0010	0.0004
		4YY	-0.0038	0.0017	-0.0006	0.0013	-0.0013	-0.0005	-0.0010	-0.0004	0.0008	0.0009
		4ZZ	0.0028	0.0005	-0.0001	0.0007	0.0017	0.0008	0.0012	-0.0003	0.0004	0.0011
		4XY	-0.0076	0.0052	0.0007	0.0002	0.0005	0.0004	0.0012	0.0002	-0.0008	-0.0007
		4XZ	0.0044	-0.0020	0.0011	0.0018	-0.0023	0.0004	0.0003	0.0000	0.0001	0.0000
		4YZ	-0.0026	-0.0028	-0.0013	0.0029	-0.0031	-0.0004	-0.0005	-0.0007	-0.0003	-0.0021
12	N	1S	0.0120	0.0142	0.0479	-0.0335	-0.0555	0.0038	0.0137	-0.0010	-0.0033	-0.0008
		2S	-0.0266	-0.0297	-0.0968	0.0715	0.1128	-0.0081	-0.0300	0.0018	0.0075	0.0002
		2PX	0.1049	0.0402	0.2308	-0.1579	-0.2364	0.0056	0.0274	0.0011	-0.0028	-0.0199
		2PY	-0.0062	-0.0149	-0.0870	0.0006	0.0472	0.0188	0.0570	-0.0082	-0.0164	0.0226
		2PZ	-0.0111	-0.0106	0.0676	-0.0269	-0.1948	0.0009	-0.0274	-0.0058	0.0008	0.0222
		3S	-0.0226	-0.0678	-0.1993	0.1386	0.2424	-0.0272	-0.1016	0.0099	0.0218	0.0092
		3PX	0.0697	0.0223	0.1541	-0.0968	-0.1512	0.0007	-0.0093	0.0063	0.0043	-0.0241
		3PY	-0.0089	-0.0027	-0.0382	0.0063	0.0228	0.0150	0.0285	-0.0027	-0.0089	0.0111
		3PZ	-0.0030	-0.0089	0.0394	-0.0177	-0.1251	0.0014	-0.0265	-0.0051	0.0002	0.0182
		4XX	0.0073	0.0039	0.0156	-0.0103	-0.0136	0.0012	0.0042	0.0000	-0.0006	-0.0016
		4YY	-0.0020	0.0009	0.0047	-0.0018	-0.0045	-0.0005	-0.0004	-0.0001	-0.0002	0.0009
		4ZZ	-0.0021	0.0004	-0.0009	0.0010	-0.0031	0.0005	0.0005	-0.0003	-0.0001	-0.0003
		4XY	-0.0030	-0.0012	-0.0064	0.0001	0.0014	0.0009	0.0039	-0.0005	-0.0010	-0.0002
		4XZ	0.0009	-0.0008	0.0072	-0.0039	-0.0124	0.0004	-0.0012	-0.0002	-0.0002	0.0012
		4YZ	0.0000	-0.0030	-0.0045	0.0005	0.0048	0.0001	-0.0003	0.0000	-0.0001	0.0021
13	N	1S	-0.0084	-0.0118	-0.0041	0.0198	0.0148	-0.0002	-0.0015	0.0005	-0.0002	-0.0065
		2S	0.0180	0.0257	0.0125	-0.0446	-0.0344	0.0035	0.0033	0.0000	-0.0010	0.0078
		2PX	0.0256	0.0094	0.0197	0.0514	0.0945	0.0000	-0.0015	-0.0018	-0.0023	0.0384
		2PY	-0.0126	0.0271	0.1150	0.0257	-0.0692	-0.0031	-0.0021	0.0017	0.0011	-0.0235
		2PZ	-0.0092	0.0466	-0.0357	0.0313	0.0281	0.0086	0.0434	-0.0010	-0.0028	-0.0391
		3S	0.0521	0.0781	0.0098	-0.1270	-0.0921	-0.0143	0.0130	-0.0143	0.0161	0.0922
		3PX	0.0273	0.0037	0.0529	0.0327	0.0273	-0.0410	-0.0041	-0.0055	0.0055	0.0900
		3PY	-0.0218	0.0133	0.0850	0.0327	-0.0437	-0.0039	0.0280	0.0047	-0.0068	-0.0192
		3PZ	-0.0028	0.0278	-0.0157	0.0150	0.0032	-0.0084	0.0212	-0.0017	0.0009	-0.0184
		4XX	-0.0031	-0.0023	-0.0001	0.0027	0.0027	0.0037	0.0131	-0.0017	-0.0037	-0.0013

		4YY	-0.0003	-0.0025	0.0019	0.0022	-0.0062	-0.0025	-0.0150	0.0011	0.0028	-0.0038
		4ZZ	0.0000	0.0006	-0.0009	0.0006	0.0066	0.0007	0.0016	0.0010	0.0001	-0.0015
		4XY	0.0048	0.0030	0.0105	-0.0083	-0.0087	0.0006	0.0006	0.0006	-0.0002	-0.0003
		4XZ	-0.0015	0.0011	-0.0018	-0.0011	0.0054	0.0010	0.0073	-0.0001	-0.0009	0.0011
		4YZ	-0.0005	0.0003	0.0009	-0.0038	-0.0050	0.0021	0.0057	-0.0011	-0.0020	0.0010
14	C	1S	0.0091	0.0015	0.0011	-0.0083	-0.0083	-0.0071	-0.0185	0.0019	-0.0008	0.0022
		2S	-0.0235	-0.0056	-0.0039	0.0239	0.0227	0.0124	0.0480	-0.0037	0.0010	0.0030
		2PX	-0.0141	-0.0196	0.0242	-0.0228	-0.1047	-0.0098	-0.0449	0.0020	0.0163	-0.0052
		2PY	-0.0128	0.0147	-0.0151	-0.0208	0.0337	-0.0105	-0.0289	0.0056	-0.0104	0.0122
		2PZ	0.0317	0.0566	0.0404	-0.0589	0.0357	0.0055	0.0216	0.0041	0.0075	0.0314
		3S	-0.0412	0.0070	-0.0346	0.0312	0.0663	0.0865	0.0903	-0.0104	0.0075	-0.0763
		3PX	0.0216	0.0170	0.0364	-0.0089	-0.0434	-0.0324	-0.0003	-0.0174	0.0259	0.0883
		3PY	0.0228	0.0325	-0.0180	-0.0280	0.0485	0.0170	-0.0189	-0.0060	-0.0078	0.0296
		3PZ	0.0182	0.0322	0.0333	-0.0267	0.0117	-0.0130	0.0263	-0.0045	0.0113	0.0494
		4XX	0.0054	0.0063	0.0001	-0.0006	0.0022	-0.0008	0.0003	0.0003	0.0002	0.0047
		4YY	-0.0072	-0.0099	-0.0030	0.0016	-0.0036	-0.0015	-0.0011	0.0007	-0.0004	-0.0080
		4ZZ	0.0034	0.0028	0.0016	-0.0008	0.0012	0.0010	-0.0015	-0.0002	0.0003	0.0045
		4XY	-0.0022	-0.0060	-0.0042	0.0006	-0.0033	-0.0018	-0.0028	0.0001	-0.0001	-0.0012
		4XZ	0.0047	0.0028	0.0020	-0.0027	0.0053	0.0006	-0.0014	0.0001	0.0007	0.0055
		4YZ	-0.0001	-0.0009	0.0000	-0.0033	0.0023	0.0006	0.0003	0.0003	0.0000	-0.0031
15	C	1S	-0.0008	-0.0003	-0.0184	-0.0102	-0.0023	-0.0001	0.0009	-0.0002	-0.0001	-0.0001
		2S	0.0062	0.0063	0.0476	0.0187	0.0053	0.0072	-0.0034	-0.0005	0.0022	-0.0065
		2PX	0.0113	-0.0154	-0.0669	-0.0195	-0.0185	-0.0470	-0.1912	0.0155	0.0424	-0.0084
		2PY	-0.0034	-0.0002	0.0331	-0.0675	-0.0471	0.0560	0.2251	-0.0175	-0.0525	0.0028
		2PZ	-0.0025	-0.0021	-0.0311	0.1072	0.0425	-0.0383	-0.1686	0.0131	0.0386	-0.0040
		3S	-0.0135	-0.0130	0.0280	0.0145	-0.0253	-0.0246	0.0066	0.0079	-0.0042	0.0265
		3PX	-0.0043	-0.0229	0.0182	0.0571	0.0052	-0.0592	-0.1252	0.0121	0.0239	0.0216
		3PY	0.0023	-0.0022	0.0700	0.0142	0.0029	0.0204	0.1587	-0.0127	-0.0335	0.0220
		3PZ	0.0071	0.0003	-0.0074	0.0585	0.0144	-0.0333	-0.1002	0.0098	0.0284	0.0019
		4XX	0.0008	0.0001	-0.0054	-0.0052	-0.0004	0.0003	-0.0011	-0.0041	-0.0049	0.0005
		4YY	-0.0001	0.0008	-0.0052	-0.0035	-0.0027	0.0003	-0.0019	-0.0046	-0.0047	-0.0015
		4ZZ	0.0002	0.0005	0.0056	0.0034	0.0019	0.0010	0.0027	0.0085	0.0103	-0.0009
		4XY	0.0002	0.0002	-0.0073	-0.0073	-0.0037	-0.0001	0.0017	0.0050	0.0061	0.0008
		4XZ	-0.0010	0.0000	-0.0034	-0.0042	-0.0017	0.0000	0.0032	0.0039	0.0042	-0.0018
		4YZ	0.0006	0.0015	0.0021	-0.0011	-0.0007	0.0004	-0.0003	-0.0052	-0.0062	-0.0017
16	C	1S	-0.0007	-0.0003	0.0069	0.0064	-0.0003	-0.0001	0.0015	-0.0001	-0.0004	-0.0021
		2S	0.0040	0.0038	-0.0143	-0.0164	0.0021	0.0045	-0.0040	0.0009	0.0041	-0.0007
		2PX	-0.0001	-0.0114	0.0847	0.1396	0.0681	-0.0097	-0.0452	0.1022	0.1355	0.0018
		2PY	0.0171	-0.0055	0.1522	0.0112	0.0147	0.0155	0.0438	-0.1222	-0.1588	0.0053
		2PZ	0.0049	-0.0174	-0.0011	-0.0216	-0.0027	-0.0100	-0.0264	0.0870	0.1127	-0.0087
		3S	-0.0101	-0.0102	-0.0301	-0.0118	0.0003	-0.0145	-0.0049	-0.0028	-0.0080	0.0281
		3PX	-0.0019	-0.0064	0.0313	0.0566	0.0292	-0.0040	-0.0396	0.0683	0.0864	-0.0029
		3PY	0.0062	0.0054	0.0407	-0.0169	-0.0022	0.0263	0.0290	-0.0830	-0.1067	-0.0160
		3PZ	0.0020	0.0018	-0.0386	-0.0178	-0.0134	-0.0007	-0.0202	0.0612	0.0798	-0.0118

		4XX	0.0004	0.0004	-0.0016	0.0007	-0.0004	-0.0032	-0.0149	-0.0043	-0.0033	-0.0010
		4YY	0.0011	-0.0002	-0.0040	-0.0003	0.0003	0.0023	0.0071	0.0067	0.0077	-0.0013
		4ZZ	-0.0007	0.0008	0.0088	0.0003	0.0011	0.0025	0.0077	-0.0025	-0.0036	-0.0003
		4XY	0.0002	0.0001	-0.0027	-0.0050	-0.0028	0.0018	0.0069	-0.0003	-0.0012	-0.0004
		4XZ	0.0003	-0.0006	-0.0016	-0.0084	-0.0037	-0.0007	-0.0012	-0.0039	-0.0047	0.0004
		4YZ	0.0006	-0.0004	0.0011	-0.0007	0.0006	-0.0022	-0.0088	-0.0008	0.0003	0.0000
17	C	1S	0.0012	-0.0016	0.0074	0.0032	0.0014	-0.0004	-0.0014	-0.0001	0.0002	0.0015
		2S	-0.0015	0.0049	-0.0162	-0.0098	-0.0039	0.0018	0.0025	-0.0002	-0.0012	-0.0013
		2PX	0.0076	0.0142	0.0978	0.1676	0.0638	-0.0143	-0.1002	-0.0926	-0.1023	-0.0011
		2PY	-0.0046	0.0037	0.1312	0.0206	0.0001	0.0225	0.1268	0.1114	0.1189	-0.0027
		2PZ	0.0130	0.0067	-0.0416	-0.0461	-0.0040	-0.0143	-0.0764	-0.0784	-0.0819	-0.0056
		3S	-0.0007	0.0035	-0.0224	0.0032	-0.0010	-0.0094	0.0134	0.0027	0.0028	-0.0002
		3PX	0.0074	0.0081	0.0093	0.0267	0.0162	0.0069	-0.0754	-0.0647	-0.0719	-0.0228
		3PY	0.0039	0.0059	0.0650	0.0044	0.0060	0.0193	0.0923	0.0722	0.0808	-0.0047
		3PZ	0.0092	0.0007	0.0205	0.0514	0.0258	-0.0141	-0.0533	-0.0537	-0.0501	-0.0063
		4XX	0.0007	0.0012	0.0009	-0.0027	-0.0020	-0.0020	-0.0032	0.0068	0.0091	0.0005
		4YY	0.0003	0.0003	-0.0010	-0.0041	-0.0011	0.0037	0.0123	-0.0065	-0.0099	0.0012
		4ZZ	0.0000	-0.0009	0.0036	0.0090	0.0041	-0.0018	-0.0095	-0.0003	0.0007	0.0001
		4XY	0.0002	-0.0002	-0.0055	-0.0019	-0.0010	-0.0008	-0.0044	-0.0015	-0.0012	0.0003
		4XZ	0.0001	-0.0007	-0.0037	-0.0059	-0.0020	-0.0021	-0.0081	0.0030	0.0049	-0.0010
		4YZ	0.0004	0.0002	0.0046	-0.0036	-0.0010	0.0003	0.0029	0.0027	0.0031	0.0002
18	C	1S	-0.0014	0.0020	-0.0010	0.0045	0.0029	0.0001	-0.0005	0.0003	0.0005	0.0009
		2S	0.0024	-0.0048	-0.0016	-0.0141	-0.0079	-0.0005	0.0019	-0.0010	-0.0014	-0.0016
		2PX	-0.0102	0.0041	-0.1354	-0.0605	-0.0254	0.0326	0.1326	0.0987	0.1058	-0.0077
		2PY	-0.0002	0.0158	-0.0833	-0.0870	-0.0543	-0.0396	-0.1511	-0.1148	-0.1243	0.0027
		2PZ	0.0030	0.0047	-0.0623	0.0775	0.0218	0.0267	0.1050	0.0843	0.0916	-0.0028
		3S	0.0094	0.0000	0.0186	-0.0067	-0.0044	0.0152	-0.0008	0.0066	0.0079	-0.0209
		3PX	-0.0016	0.0032	-0.0340	0.0032	0.0023	0.0315	0.0958	0.0728	0.0794	-0.0150
		3PY	0.0013	0.0060	-0.0060	-0.0388	-0.0237	-0.0260	-0.1201	-0.0899	-0.0985	-0.0021
		3PZ	-0.0021	-0.0027	-0.0341	0.0219	0.0109	0.0182	0.0763	0.0577	0.0627	-0.0035
		4XX	-0.0004	0.0004	-0.0056	0.0031	0.0012	-0.0004	-0.0020	0.0052	0.0068	-0.0001
		4YY	-0.0001	0.0004	-0.0029	-0.0053	-0.0016	0.0025	0.0091	-0.0056	-0.0084	0.0003
		4ZZ	0.0003	-0.0004	0.0091	0.0053	0.0018	-0.0020	-0.0071	0.0007	0.0019	0.0000
		4XY	-0.0004	0.0006	-0.0054	-0.0062	-0.0026	-0.0009	-0.0031	-0.0006	-0.0003	0.0000
		4XZ	-0.0006	-0.0003	-0.0048	-0.0084	-0.0030	-0.0019	-0.0057	0.0029	0.0045	-0.0004
		4YZ	0.0000	-0.0006	0.0014	0.0005	0.0008	0.0007	0.0022	0.0020	0.0022	-0.0003
19	C	1S	-0.0023	-0.0020	-0.0018	-0.0028	0.0004	0.0005	0.0005	-0.0002	-0.0007	-0.0006
		2S	0.0048	0.0040	0.0006	0.0071	-0.0012	-0.0016	-0.0008	0.0008	0.0020	0.0022
		2PX	-0.0025	-0.0056	-0.1586	-0.1128	-0.0265	0.0266	0.0626	-0.1129	-0.1480	0.0061
		2PY	-0.0048	-0.0125	-0.0559	-0.1001	-0.0490	-0.0362	-0.0799	0.1304	0.1745	-0.0040
		2PZ	0.0089	-0.0036	0.0061	0.1252	0.0406	0.0258	0.0533	-0.0902	-0.1215	0.0043
		3S	0.0127	0.0122	0.0188	-0.0044	0.0011	0.0139	-0.0055	-0.0100	-0.0096	-0.0138
		3PX	0.0035	-0.0005	-0.0445	-0.0184	0.0040	0.0244	0.0485	-0.0815	-0.1073	0.0034
		3PY	0.0002	-0.0051	0.0077	-0.0461	-0.0230	-0.0197	-0.0619	0.0977	0.1304	-0.0117

		3PZ	0.0040	0.0008	0.0000	0.0377	0.0158	0.0213	0.0428	-0.0717	-0.0984	0.0030
		4XX	-0.0001	0.0000	-0.0049	-0.0002	-0.0002	-0.0028	-0.0117	-0.0043	-0.0036	-0.0001
		4YY	-0.0006	-0.0002	-0.0011	-0.0070	-0.0026	0.0008	0.0054	0.0048	0.0052	-0.0002
		4ZZ	0.0002	-0.0002	0.0062	0.0060	0.0029	0.0021	0.0065	-0.0008	-0.0020	0.0000
		4XY	-0.0004	-0.0001	-0.0070	-0.0040	-0.0012	0.0016	0.0053	0.0003	-0.0004	-0.0002
		4XZ	0.0001	0.0003	-0.0050	-0.0045	-0.0009	0.0000	-0.0007	-0.0023	-0.0027	0.0000
		4YZ	0.0004	0.0004	0.0038	-0.0024	-0.0003	-0.0019	-0.0068	-0.0014	-0.0006	-0.0002
20	C	1S	0.0015	0.0008	-0.0011	-0.0012	-0.0009	-0.0001	0.0007	-0.0001	0.0001	0.0001
		2S	-0.0031	-0.0014	0.0019	0.0025	0.0021	0.0011	0.0002	0.0001	-0.0006	-0.0007
		2PX	0.0126	-0.0062	0.1367	0.1809	0.0664	0.0510	0.1674	-0.0105	-0.0378	0.0018
		2PY	0.0078	-0.0116	0.1675	0.0354	0.0102	-0.0546	-0.1895	0.0124	0.0414	-0.0028
		2PZ	-0.0034	-0.0093	-0.0117	-0.0655	-0.0019	0.0394	0.1389	-0.0100	-0.0305	0.0008
		3S	-0.0057	-0.0081	0.0227	0.0220	0.0107	-0.0051	-0.0116	0.0001	0.0010	0.0016
		3PX	0.0007	-0.0034	-0.0011	0.0462	0.0167	0.0278	0.1138	-0.0018	-0.0187	0.0072
		3PY	-0.0012	-0.0037	0.0264	-0.0236	-0.0120	-0.0413	-0.1291	0.0037	0.0232	0.0027
		3PZ	-0.0021	-0.0030	-0.0140	-0.0252	0.0001	0.0259	0.0882	-0.0182	-0.0350	-0.0007
		4XX	0.0002	0.0006	-0.0080	0.0021	0.0007	0.0022	0.0061	-0.0044	-0.0063	0.0003
		4YY	-0.0003	-0.0001	-0.0014	-0.0089	-0.0036	-0.0026	-0.0089	-0.0043	-0.0041	0.0002
		4ZZ	0.0003	-0.0004	0.0073	0.0053	0.0021	0.0004	0.0034	0.0086	0.0103	-0.0003
		4XY	-0.0006	-0.0001	-0.0079	-0.0067	-0.0028	-0.0004	0.0007	0.0051	0.0063	-0.0002
		4XZ	-0.0006	-0.0009	-0.0053	-0.0054	-0.0012	0.0011	0.0046	0.0036	0.0039	-0.0003
		4YZ	0.0000	-0.0007	0.0014	-0.0002	0.0009	0.0010	0.0018	-0.0057	-0.0073	0.0002
21	H	1S	0.0071	-0.0012	0.0436	0.0801	0.0267	0.0002	-0.0024	0.0003	0.0007	0.0022
		2S	0.0066	0.0022	0.0578	0.1008	0.0337	0.0020	-0.0016	0.0014	0.0020	0.0029
		3PX	0.0000	-0.0001	-0.0011	0.0013	0.0003	0.0006	0.0030	0.0025	0.0027	0.0000
		3PY	-0.0001	0.0002	-0.0012	-0.0013	-0.0009	-0.0010	-0.0037	-0.0028	-0.0031	0.0001
		3PZ	-0.0004	0.0002	-0.0024	-0.0009	-0.0003	0.0006	0.0027	0.0021	0.0023	-0.0001
22	H	1S	0.0003	0.0077	0.0382	-0.0171	0.0007	-0.0002	0.0028	-0.0002	0.0004	-0.0011
		2S	0.0004	0.0043	0.0502	-0.0198	0.0016	0.0020	0.0055	-0.0017	-0.0029	-0.0030
		3PX	-0.0001	-0.0001	-0.0026	-0.0018	-0.0004	0.0006	0.0014	-0.0028	-0.0037	0.0002
		3PY	-0.0001	0.0001	0.0001	-0.0023	-0.0009	-0.0009	-0.0019	0.0033	0.0043	-0.0001
		3PZ	0.0002	0.0005	0.0012	0.0014	0.0007	0.0006	0.0013	-0.0022	-0.0029	0.0001
23	C	1S	-0.0007	0.0017	-0.0061	0.0031	0.0008	-0.0001	-0.0014	0.0004	-0.0001	-0.0007
		2S	0.0015	-0.0020	0.0118	-0.0068	0.0011	0.0020	0.0020	-0.0011	0.0000	-0.0010
		2PX	0.0082	-0.0135	-0.0573	-0.0843	-0.0385	0.0063	0.0224	-0.0353	-0.0420	0.0028
		2PY	0.0241	0.0037	-0.1012	0.0115	-0.0094	-0.0099	-0.0208	0.0408	0.0498	0.0003
		2PZ	-0.0364	0.0161	-0.0202	0.0135	-0.0052	0.0041	0.0132	-0.0292	-0.0368	0.0022
		3S	0.0049	-0.0163	0.0566	-0.0063	-0.0119	-0.0104	0.0166	-0.0013	0.0017	0.0161
		3PX	0.0002	-0.0104	-0.0356	-0.0394	-0.0236	0.0016	0.0225	-0.0121	-0.0132	0.0074
		3PY	0.0156	0.0068	-0.0490	-0.0048	-0.0112	-0.0015	-0.0195	0.0115	0.0165	-0.0082
		3PZ	-0.0199	0.0045	-0.0186	0.0009	-0.0106	0.0039	0.0169	-0.0097	-0.0126	0.0035
		4XX	-0.0017	0.0008	-0.0001	-0.0012	-0.0008	0.0004	0.0005	-0.0040	-0.0050	-0.0003
		4YY	0.0017	-0.0002	-0.0061	0.0002	0.0003	-0.0006	-0.0027	0.0081	0.0105	-0.0007
		4ZZ	-0.0001	0.0003	0.0050	0.0013	0.0014	0.0009	0.0019	-0.0042	-0.0054	-0.0001

		4XY	-0.0002	0.0005	-0.0001	-0.0004	-0.0002	0.0005	0.0010	-0.0011	-0.0014	-0.0004
		4XZ	0.0009	-0.0008	-0.0037	-0.0072	-0.0030	0.0005	0.0018	-0.0048	-0.0062	0.0004
		4YZ	0.0000	-0.0006	0.0030	-0.0005	0.0007	-0.0002	-0.0009	0.0003	0.0006	0.0001
24	H	1S	-0.0077	-0.0024	-0.0234	-0.0541	-0.0250	0.0071	0.0207	-0.0480	-0.0600	0.0014
		2S	0.0010	0.0137	-0.0168	-0.0554	-0.0110	0.0134	-0.0009	-0.0628	-0.0812	-0.0158
		3PX	0.0006	0.0001	0.0001	0.0008	0.0004	-0.0004	-0.0010	0.0013	0.0014	-0.0002
		3PY	0.0004	0.0002	-0.0023	-0.0007	-0.0003	0.0004	0.0007	-0.0002	-0.0001	-0.0003
		3PZ	-0.0005	0.0002	0.0002	0.0013	0.0005	0.0003	0.0005	-0.0004	-0.0004	0.0001
25	H	1S	0.0212	-0.0023	-0.0633	0.0051	-0.0043	-0.0082	-0.0187	0.0472	0.0591	-0.0001
		2S	0.0087	-0.0070	-0.0836	0.0195	0.0104	-0.0096	-0.0144	0.0627	0.0774	0.0078
		3PX	0.0000	-0.0002	-0.0016	-0.0015	-0.0008	0.0002	0.0005	-0.0007	-0.0009	-0.0001
		3PY	-0.0005	0.0003	0.0012	-0.0002	-0.0001	0.0002	0.0000	-0.0007	-0.0007	-0.0002
		3PZ	-0.0001	0.0003	-0.0010	0.0001	-0.0002	-0.0003	-0.0008	0.0006	0.0009	0.0001
26	H	1S	-0.0216	0.0123	0.0424	0.0525	0.0213	0.0002	-0.0026	0.0002	-0.0004	-0.0007
		2S	-0.0189	0.0122	0.0359	0.0571	0.0242	0.0006	-0.0052	0.0001	-0.0002	-0.0021
		3PX	-0.0007	0.0002	0.0003	0.0000	0.0001	0.0002	0.0004	-0.0008	-0.0010	0.0000
		3PY	0.0002	0.0001	-0.0016	0.0006	0.0001	-0.0004	-0.0007	0.0009	0.0011	0.0002
		3PZ	0.0001	0.0000	-0.0013	-0.0012	-0.0006	0.0002	0.0005	-0.0006	-0.0008	0.0000
27	C	1S	0.0006	-0.0003	0.0159	0.0121	0.0050	0.0001	-0.0002	0.0001	0.0000	0.0000
		2S	-0.0014	0.0004	-0.0332	-0.0250	-0.0104	-0.0005	-0.0003	0.0000	0.0002	-0.0001
		2PX	-0.0126	-0.0029	-0.1191	-0.1551	-0.0561	-0.0202	-0.0597	0.0018	0.0109	0.0001
		2PY	-0.0092	0.0166	-0.1750	-0.0538	-0.0192	0.0196	0.0653	-0.0025	-0.0114	0.0002
		2PZ	0.0027	0.0324	0.0193	0.0183	-0.0089	-0.0148	-0.0455	0.0065	0.0140	-0.0009
		3S	-0.0055	0.0024	-0.1057	-0.0779	-0.0323	-0.0032	0.0044	-0.0001	-0.0002	0.0036
		3PX	-0.0060	0.0001	-0.0650	-0.0824	-0.0302	-0.0093	-0.0258	-0.0059	-0.0033	0.0014
		3PY	-0.0049	0.0077	-0.1009	-0.0359	-0.0134	0.0074	0.0281	0.0055	0.0036	0.0006
		3PZ	0.0015	0.0144	0.0141	0.0085	-0.0037	-0.0061	-0.0144	0.0159	0.0219	-0.0006
		4XX	-0.0001	0.0012	-0.0035	0.0034	0.0011	0.0028	0.0095	-0.0008	-0.0024	0.0002
		4YY	-0.0002	0.0002	0.0018	-0.0041	-0.0020	-0.0037	-0.0125	0.0004	0.0023	-0.0001
		4ZZ	0.0003	-0.0015	0.0046	0.0031	0.0018	0.0008	0.0029	0.0004	0.0002	0.0000
		4XY	-0.0007	-0.0003	-0.0074	-0.0059	-0.0018	0.0001	0.0003	0.0003	0.0004	0.0000
		4XZ	-0.0002	-0.0012	-0.0004	-0.0044	-0.0009	0.0003	0.0014	0.0001	0.0000	0.0001
		4YZ	0.0000	-0.0004	-0.0022	0.0009	0.0012	0.0025	0.0082	-0.0009	-0.0023	0.0002
28	H	1S	0.0030	0.0005	0.0713	-0.0060	-0.0087	-0.0271	-0.0888	0.0057	0.0190	-0.0009
		2S	0.0027	0.0002	0.0687	-0.0014	-0.0066	-0.0320	-0.1079	0.0080	0.0247	-0.0013
		3PX	-0.0003	-0.0001	-0.0035	-0.0028	-0.0009	0.0003	0.0012	-0.0001	-0.0003	0.0000
		3PY	0.0000	0.0003	-0.0003	-0.0009	-0.0005	-0.0003	-0.0007	0.0001	0.0002	0.0000
		3PZ	0.0000	0.0006	-0.0014	0.0006	0.0000	0.0003	0.0010	0.0001	-0.0001	0.0000
29	H	1S	0.0054	0.0157	0.0190	0.0768	0.0224	0.0149	0.0472	-0.0024	-0.0098	0.0002
		2S	0.0057	0.0144	0.0303	0.0846	0.0264	0.0178	0.0524	-0.0152	-0.0268	0.0009
		3PX	0.0000	0.0006	-0.0011	0.0002	-0.0002	-0.0001	-0.0004	-0.0002	-0.0002	0.0000
		3PY	-0.0002	0.0000	-0.0033	-0.0022	-0.0007	0.0000	-0.0001	-0.0004	-0.0004	0.0001
		3PZ	-0.0001	0.0002	0.0000	-0.0010	-0.0006	-0.0007	-0.0022	0.0002	0.0005	0.0000
30	H	1S	0.0011	-0.0227	0.0211	0.0083	0.0136	0.0125	0.0402	-0.0031	-0.0092	0.0006

		2S	0.0016	-0.0201	0.0332	0.0130	0.0165	0.0150	0.0515	0.0075	0.0028	-0.0001
		3PX	-0.0002	-0.0003	-0.0016	-0.0027	-0.0009	-0.0005	-0.0016	0.0003	0.0006	0.0000
		3PY	-0.0001	0.0000	-0.0028	-0.0007	-0.0002	0.0004	0.0015	0.0002	0.0001	0.0000
		3PZ	0.0001	-0.0005	0.0013	0.0008	0.0005	0.0002	0.0006	-0.0001	-0.0002	0.0000
31	C	1S	-0.0015	-0.0026	-0.0062	-0.0113	-0.0022	0.0024	-0.0011	0.0016	-0.0011	-0.0019
		2S	0.0011	0.0036	0.0124	0.0229	0.0072	-0.0009	0.0008	-0.0002	0.0002	0.0021
		2PX	0.0211	0.0397	-0.0706	-0.1570	-0.0496	-0.0094	0.0396	0.0217	0.0380	0.0068
		2PY	-0.0156	-0.0007	-0.0885	-0.0159	-0.0167	-0.0043	-0.0426	-0.0319	-0.0366	-0.0039
		2PZ	0.0089	0.0422	0.0486	0.0475	0.0155	-0.0021	0.0291	0.0218	0.0288	0.0067
		3S	0.0150	0.0187	0.0547	0.0880	0.0074	-0.0392	0.0137	-0.0228	0.0182	0.0327
		3PX	0.0156	0.0273	-0.0447	-0.0916	-0.0363	-0.0179	0.0260	-0.0028	0.0176	0.0174
		3PY	-0.0090	-0.0042	-0.0403	-0.0130	-0.0171	0.0035	-0.0321	0.0004	-0.0067	-0.0061
		3PZ	0.0049	0.0197	0.0276	0.0369	0.0154	-0.0069	0.0151	0.0033	0.0137	0.0058
		4XX	0.0004	0.0016	0.0003	-0.0052	-0.0016	0.0008	0.0069	0.0070	0.0078	0.0002
		4YY	-0.0008	-0.0014	-0.0051	-0.0025	-0.0007	0.0005	-0.0029	-0.0031	-0.0045	-0.0001
		4ZZ	-0.0002	-0.0012	0.0036	0.0055	0.0025	-0.0002	-0.0045	-0.0028	-0.0040	-0.0003
		4XY	-0.0004	-0.0015	-0.0018	0.0019	0.0008	-0.0002	-0.0049	-0.0037	-0.0044	-0.0003
		4XZ	0.0007	0.0001	-0.0016	-0.0051	-0.0016	-0.0005	0.0002	0.0007	0.0012	0.0001
		4YZ	0.0000	-0.0015	0.0057	0.0019	0.0010	0.0009	0.0036	0.0034	0.0034	0.0002
32	H	1S	-0.0091	-0.0058	-0.0725	-0.0210	-0.0126	-0.0056	-0.0419	-0.0374	-0.0413	-0.0027
		2S	-0.0105	-0.0065	-0.0847	-0.0170	0.0111	-0.0053	-0.0428	-0.0524	-0.0608	-0.0043
		3PX	0.0005	0.0007	-0.0011	-0.0029	-0.0009	-0.0001	0.0001	0.0004	0.0006	0.0000
		3PY	0.0003	0.0002	0.0019	0.0006	0.0004	0.0003	0.0009	0.0009	0.0008	0.0001
		3PZ	0.0000	0.0006	-0.0005	0.0003	0.0006	0.0000	0.0009	0.0004	0.0005	0.0003
33	H	1S	0.0154	0.0314	-0.0089	-0.0778	-0.0239	-0.0007	0.0517	0.0404	0.0516	0.0039
		2S	-0.0026	0.0059	-0.0029	-0.0820	-0.0174	0.0416	0.0406	0.0814	0.0501	-0.0277
		3PX	-0.0006	-0.0008	-0.0008	0.0005	0.0000	0.0001	-0.0005	-0.0005	-0.0008	0.0001
		3PY	-0.0002	0.0003	-0.0020	-0.0017	-0.0006	0.0001	-0.0003	0.0000	-0.0002	-0.0002
		3PZ	-0.0004	-0.0003	0.0009	0.0024	0.0004	0.0001	-0.0013	-0.0005	-0.0007	-0.0007
34	H	1S	-0.0013	-0.0269	0.0345	0.0243	0.0120	0.0034	-0.0078	-0.0048	-0.0089	-0.0024
		2S	-0.0013	-0.0244	0.0295	0.0135	0.0091	0.0045	-0.0143	-0.0026	-0.0073	-0.0060
		3PX	0.0003	0.0003	-0.0008	-0.0022	-0.0006	0.0001	0.0008	0.0003	0.0004	-0.0001
		3PY	-0.0003	-0.0008	-0.0009	0.0006	0.0001	-0.0002	-0.0012	-0.0010	-0.0010	-0.0002
		3PZ	0.0002	-0.0003	0.0020	0.0014	0.0005	0.0002	0.0005	0.0005	0.0005	0.0000
35	C	1S	0.0018	0.0009	0.0033	0.0038	-0.0005	0.0003	0.0020	-0.0002	0.0015	0.0002
		2S	-0.0068	-0.0024	-0.0057	-0.0075	-0.0007	-0.0003	0.0033	-0.0003	-0.0025	0.0012
		2PX	0.0901	0.1529	-0.0199	-0.0494	0.1310	0.0101	-0.0263	0.0004	0.0075	0.0861
		2PY	0.1083	0.1482	0.0451	-0.0392	0.0709	0.0158	-0.0084	-0.0020	0.0175	0.1064
		2PZ	0.0888	0.1056	-0.0055	-0.0280	0.0831	0.0107	-0.0191	-0.0029	0.0117	0.0911
		3S	0.0054	0.0021	-0.0323	-0.0183	0.0242	0.0127	-0.0387	0.0044	-0.0104	-0.0271
		3PX	0.0335	0.0667	-0.0070	-0.0233	0.0602	0.0221	0.0183	0.0024	0.0048	0.0299
		3PY	0.0652	0.0783	0.0148	-0.0357	0.0575	0.0132	-0.0312	0.0047	-0.0031	0.0757
		3PZ	0.0537	0.0709	0.0112	-0.0155	0.0625	0.0112	-0.0129	0.0008	0.0189	0.0704
		4XX	0.0000	-0.0006	-0.0015	0.0048	-0.0052	-0.0166	0.0006	0.0025	-0.0042	0.0173

		4YY	-0.0024	-0.0023	0.0030	-0.0016	-0.0020	0.0029	0.0043	-0.0015	0.0022	0.0011
		4ZZ	0.0025	0.0040	0.0008	-0.0024	0.0067	0.0139	-0.0023	-0.0009	0.0030	-0.0178
		4XY	-0.0016	-0.0043	-0.0024	0.0033	-0.0065	-0.0099	0.0025	0.0012	-0.0006	0.0122
		4XZ	0.0014	0.0023	0.0002	0.0007	0.0011	-0.0002	0.0035	0.0004	0.0007	0.0006
		4YZ	0.0014	0.0027	0.0013	-0.0038	0.0064	0.0079	-0.0075	-0.0008	-0.0005	-0.0109
36	0	1S	-0.0014	-0.0059	-0.0022	0.0004	-0.0021	-0.0002	-0.0024	-0.0006	-0.0002	-0.0002
		2S	0.0038	0.0116	0.0041	0.0005	0.0051	0.0010	0.0038	0.0005	0.0001	0.0005
		2PX	0.0716	0.0961	-0.0136	-0.0444	0.1230	0.1433	0.0123	-0.0239	0.0507	-0.1360
		2PY	0.0952	0.1296	0.0349	-0.0623	0.1147	0.1246	-0.1306	-0.0185	0.0026	-0.1742
		2PZ	0.0926	0.1626	0.0211	-0.0640	0.1567	0.1431	-0.0245	-0.0201	0.0380	-0.1468
		3S	-0.0015	0.0242	0.0092	-0.0053	0.0021	0.0007	0.0235	0.0036	-0.0033	-0.0050
		3PX	0.0439	0.0616	-0.0069	-0.0314	0.0799	0.1073	0.0126	-0.0204	0.0310	-0.1178
		3PY	0.0575	0.0819	0.0231	-0.0411	0.0740	0.0930	-0.0906	-0.0143	0.0005	-0.1501
		3PZ	0.0588	0.0999	0.0127	-0.0409	0.1038	0.1070	-0.0221	-0.0153	0.0277	-0.1263
		4XX	0.0053	0.0070	-0.0014	-0.0024	0.0081	0.0053	-0.0014	-0.0008	0.0018	-0.0022
		4YY	0.0035	0.0044	0.0014	-0.0020	0.0042	0.0042	-0.0027	-0.0015	0.0003	-0.0028
		4ZZ	-0.0084	-0.0140	-0.0013	0.0052	-0.0120	-0.0089	0.0020	0.0010	-0.0032	0.0047
		4XY	0.0048	0.0068	0.0010	-0.0025	0.0056	0.0047	-0.0031	-0.0006	0.0011	-0.0030
		4XZ	-0.0008	-0.0008	0.0009	0.0013	-0.0018	-0.0025	-0.0016	0.0011	-0.0003	0.0011
		4YZ	-0.0038	-0.0049	-0.0019	0.0018	-0.0029	-0.0026	0.0034	0.0003	0.0001	0.0019
37	C	1S	-0.0015	-0.0001	-0.0010	-0.0003	-0.0021	0.0018	0.0040	-0.0005	0.0022	-0.0011
		2S	0.0005	0.0007	0.0027	0.0012	0.0040	-0.0018	-0.0070	0.0006	-0.0047	0.0000
		2PX	0.0716	0.0635	-0.0029	0.0435	-0.0435	-0.1309	0.0499	0.0177	-0.0099	0.1385
		2PY	0.0854	0.1222	-0.0553	0.0275	0.0262	-0.1700	0.0267	0.0275	-0.0314	0.1702
		2PZ	0.0691	0.0977	-0.0168	0.0250	-0.0073	-0.1357	0.0216	0.0171	-0.0202	0.1272
		3S	0.0178	0.0014	0.0091	-0.0009	0.0145	-0.0265	-0.0409	-0.0005	-0.0105	0.0368
		3PX	0.0333	0.0391	-0.0208	0.0263	-0.0144	-0.0913	0.0349	0.0095	-0.0110	0.1149
		3PY	0.0520	0.0703	-0.0210	0.0252	0.0020	-0.1200	0.0208	0.0196	-0.0106	0.1699
		3PZ	0.0407	0.0408	-0.0125	0.0151	-0.0185	-0.1011	0.0143	0.0117	-0.0228	0.1423
		4XX	-0.0025	-0.0028	-0.0042	0.0032	-0.0053	-0.0036	0.0020	0.0002	-0.0009	-0.0101
		4YY	0.0012	0.0015	0.0024	-0.0024	0.0027	-0.0001	0.0007	-0.0095	0.0079	0.0076
		4ZZ	0.0002	0.0012	0.0014	-0.0009	0.0024	0.0043	-0.0017	0.0089	-0.0066	0.0023
		4XY	-0.0002	-0.0017	-0.0003	0.0025	-0.0031	-0.0026	0.0017	-0.0042	0.0031	-0.0034
		4XZ	-0.0010	-0.0008	0.0009	0.0018	-0.0037	0.0002	-0.0002	0.0056	-0.0046	-0.0045
		4YZ	0.0011	0.0017	-0.0006	-0.0037	0.0056	0.0032	-0.0020	0.0031	-0.0019	0.0054
38	C	1S	0.0023	0.0012	-0.0002	0.0003	0.0024	0.0007	0.0006	0.0006	-0.0003	0.0008
		2S	-0.0051	-0.0026	0.0002	-0.0009	-0.0047	-0.0016	-0.0009	-0.0021	0.0007	-0.0017
		2PX	0.0310	0.0596	-0.0837	0.0241	0.0003	-0.0595	0.0071	0.1349	-0.1122	-0.0382
		2PY	0.0544	0.0620	-0.0051	0.0693	-0.0875	-0.0747	0.0126	0.1608	-0.1323	-0.0512
		2PZ	0.0456	0.0545	-0.0191	0.0507	-0.0444	-0.0589	-0.0027	0.1307	-0.1114	-0.0355
		3S	-0.0096	-0.0069	0.0049	0.0006	-0.0146	-0.0036	-0.0083	0.0024	0.0053	-0.0055
		3PX	0.0211	0.0258	-0.0323	0.0176	-0.0151	-0.0474	-0.0044	0.0973	-0.0840	-0.0417
		3PY	0.0320	0.0494	-0.0095	0.0363	-0.0331	-0.0431	0.0174	0.1164	-0.0888	-0.0677
		3PZ	0.0243	0.0309	-0.0178	0.0264	-0.0204	-0.0441	-0.0053	0.0902	-0.0836	-0.0475

		4XX	-0.0001	0.0008	-0.0029	0.0025	-0.0028	0.0049	-0.0016	0.0062	-0.0050	-0.0118
		4YY	0.0030	0.0032	0.0000	-0.0002	0.0018	-0.0087	0.0023	-0.0036	0.0028	0.0127
		4ZZ	-0.0024	-0.0038	0.0035	-0.0020	0.0012	0.0040	-0.0008	-0.0026	0.0024	-0.0010
		4XY	0.0013	0.0014	-0.0003	0.0026	-0.0034	-0.0007	0.0002	0.0029	-0.0025	-0.0020
		4XZ	-0.0014	-0.0027	0.0003	-0.0002	-0.0012	0.0049	-0.0012	0.0018	-0.0013	-0.0073
		4YZ	-0.0011	-0.0002	-0.0002	-0.0028	0.0044	-0.0012	0.0003	-0.0036	0.0028	0.0050
39	C	1S	0.0026	-0.0010	0.0016	0.0002	-0.0028	0.0001	-0.0009	0.0003	0.0002	-0.0011
		2S	-0.0076	0.0027	-0.0042	0.0009	0.0065	-0.0002	0.0007	-0.0015	-0.0011	0.0015
		2PX	0.0519	0.0458	-0.0513	0.0308	-0.0426	-0.1150	0.0369	-0.1076	0.0789	-0.0428
		2PY	0.0534	0.0879	-0.0252	0.0763	-0.0596	-0.1474	0.0538	-0.1429	0.1015	-0.0475
		2PZ	0.0511	0.0261	-0.0340	0.0491	-0.0480	-0.0976	0.0449	-0.0997	0.0767	-0.0356
		3S	0.0004	-0.0071	-0.0041	-0.0104	0.0081	-0.0039	0.0133	0.0011	-0.0012	0.0311
		3PX	0.0314	0.0280	-0.0224	0.0204	-0.0190	-0.0866	0.0330	-0.0760	0.0584	-0.0230
		3PY	0.0329	0.0437	-0.0178	0.0449	-0.0307	-0.1059	0.0344	-0.1006	0.0674	-0.0632
		3PZ	0.0284	0.0146	-0.0193	0.0277	-0.0389	-0.0728	0.0304	-0.0689	0.0474	-0.0386
		4XX	-0.0004	-0.0002	-0.0024	0.0023	-0.0036	0.0036	-0.0002	-0.0070	0.0055	-0.0134
		4YY	-0.0019	-0.0028	0.0030	-0.0030	0.0035	0.0023	-0.0011	0.0030	-0.0024	0.0042
		4ZZ	0.0024	0.0032	0.0000	0.0015	-0.0004	-0.0062	0.0013	0.0034	-0.0031	0.0096
		4XY	-0.0012	-0.0024	0.0001	0.0003	-0.0014	0.0041	-0.0004	-0.0034	0.0030	-0.0080
		4XZ	0.0016	0.0027	-0.0006	0.0023	-0.0024	-0.0021	0.0012	-0.0016	0.0016	-0.0014
		4YZ	0.0016	0.0009	-0.0009	-0.0019	0.0028	-0.0038	-0.0001	0.0044	-0.0036	0.0088
40	C	1S	-0.0003	-0.0030	-0.0007	-0.0002	-0.0013	-0.0003	0.0000	0.0002	-0.0001	0.0000
		2S	0.0001	0.0062	0.0007	0.0000	0.0034	0.0004	-0.0006	-0.0004	0.0003	0.0001
		2PX	0.0412	0.0377	0.0166	0.0788	-0.1106	0.0456	-0.0181	0.1179	-0.0933	-0.1065
		2PY	0.0247	0.0658	-0.0644	0.0621	-0.0632	0.0558	-0.0252	0.1471	-0.1179	-0.1313
		2PZ	0.0317	0.0202	-0.0632	0.0407	-0.0483	0.0422	-0.0160	0.1127	-0.0896	-0.1005
		3S	0.0030	0.0194	0.0110	0.0072	0.0022	0.0066	0.0082	-0.0036	0.0013	-0.0082
		3PX	0.0163	0.0135	-0.0068	0.0426	-0.0656	0.0310	-0.0183	0.0848	-0.0689	-0.0886
		3PY	0.0184	0.0348	-0.0285	0.0469	-0.0534	0.0428	-0.0165	0.1033	-0.0847	-0.1123
		3PZ	0.0163	0.0180	-0.0382	0.0265	-0.0294	0.0363	-0.0084	0.0817	-0.0612	-0.0859
		4XX	-0.0021	-0.0024	-0.0007	-0.0018	0.0012	0.0081	-0.0015	-0.0081	0.0070	0.0057
		4YY	0.0028	0.0027	-0.0020	0.0040	-0.0049	-0.0010	0.0003	0.0047	-0.0038	-0.0033
		4ZZ	-0.0007	-0.0009	0.0032	-0.0020	0.0028	-0.0072	0.0013	0.0033	-0.0031	-0.0025
		4XY	0.0002	0.0007	0.0003	0.0015	-0.0019	0.0053	-0.0015	-0.0033	0.0029	0.0026
		4XZ	-0.0009	-0.0023	0.0019	-0.0020	0.0018	0.0002	0.0004	-0.0026	0.0023	0.0016
		4YZ	-0.0004	0.0005	-0.0017	-0.0013	0.0024	-0.0058	0.0010	0.0047	-0.0042	-0.0033
41	H	1S	0.0035	0.0000	0.0171	0.0088	-0.0121	-0.0001	-0.0038	0.0017	-0.0022	0.0007
		2S	0.0058	0.0039	0.0178	0.0080	-0.0081	0.0068	0.0087	0.0025	0.0037	0.0024
		3PX	0.0008	0.0013	-0.0011	0.0007	-0.0004	-0.0014	-0.0004	0.0034	-0.0029	-0.0010
		3PY	0.0013	0.0015	0.0000	0.0014	-0.0016	-0.0015	0.0004	0.0039	-0.0032	-0.0012
		3PZ	0.0008	0.0012	-0.0012	0.0006	-0.0004	-0.0012	0.0001	0.0031	-0.0026	-0.0009
42	C	1S	-0.0020	0.0022	0.0018	0.0005	-0.0001	0.0000	0.0009	-0.0002	0.0002	0.0010
		2S	0.0038	-0.0045	-0.0045	-0.0019	0.0010	-0.0003	-0.0018	0.0009	-0.0012	-0.0001
		2PX	0.0346	0.0398	-0.0202	0.0773	-0.0799	0.0002	0.0216	-0.1226	0.0980	-0.1119

		2PY	0.0340	0.0439	-0.0530	0.0651	-0.0888	0.0013	0.0169	-0.1469	0.1169	-0.1414
		2PZ	0.0387	0.0396	-0.0439	0.0478	-0.0564	-0.0039	0.0126	-0.1099	0.0860	-0.1056
		3S	0.0072	-0.0051	-0.0025	0.0084	-0.0063	0.0045	-0.0088	-0.0024	-0.0013	-0.0306
		3PX	0.0202	0.0193	-0.0226	0.0389	-0.0439	0.0045	0.0178	-0.0881	0.0738	-0.0877
		3PY	0.0185	0.0264	-0.0347	0.0436	-0.0611	0.0060	0.0092	-0.1091	0.0847	-0.1313
		3PZ	0.0219	0.0243	-0.0175	0.0397	-0.0430	0.0041	0.0075	-0.0822	0.0654	-0.1019
		4XX	-0.0025	-0.0026	0.0002	-0.0022	0.0014	0.0106	-0.0035	0.0059	-0.0041	0.0057
		4YY	-0.0002	0.0004	0.0013	-0.0018	0.0034	-0.0120	0.0034	-0.0039	0.0022	-0.0046
		4ZZ	0.0020	0.0027	-0.0009	0.0044	-0.0050	0.0016	0.0003	-0.0019	0.0017	-0.0010
		4XY	-0.0013	-0.0020	0.0021	-0.0015	0.0015	0.0023	-0.0007	0.0025	-0.0017	0.0024
		4XZ	0.0002	0.0013	-0.0007	0.0014	-0.0016	0.0059	-0.0019	0.0017	-0.0011	0.0026
		4YZ	0.0015	0.0011	-0.0024	0.0009	-0.0012	-0.0041	0.0015	-0.0031	0.0023	-0.0030
43	H	1S	-0.0081	0.0196	0.0138	0.0109	-0.0009	-0.0031	0.0013	-0.0030	-0.0002	0.0030
		2S	-0.0075	0.0161	0.0117	0.0078	-0.0140	-0.0004	0.0032	0.0007	-0.0003	0.0025
		3PX	0.0011	0.0015	-0.0007	0.0008	-0.0005	-0.0030	0.0008	-0.0030	0.0019	-0.0008
		3PY	0.0021	0.0009	-0.0010	0.0015	-0.0016	-0.0036	0.0014	-0.0039	0.0029	-0.0012
		3PZ	0.0009	0.0013	-0.0003	0.0015	-0.0011	-0.0026	0.0010	-0.0028	0.0020	-0.0007
44	C	1S	0.0012	-0.0018	-0.0002	-0.0002	-0.0009	0.0006	0.0007	0.0000	0.0004	-0.0002
		2S	-0.0027	0.0036	0.0011	0.0007	0.0016	-0.0015	-0.0014	-0.0001	-0.0010	0.0002
		2PX	0.0173	0.0147	-0.0804	0.0477	-0.0747	0.1475	-0.0325	-0.0143	0.0213	0.0379
		2PY	0.0445	0.0546	-0.0445	0.0959	-0.1151	0.1802	-0.0412	-0.0205	0.0260	0.0479
		2PZ	0.0260	0.0472	-0.0125	0.0778	-0.1058	0.1409	-0.0352	-0.0132	0.0186	0.0360
		3S	-0.0021	0.0131	0.0026	0.0011	0.0036	-0.0019	-0.0020	0.0014	-0.0018	0.0020
		3PX	0.0172	0.0200	-0.0182	0.0437	-0.0568	0.0934	-0.0211	-0.0097	0.0126	0.0207
		3PY	0.0185	0.0264	-0.0347	0.0461	-0.0630	0.1123	-0.0286	-0.0115	0.0144	0.0379
		3PZ	0.0155	0.0218	-0.0221	0.0363	-0.0472	0.0903	-0.0202	-0.0066	0.0139	0.0289
		4XX	-0.0017	-0.0017	-0.0004	-0.0027	0.0027	0.0066	-0.0020	-0.0013	0.0016	0.0186
		4YY	0.0015	0.0004	-0.0012	0.0012	-0.0010	-0.0062	0.0026	-0.0077	0.0057	-0.0128
		4ZZ	0.0006	0.0013	0.0016	0.0014	-0.0016	-0.0004	-0.0006	0.0090	-0.0073	-0.0058
		4XY	-0.0005	-0.0001	0.0023	0.0003	-0.0006	0.0020	-0.0002	-0.0047	0.0040	0.0074
		4XZ	-0.0001	-0.0015	-0.0001	-0.0006	0.0007	0.0032	-0.0014	0.0047	-0.0036	0.0067
		4YZ	0.0002	0.0010	-0.0019	0.0000	0.0002	-0.0030	0.0005	0.0036	-0.0032	-0.0099
45	H	1S	0.0105	-0.0121	0.0142	0.0056	-0.0151	0.0001	0.0029	-0.0013	0.0018	0.0001
		2S	0.0111	-0.0123	0.0170	0.0078	-0.0182	-0.0009	0.0033	-0.0021	0.0017	0.0000
		3PX	0.0006	0.0011	-0.0001	0.0015	-0.0018	0.0013	-0.0004	0.0029	-0.0023	-0.0029
		3PY	0.0010	0.0008	-0.0008	0.0015	-0.0019	0.0015	-0.0006	0.0036	-0.0029	-0.0035
		3PZ	0.0003	0.0009	-0.0016	0.0008	-0.0007	0.0011	-0.0006	0.0028	-0.0023	-0.0027
46	H	1S	-0.0031	-0.0051	0.0096	0.0080	-0.0093	0.0037	0.0018	0.0006	0.0009	0.0012
		2S	-0.0021	-0.0021	0.0161	0.0118	-0.0124	0.0044	0.0023	0.0001	0.0019	-0.0014
		3PX	0.0008	0.0009	-0.0006	0.0015	-0.0016	0.0000	0.0004	-0.0031	0.0024	-0.0032
		3PY	0.0008	0.0010	-0.0012	0.0013	-0.0017	0.0001	0.0004	-0.0037	0.0030	-0.0036
		3PZ	0.0006	0.0005	-0.0005	0.0013	-0.0016	0.0001	0.0004	-0.0027	0.0022	-0.0028
47	C	1S	0.0008	0.0006	0.0043	0.0026	-0.0028	-0.0001	0.0001	-0.0002	0.0001	-0.0001
		2S	-0.0016	-0.0011	-0.0089	-0.0056	0.0061	-0.0001	-0.0002	0.0006	-0.0004	0.0001

		2PX	0.0235	0.0338	0.0147	0.0547	-0.0659	0.1239	-0.0319	-0.0151	0.0199	0.1744
		2PY	0.0096	0.0198	-0.0259	0.0354	-0.0625	0.1568	-0.0401	-0.0168	0.0245	0.2190
		2PZ	0.0049	-0.0044	-0.0569	0.0218	-0.0241	0.1182	-0.0292	-0.0138	0.0193	0.1661
		3S	-0.0062	-0.0079	-0.0274	-0.0173	0.0169	-0.0004	-0.0010	0.0014	-0.0003	0.0058
		3PX	0.0117	0.0179	0.0052	0.0318	-0.0394	0.0965	-0.0258	-0.0120	0.0158	0.1674
		3PY	0.0053	0.0088	-0.0202	0.0223	-0.0370	0.1228	-0.0317	-0.0143	0.0208	0.2108
		3PZ	0.0030	0.0002	-0.0252	0.0154	-0.0231	0.0922	-0.0235	-0.0114	0.0151	0.1615
		4XX	-0.0016	-0.0021	0.0019	-0.0039	0.0051	-0.0090	0.0021	0.0009	-0.0013	-0.0034
		4YY	0.0011	0.0010	-0.0020	0.0026	-0.0030	0.0058	-0.0012	-0.0017	0.0017	0.0024
		4ZZ	0.0008	0.0014	0.0014	0.0020	-0.0029	0.0030	-0.0009	0.0008	-0.0004	0.0012
		4XY	-0.0004	-0.0001	0.0024	-0.0010	0.0011	-0.0037	0.0008	0.0000	-0.0002	-0.0015
		4XZ	-0.0003	-0.0011	-0.0005	-0.0015	0.0028	-0.0031	0.0008	0.0009	-0.0009	-0.0012
		4YZ	0.0003	0.0007	-0.0018	0.0015	-0.0025	0.0049	-0.0013	-0.0001	0.0004	0.0019
48	H	1S	0.0053	0.0159	0.0301	0.0094	-0.0174	0.0003	-0.0010	0.0005	-0.0005	-0.0001
		2S	0.0050	0.0150	0.0334	0.0113	-0.0213	0.0010	-0.0008	0.0002	-0.0005	-0.0004
		3PX	0.0003	0.0003	-0.0006	0.0009	-0.0009	0.0029	-0.0008	-0.0005	0.0006	0.0048
		3PY	0.0002	0.0002	-0.0009	0.0007	-0.0012	0.0036	-0.0009	-0.0006	0.0007	0.0060
		3PZ	0.0004	0.0007	0.0002	0.0009	-0.0013	0.0028	-0.0007	-0.0004	0.0005	0.0045
49	H	1S	0.0030	-0.0033	-0.0091	0.0027	0.0078	-0.0009	0.0008	-0.0009	0.0004	-0.0001
		2S	0.0036	-0.0034	-0.0079	0.0041	0.0071	-0.0004	0.0017	-0.0014	0.0013	-0.0014
		3PX	0.0004	0.0008	0.0003	0.0010	-0.0015	0.0029	-0.0008	-0.0002	0.0004	0.0048
		3PY	0.0003	0.0003	-0.0010	0.0009	-0.0011	0.0037	-0.0010	-0.0002	0.0005	0.0060
		3PZ	0.0001	0.0001	-0.0007	0.0005	-0.0009	0.0028	-0.0007	-0.0002	0.0003	0.0046

3.2.2 Combined coefficients and computational details of HFV index (F) of M3

Table S5. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of **M3**

i/j \ k ($\|c_{ki}\|/\|c_{kj}\|$)	73	74	79	80	83	87	88	89	90	92
35	0.2636	0.3797	0.0779	0.1101	0.2555	0.0615	0.0826	0.0115	0.0432	0.2324
37	0.2104	0.2707	0.0830	0.0901	0.0751	0.4254	0.1085	0.0635	0.0672	0.4149
38	0.1257	0.1703	0.1167	0.1310	0.1367	0.1861	0.0323	0.4120	0.3400	0.1387
39	0.1463	0.1642	0.0931	0.1444	0.1307	0.3556	0.1250	0.3394	0.2420	0.1309
40	0.0900	0.1289	0.1291	0.1659	0.2067	0.1444	0.0565	0.3660	0.2883	0.2992
42	0.0998	0.1166	0.1050	0.1712	0.2004	0.0280	0.0489	0.3716	0.2921	0.3278
44	0.0862	0.1199	0.1277	0.1952	0.2517	0.4372	0.0959	0.0483	0.0623	0.1066
47	0.0413	0.0636	0.0963	0.1066	0.1427	0.4004	0.0961	0.0467	0.0640	0.5241

Table S6. The computational details of HFV index (F) of **M3**

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	$\sum P$	HFV (F)
α (37)	37-35	73 (1), 74 (1), 80 (-1), 87 (-1), 92 (1)	0.46 [a]	1.08	0.68
	37-38	73 (1), 74 (1), 80 (1), 87 (1), 92 (-1)	0.23 [b]		
	37-39	73 (1), 74 (1), 80 (1), 87 (1),88 (1), 92 (-1)	0.39 [c]		
γ (42)	42-39	73 (1), 74 (1), 79 (1), 80 (1), 83 (1), 89 (1), 90 (1),92 (1)	0.65 [d]	0.82	0.94
	42-44	73 (1), 74 (1), 79 (1) 80 (1), 83 (1), 92 (-1)	0.17 [e]		
ε (47)	47-44	80 (1), 83 (1), 87 (1), 88 (1), 92 (1)	0.59 [f]	0.59	1.17

a : $P_{37\text{-}35}$=2*0.2636*0.2104+2*0.3797*0.2707-2*0.1101*0.0901-2*0.0615*0.4254+2*0.2324*0.4149=0.46

b : $P_{37\text{-}38}$=2*0.2104*0.1257+2*0.2707*0.1703+2*0.0901*0.1310+2*0.4254*0.1861-2*0.4149*0.1387=0.23

c : $P_{37\text{-}39}$=2*0.2104*0.1463+2*0.2707*0.1642+2*0.0901*0.144+2*0.4254*0.3556+2*0.1085*0.12500-2*0.4149*0.1309=0.39

d : $P_{42\text{-}39}$=2*0.0998*0.1463+2*0.1166*0.1642+2*0.1050*0.0931+2*0.1712*0.144+2*0.2004*0.1307+2*0.3716*0.3394+2*0.2921*0.2420+2*0.3278*0.1309=0.65

e : $P_{42\text{-}44}$=2*0.0998*0.0862+2*0.1166*0.1199+2*0.1050*0.1277+2*0.1712*0.1952+2*0.2004*0.2517-2*0.3278*0.1066=0.17

f : $P_{47\text{-}44}$=2*0.1066*0.1952+2*0.1427*0.2517+2*0.4004*0.4372+2*0.0961*0.0959+2*0.5241*0.1066=0.59

3.3 The occupied π-type molecular orbitals associated with the active sites of M1b

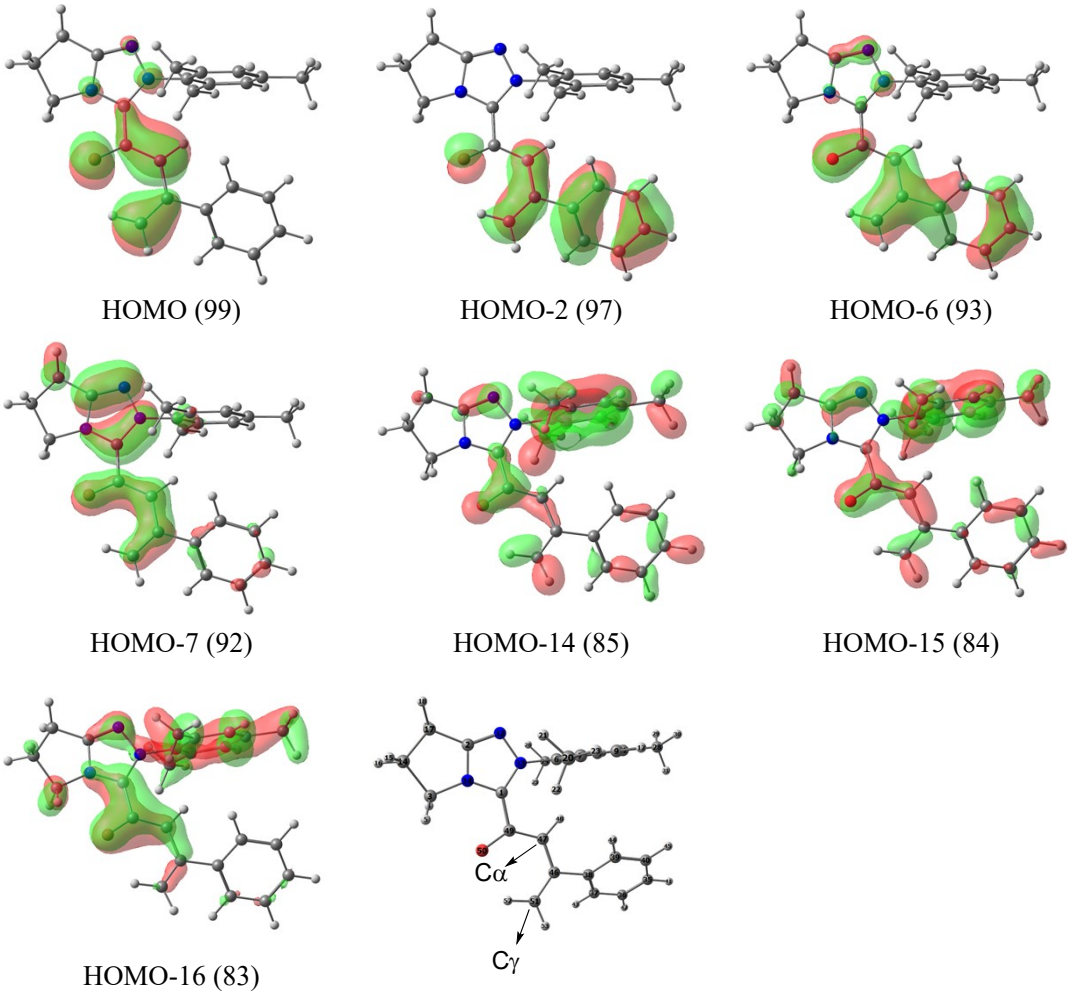


Fig. S6. The occupied π-type molecular orbitals associated with the active sites of **M1b**

3.3.1 Molecular orbital coefficients of M1b

		83	84	85	89	92	93	97	99
1C	1S	0.00908	-0.00616	-0.00382	0.00207	0.00118	0.00087	-0.00447	0.00002
	2S	-0.02221	0.01307	0.007	-0.00449	-0.00168	-0.00282	0.0115	0.00427
	2PX	0.01558	-0.01177	-0.0191	0.01196	0.02035	0.00165	-0.01246	0.00048
	2PY	-0.01986	0.00655	0.00293	0.01868	0.02856	-0.00108	-0.01145	0.0046
	2PZ	0.14536	-0.05257	0.07879	0.04072	-0.23833	0.05779	-0.00252	-0.0762
	3S	-0.03293	0.02998	0.00914	-0.01259	-0.01041	-0.00234	0.01625	-0.01784
	3PX	0.01294	0.00433	0.00333	0.00609	0.01474	0.00452	-0.00942	-0.01865
	3PY	-0.01204	0.0031	-0.0128	-0.01172	0.01677	0.00704	-0.00572	0.02201
	3PZ	0.09066	-0.03629	0.05192	0.01162	-0.14842	0.03227	-0.00219	-0.10782
	4XX	0.0004	-0.00119	-0.00224	-0.00211	0.00047	0.00101	0.00067	0.00049
	4YY	0.00236	-0.0018	0.00033	0.00193	0.00249	-0.00276	-0.001	-0.00165
	4ZZ	-0.00132	0.00107	-0.00071	0.00011	-0.00273	0.00175	-0.00006	0.0022
	4XY	-0.00107	-0.00035	0.00023	-0.00093	0.00185	-0.00071	0.00005	-0.0023
	4XZ	0.00006	0.00499	-0.0022	0.01586	-0.0057	0.00439	0.00058	0.0109
	4YZ	-0.00747	0.0023	-0.00386	-0.00908	-0.01557	0.0078	-0.00175	0.00742
2C	1S	-0.00179	0.00011	-0.00487	0.00432	0.00143	0	-0.00079	-0.00038
	2S	0.00402	0.00135	0.01235	-0.00908	-0.00247	0.00025	0.00191	0.00104
	2PX	-0.00696	-0.02552	-0.02115	-0.00976	-0.01998	0.0071	-0.00051	0.00084
	2PY	0.01154	-0.00436	0.03554	-0.02061	-0.02167	0.01246	0.00165	0.00384
	2PZ	-0.05586	0.09904	-0.07435	0.08725	0.25883	-0.069	0.0006	-0.04191
	3S	0.00732	-0.00605	0.01256	-0.03015	-0.01221	-0.00084	0.00046	-0.00609
	3PX	-0.00224	0.00056	0.00487	-0.00566	-0.00938	-0.00258	0.00651	0.01654
	3PY	0.01059	-0.00518	0.01245	0.00541	-0.0176	0.00895	0.00021	0.00244
	3PZ	-0.04136	0.0652	-0.04847	0.04923	0.17588	-0.04598	-0.00324	-0.04558
	4XX	0.00003	-0.00032	-0.00206	-0.00033	0.00116	0.0001	0.00016	0.00006
	4YY	0.00044	0.00138	-0.00006	0.00476	-0.00085	0.00052	-0.0007	0.00016
	4ZZ	-0.00107	-0.00115	-0.00021	-0.00329	0.00018	-0.00043	0.00011	-0.00088
	4XY	-0.00037	0.00041	-0.00094	0.00158	0.00012	0.0002	-0.00036	0.00019
	4XZ	0.00268	-0.0082	0.0053	-0.00397	-0.01003	0.00224	-0.00005	0.0005
	4YZ	-0.00727	0.00251	-0.00456	-0.01671	0.01219	-0.006	0.00084	-0.00631
3C	1S	-0.00164	-0.00211	0.00065	-0.00401	-0.00148	-0.00029	-0.00131	-0.00049
	2S	0.00414	0.005	-0.00023	0.00667	0.00128	0.00113	0.00322	0.00068
	2PX	0.00993	0.01395	0.00151	0.01129	0.00599	-0.00309	-0.00352	0.00007
	2PY	-0.0032	0.0086	0.02234	-0.00026	0.00362	-0.00056	-0.00433	-0.00039
	2PZ	-0.09309	-0.04368	-0.0012	-0.14635	-0.00029	0.00048	-0.00993	-0.02072
	3S	0.00487	0.00719	-0.0054	0.03451	0.01727	0.00014	0.008	0.00847
	3PX	-0.00565	0.00946	-0.01647	0.01197	0.00009	0.01455	-0.00675	-0.02792
	3PY	-0.01532	0.0065	0.00531	0.00554	-0.00275	0.01703	-0.01668	-0.02854
	3PZ	-0.05129	-0.01968	0.00052	-0.07318	0.00619	0.00429	-0.01476	-0.03236
	4XX	0.00177	0.00095	0.00102	0.00262	-0.0003	0.00027	-0.00068	0.00084
	4YY	0.00008	0.00075	0.00016	0.00086	0.00025	-0.00023	0.00014	-0.0001
	4ZZ	-0.00239	-0.00198	-0.0005	-0.00463	-0.00039	-0.00003	0.00008	-0.00108

	4XY	0.00191	0.0016	-0.0003	0.00326	0.00103	-0.00055	-0.00028	0.00076
	4XZ	0.00033	0.0016	-0.00131	-0.00234	0.00219	-0.00121	0.00017	-0.00173
	4YZ	0.00627	0.00394	-0.00019	0.01717	-0.00077	0.00175	-0.00004	0.00454
4H	1S	-0.05778	-0.03185	-0.00763	-0.10668	0.00061	-0.00293	-0.00215	-0.02234
	2S	-0.04821	-0.03679	-0.00029	-0.11926	0.0006	-0.01495	0.0057	-0.01638
	3PX	-0.00051	0.00027	-0.00018	-0.00104	0.00018	0.00002	-0.00016	-0.00065
	3PY	-0.00114	-0.00065	0.00026	-0.00191	-0.0001	-0.00009	0.00005	0.00041
	3PZ	0.00068	0.00044	0.00036	0.0013	-0.00012	0.00012	-0.0001	0
5H	1S	0.04491	0.02319	-0.00947	0.08681	-0.0019	0.00546	0.00316	0.01069
	2S	0.01718	0.03172	-0.01045	0.08174	-0.00817	0.03003	-0.02461	-0.0325
	3PX	0.00197	-0.00013	-0.0001	0.00222	-0.00007	-0.00035	0.00111	0.00143
	3PY	0.00116	0.00086	-0.00025	0.00221	0	0.00036	-0.00015	-0.00071
	3PZ	-0.00015	-0.00009	-0.00034	-0.0001	-0.00012	0.00021	-0.00002	-0.00019
6C	1S	0.00846	0.00003	0.00088	0.00124	-0.00029	0.00004	0.00048	-0.00003
	2S	-0.01876	-0.0006	-0.00052	-0.00526	0.00178	0.00243	-0.00087	-0.00566
	2PX	0.00322	0.06929	0.10231	-0.00314	0.00675	0.00474	0.00421	0.0039
	2PY	-0.05353	0.07139	0.12148	-0.00053	0.00965	0.00334	0.00391	0.00492
	2PZ	-0.09472	-0.13652	0.08469	0.0875	0.0592	-0.01574	0.00276	-0.00106
	3S	-0.01269	0.00239	-0.00447	0.00355	-0.0004	-0.01001	-0.00323	0.0207
	3PX	-0.04069	0.03986	0.05172	0.01209	0.00595	-0.00008	0.00635	0.01242
	3PY	0.00159	0.04266	0.07828	-0.0074	0.00725	0.01011	0.00183	-0.01455
	3PZ	-0.01667	-0.08526	0.05836	-0.00044	-0.02471	-0.00496	0.00045	-0.03006
	4XX	0.00576	-0.00249	-0.00289	0.00111	0.00142	-0.00011	0.00026	-0.00151
	4YY	0.00126	0.00265	0.00478	0.00043	-0.00058	0.00031	0.0002	0.0004
	4ZZ	-0.0037	-0.00024	-0.00124	-0.00152	-0.00048	0.00045	-0.00008	-0.00021
	4XY	-0.00344	-0.00164	-0.00305	0.00013	-0.00039	0.00026	0.00032	-0.00005
	4XZ	0.00187	0.00436	-0.00329	-0.00937	-0.00905	0.00259	-0.00006	0.00565
	4YZ	-0.00145	-0.0035	0.00223	0.0066	0.0075	-0.00309	0.00008	-0.00354
7C	1S	0.00014	0.00159	-0.00169	0.00865	0.00933	-0.00315	0.00055	-0.00377
	2S	0.00062	-0.00169	0.00264	-0.01926	-0.01716	0.00796	-0.00376	0.003
	2PX	-0.12378	0.01756	0.05669	-0.03001	-0.02329	0.0141	0.00354	0.0154
	2PY	0.03796	0.08342	0.10322	0.0278	0.02989	-0.00017	0.00662	0.00514
	2PZ	0.10586	0.14096	-0.0711	-0.07648	-0.05217	0.01483	-0.00197	0.01148
	3S	0.00693	-0.02154	0.02114	-0.04854	-0.06461	0.01028	0.00253	0.0176
	3PX	-0.01879	0.01988	0.03969	-0.02437	-0.031	0.01456	-0.00172	-0.01606
	3PY	-0.00981	0.03892	0.06222	0.02237	0.02781	0.00135	-0.00228	-0.00018
	3PZ	-0.01417	-0.00496	0.00293	-0.01769	-0.03244	0.00238	0.00354	0.00518
	4XX	0.00386	-0.00249	-0.00344	0.00079	0.00185	-0.00039	-0.00047	-0.00205
	4YY	0.00079	0.00292	0.00393	0.00111	0.00103	-0.00018	0.00014	-0.0004
	4ZZ	-0.00616	-0.00232	-0.00002	-0.00036	-0.00007	0.00028	-0.00053	-0.00144
	4XY	-0.00194	-0.00121	-0.00233	-0.0005	-0.00109	0.00025	0.00025	0.00152
	4XZ	0.00541	0.01093	0.00146	-0.00289	-0.00166	0.00055	0.00005	-0.00021
	4YZ	-0.00615	-0.00199	0.01049	0.00238	0.0016	0	-0.00002	0.00001
8C	1S	-0.00621	-0.00318	-0.00083	-0.00782	-0.00909	0.00318	0	0.00389

	2S	0.01455	0.00477	0.00286	0.01589	0.01771	-0.00697	0.00039	-0.00738
	2PX	-0.06201	0.04143	0.06055	0.03412	0.02625	-0.01261	0.00177	-0.00517
	2PY	0.01661	0.04802	0.11732	-0.02098	-0.03097	0.00373	0.00034	0.01238
	2PZ	0.08928	0.13832	-0.08162	-0.06979	-0.05031	0.0138	-0.0006	0.0123
	3S	0.00388	0.03098	-0.01022	0.05536	0.06182	-0.01474	0.00081	-0.00385
	3PX	-0.03888	0.0228	0.03787	0.02048	0.03194	-0.00653	0.00141	0.00949
	3PY	0.00505	0.03711	0.0604	-0.01498	-0.02526	-0.00504	0.00491	0.02155
	3PZ	0.03154	-0.00514	0.00842	-0.0239	-0.02795	0.00483	0.00046	-0.00264
	4XX	0.00143	-0.00291	-0.0027	-0.00106	-0.00025	0.00084	0.00027	0.00174
	4YY	-0.00031	0.0014	0.00406	-0.00008	-0.00194	-0.00002	0.00003	-0.0001
	4ZZ	-0.00191	0.00237	-0.00313	-0.0005	-0.00012	-0.00007	0.00011	0.00067
	4XY	-0.00038	-0.00034	-0.00176	0.00043	0.0011	-0.00019	0.00006	-0.0012
	4XZ	0.00819	0.0039	-0.00951	-0.00282	-0.00239	0.00044	-0.00012	-0.00035
	4YZ	-0.00257	-0.01048	-0.00362	0.00251	0.00114	-0.00015	-0.00017	-0.00055
9C	1S	0.00344	0.00555	-0.00434	-0.0048	-0.00447	0.00112	0.00003	0.00222
	2S	-0.00966	-0.01566	0.01273	0.01218	0.01125	-0.00305	-0.00126	-0.00515
	2PX	0.08424	0.09571	0.08014	0.0212	0.01504	-0.0029	0.00343	-0.00296
	2PY	-0.10906	0.03517	0.09601	-0.00533	-0.01555	0.00621	0.00477	0.00948
	2PZ	-0.13298	-0.14549	0.07129	0.04363	0.02216	-0.00493	0.00028	-0.00071
	3S	0.00577	-0.006	0.0011	0.00588	0.00378	0.00216	0.00115	-0.01921
	3PX	0.02062	0.04612	0.04472	0.00821	0.00269	-0.00038	0.0035	-0.00561
	3PY	-0.04631	0.03091	0.06016	0.0015	-0.00331	0.00091	0.00334	0.02011
	3PZ	-0.02839	-0.01819	0.00274	0.00556	0.00524	0.00243	-0.00009	0.00603
	4XX	0.0015	0.00193	0.00368	0.00024	0.00041	0.00035	0.00015	0.00115
	4YY	0.00298	-0.00185	-0.00218	0.00008	-0.00065	-0.00036	-0.00039	-0.00064
	4ZZ	-0.00253	0.00361	-0.00372	-0.00232	-0.00147	0.00039	-0.00028	0.00018
	4XY	-0.00297	0.00003	-0.00005	-0.00032	0.00015	-0.00001	0.00021	0.00027
	4XZ	0.00594	0.01055	-0.00137	-0.00341	-0.00244	0.00046	-0.00013	0.0001
	4YZ	-0.00611	-0.00426	0.00781	0.00317	0.00131	-0.00068	0.00014	-0.0006
10C	1S	-0.00425	-0.00572	0.00269	0.00451	0.00436	-0.00137	0	-0.00197
	2S	0.01334	0.01784	-0.00815	-0.01172	-0.01075	0.00297	-0.00122	0.00626
	2PX	0.01918	0.02778	0.10605	-0.01067	-0.02834	-0.00194	-0.00075	0.00106
	2PY	-0.0503	0.0719	0.084	0.01818	-0.00086	-0.0135	-0.00047	-0.01213
	2PZ	-0.09843	-0.14337	0.08995	0.04302	0.01976	-0.00478	0.00077	-0.00099
	3S	-0.00127	-0.00558	-0.00068	-0.0117	-0.00553	0.00865	0.00131	-0.00254
	3PX	-0.01197	0.01414	0.05784	-0.00305	-0.01204	-0.00033	-0.00216	-0.0015
	3PY	-0.01163	0.04197	0.05788	0.0095	-0.00878	-0.00967	-0.00397	-0.01332
	3PZ	-0.01562	-0.01166	0.01385	0.00708	0.00531	-0.00032	-0.00115	0.01087
	4XX	0.00173	0.00147	0.00474	0.00019	0.00009	-0.00014	-0.00023	0.00013
	4YY	0.00204	-0.00143	-0.00284	0.0001	0.00038	-0.00012	-0.00014	-0.00031
	4ZZ	-0.0072	-0.0035	-0.00008	0.00145	0.0011	-0.00031	-0.00021	-0.00004
	4XY	-0.002	0.00104	0.00007	-0.00009	-0.00028	0.00006	0.00005	0.00031
	4XZ	0.00848	0.00729	-0.00766	-0.00386	-0.00204	0.00084	-0.00007	0.00056
	4YZ	-0.00453	-0.00928	-0.00039	0.00244	0.00204	-0.00026	-0.00001	-0.00002

11C	1S	0.00131	-0.00014	0.00064	-0.0001	-0.00003	0.00003	0.00001	-0.00004
	2S	-0.00272	0.00043	-0.00171	0.00006	0.00025	0.00025	-0.00119	0.00033
	2PX	-0.10769	0.01918	0.04213	0.00687	-0.00693	-0.0045	0.00043	-0.00632
	2PY	0.04226	0.06141	0.10497	0.00968	-0.01062	-0.00604	0.00103	-0.00892
	2PZ	0.14744	0.18206	-0.09331	-0.04339	-0.01891	0.00399	-0.00058	0.00012
	3S	-0.01749	0.00252	-0.00206	0.00109	0.00023	-0.0024	0.00208	0.00274
	3PX	-0.02092	0.02278	0.04034	0.0053	-0.00331	-0.00447	-0.00144	-0.00219
	3PY	-0.00823	0.03188	0.05447	0.00362	-0.00638	-0.00162	0.00045	-0.01017
	3PZ	0.0588	0.08324	-0.04303	-0.0201	-0.00775	0.00293	-0.00086	0.01098
	4XX	0.00148	0.00461	0.00892	0.0006	-0.00033	-0.00021	-0.00005	0
	4YY	0.00408	-0.00422	-0.00666	-0.00036	0.00049	0.0002	-0.00023	0.00017
	4ZZ	-0.00444	-0.00007	-0.00193	-0.00033	-0.00005	0.00003	-0.0002	0.00014
	4XY	-0.00404	0.00139	0.00167	0	-0.00026	-0.00004	0.00009	-0.00008
	4XZ	0.00675	0.00782	-0.00368	-0.00232	-0.00166	0.00005	-0.00014	0.00019
	4YZ	-0.00508	-0.00639	0.00337	0.00176	0.00073	-0.00071	-0.00011	-0.00068
12H	1S	0.03983	0.0798	-0.04903	-0.03517	-0.02081	0.00538	-0.00063	0.00299
	2S	0.05014	0.10266	-0.06696	-0.04724	-0.02912	0.00883	-0.00108	0.00805
	3PX	0.00185	0.00304	0.00091	0.00001	0.00009	0	0.00012	0.00009
	3PY	-0.00234	-0.00017	0.00255	0.00028	-0.00014	0.00014	0.00009	0.00005
	3PZ	-0.00075	0.00033	-0.00032	-0.00045	-0.00031	0.00008	0.00004	-0.00004
13H	1S	-0.08476	-0.08553	0.04176	0.03395	0.02042	-0.00532	0.0003	-0.00327
	2S	-0.10956	-0.11218	0.0524	0.04436	0.0286	-0.00793	0.00089	-0.00948
	3PX	-0.00124	-0.00097	0.00289	0.0004	-0.00035	-0.00016	0.00002	-0.00009
	3PY	0.00007	0.00243	0.00119	-0.00002	-0.00021	-0.00027	0.00001	-0.00023
	3PZ	0.00117	0.00041	0.00002	-0.00042	-0.00031	0.00006	-0.00005	-0.00001
14C	1S	-0.00188	-0.00281	-0.00111	-0.00457	-0.00354	0.001	0.00031	-0.00169
	2S	0.00413	0.00758	0.00091	0.01591	0.0073	0.00093	-0.00208	0.00112
	2PX	-0.01838	-0.01392	-0.01309	-0.02756	-0.00226	-0.0001	0.00297	-0.00766
	2PY	-0.00702	0.01054	-0.00529	-0.00171	0.02091	-0.00336	0.00157	-0.00803
	2PZ	0.04658	0.06041	-0.01854	0.06326	0.02327	-0.00518	0.00156	0.00107
	3S	0.01306	0.00986	0.01634	-0.00373	0.02511	-0.02567	0.00594	0.02755
	3PX	-0.01402	-0.00037	-0.01347	0.00785	0.00672	0.00906	-0.00426	-0.01642
	3PY	-0.01054	0.00497	-0.00612	-0.01798	0.01664	-0.00531	0.00237	-0.0169
	3PZ	0.02004	0.03258	-0.009	0.02759	0.00896	-0.00114	-0.00097	0.00584
	4XX	0.00186	0.00152	0.00006	0.00233	-0.00003	-0.00014	0.00014	0.00021
	4YY	0.00122	0.00279	-0.00178	0.00324	0.00194	-0.00015	0.00009	-0.00018
	4ZZ	-0.00318	-0.00463	0.00141	-0.00515	-0.00262	0.00095	-0.00038	-0.00056
	4XY	0.0005	0.00057	0.00089	0.00144	0.00072	-0.00018	0.00003	0.00047
	4XZ	0.00266	0.00159	-0.00041	0.00308	-0.00064	0.0002	0.00024	-0.00008
	4YZ	0.00136	-0.00043	0.00084	0.00181	-0.00115	0.00047	0.00008	0.00059
15H	1S	-0.03601	-0.0443	0.01309	-0.05003	-0.0169	0.0047	-0.00245	-0.00195
	2S	-0.03769	-0.04661	0.01304	-0.0627	-0.02572	0.0076	-0.00368	-0.00393
	3PX	-0.00016	0.00012	-0.00037	-0.0004	0.0003	-0.00023	0.00015	-0.00001
	3PY	-0.00034	0.00032	-0.00015	-0.00021	0.00063	-0.00013	0	-0.00021

	3PZ	-0.00084	-0.0009	0.0002	-0.00109	-0.00024	0.00005	-0.00003	0.00001
16H	1S	0.01167	0.01343	-0.01107	0.01403	0.00279	-0.00158	0.00167	-0.00063
	2S	0.00991	0.00811	-0.0108	-0.00163	-0.00408	-0.0028	0.00428	-0.00721
	3PX	-0.0005	-0.00068	0.00029	-0.00076	-0.00037	0.00008	0.00003	0.00005
	3PY	0.0004	0.00039	-0.0001	0.0005	0.00016	-0.00005	0.0001	0.00001
	3PZ	0.0007	0.00075	-0.00004	0.00097	0.00027	0	-0.00003	-0.00011
17C	1S	-0.00229	-0.00052	0.00218	-0.00335	-0.00034	-0.00043	-0.00051	-0.00098
	2S	0.00443	0.00217	-0.00495	0.00412	0.00163	-0.00021	0.00153	0.00121
	2PX	0.00461	0.02449	0.01183	0.01495	0.00863	-0.00402	-0.00071	-0.00065
	2PY	-0.01737	-0.0044	-0.00372	-0.01262	0.00575	-0.00322	-0.00167	-0.0023
	2PZ	0.00263	-0.07724	0.04746	-0.0611	-0.07991	0.01702	-0.00095	0.00422
	3S	0.01321	-0.00483	-0.01438	0.03582	-0.00168	0.01185	-0.00241	0.00047
	3PX	0.00409	0.01706	0.00958	0.0001	0.00402	-0.00643	0.00295	0.00142
	3PY	-0.01567	0.00032	-0.00402	-0.02641	0.00978	-0.006	-0.00146	-0.01085
	3PZ	0.00927	-0.04135	0.0281	-0.01961	-0.03583	0.00324	0.00295	0.00801
	4XX	-0.00085	0.00037	-0.00154	0.00025	0.00209	-0.00059	0.00005	-0.00062
	4YY	0.001	0.00409	-0.00108	0.00394	0.0035	-0.00057	-0.00015	-0.00031
	4ZZ	-0.00046	-0.00441	0.00297	-0.00496	-0.0056	0.00116	-0.00001	0.00036
	4XY	-0.00013	0.00189	-0.00083	0.0024	0.00216	-0.00069	-0.00024	-0.00004
	4XZ	0.00218	-0.00491	0.00333	-0.00464	-0.01135	0.00299	0.00003	0.00184
	4YZ	-0.00078	-0.00226	0.00094	-0.00263	-0.0008	0.00002	0.00009	-0.00045
18H	1S	-0.00516	0.04315	-0.02111	0.03591	0.05121	-0.01333	-0.00063	-0.00425
	2S	-0.00167	0.04004	-0.01867	0.05085	0.05546	-0.01493	-0.0016	0.00019
	3PX	-0.00026	-0.00024	0.00031	-0.00053	0.00029	-0.00012	-0.00006	-0.00048
	3PY	0.00004	-0.00122	0.00058	-0.00092	-0.00156	0.00047	-0.0001	0.00009
	3PZ	-0.00004	-0.00035	0.00034	-0.00023	-0.0006	0.00014	-0.00006	0.00005
19H	1S	0.00394	-0.05335	0.03597	-0.04713	-0.07024	0.01582	-0.00037	0.00704
	2S	-0.0026	-0.05416	0.03404	-0.06253	-0.08348	0.02104	-0.00241	0.00539
	3PX	0.00045	0.00079	0.00004	0.00081	-0.0004	0.00016	0	0.00036
	3PY	-0.00039	0.00015	-0.00028	0.00023	0.00078	-0.00025	0	-0.00008
	3PZ	-0.00008	0.00077	-0.00059	0.00063	0.00104	-0.00024	0.00003	-0.0001
20C	1S	0.01107	0.0124	-0.00634	-0.00079	-0.00103	-0.00032	0.00115	0.00484
	2S	-0.02412	-0.02525	0.01218	0.00133	-0.00153	0.00128	-0.00147	-0.00414
	2PX	0.10064	0.02838	-0.09032	-0.02773	-0.00773	-0.00273	0.00143	0.00583
	2PY	-0.08225	-0.09171	-0.09449	0.01193	0.01298	-0.0096	0.00537	0.02052
	2PZ	-0.09929	-0.11603	0.05498	0.02552	0.01227	-0.00201	-0.00096	-0.00246
	3S	-0.07772	-0.08168	0.0442	0.01642	0.03427	-0.00359	-0.01313	-0.06787
	3PX	0.04938	0.02702	-0.05134	-0.02035	0.01134	-0.00295	0.00072	0.00225
	3PY	-0.05699	-0.04819	-0.05068	0.01004	0.00148	-0.00754	0.01195	0.04612
	3PZ	-0.06456	-0.06184	0.02783	0.02742	0.01818	-0.00635	0.00301	0.01121
	4XX	0.00488	-0.00193	-0.00742	-0.00007	0.00025	-0.00066	0.00009	0.00035
	4YY	0.00288	0.0063	0.00746	0.00019	-0.00007	0.00062	-0.00001	-0.00005
	4ZZ	-0.00602	-0.00197	-0.00132	0.00016	-0.0004	-0.00001	0.00019	0.00126
	4XY	0.00184	0.00077	-0.0009	-0.00131	-0.0011	0.00032	-0.0001	0.00017

	4XZ	0.00221	0.00503	-0.00096	-0.00044	0.00049	-0.00001	0.00011	-0.00031
	4YZ	-0.00221	-0.00144	0.00524	0.00046	-0.00035	0.00053	0.00004	0.00005
21H	1S	0.05274	-0.0084	-0.07074	-0.01228	-0.00418	-0.0033	0.00055	0.00286
	2S	0.0658	-0.01465	-0.06354	-0.00026	-0.02729	0.00141	0.00033	0.0121
	3PX	-0.00055	0.00061	0.00169	0.00059	0.00035	0.00004	-0.00001	-0.00016
	3PY	-0.00223	-0.00155	-0.00108	-0.00005	0.00007	0.00001	0	0.00023
	3PZ	-0.00134	-0.00221	0.00171	0.00151	0.00026	0.00003	-0.00006	-0.0005
22H	1S	0.03923	0.06105	0.07679	-0.0046	-0.00703	0.00738	-0.00205	-0.00624
	2S	0.01656	0.07227	0.05565	0.00275	-0.01112	-0.00078	0.0179	0.07734
	3PX	0.00218	0.00113	-0.00086	-0.00029	0.00033	-0.00001	-0.00013	-0.00022
	3PY	0.00081	0.00122	0.00194	-0.00024	-0.00047	0.00007	-0.00001	-0.00024
	3PZ	-0.00203	-0.00173	0.0005	0.00091	0.00075	-0.00038	0.00034	0.00126
23H	1S	-0.00987	0.02065	-0.03288	-0.00381	-0.00046	-0.0009	0.00108	0.00375
	2S	0.00029	0.03614	-0.04	-0.00636	0.00277	-0.00227	0.00216	0.01027
	3PX	0.0014	0.00039	-0.00216	-0.00053	-0.00039	-0.00004	0.00005	0.00035
	3PY	-0.00092	-0.0019	-0.0012	0.00025	0.00035	-0.00019	0	0.00001
	3PZ	-0.00194	-0.0013	-0.00007	0.00023	0.00024	-0.00003	-0.00002	-0.00012
	1S	-0.00625	-0.01138	0.00664	0.00117	0.00141	0.00022	-0.0008	-0.00362
	2S	0.01404	0.02293	-0.01301	-0.00197	-0.00086	-0.00031	0.00016	0.00086
	2PX	0.03774	-0.09499	-0.0151	0.02728	-0.00226	0.00402	-0.00117	-0.00333
	2PY	0.04393	-0.02665	-0.10894	-0.01352	-0.01747	0.00966	-0.00463	-0.01484
	2PZ	-0.06905	-0.11521	0.06503	0.02859	0.01488	-0.00219	-0.00046	-0.00209
	3S	0.02864	0.07804	-0.04842	-0.01586	-0.02896	-0.00094	0.01341	0.06617
	3PX	0.02216	-0.05626	0.00182	0.0149	-0.01499	0.00465	-0.00008	0.00113
	3PY	0.03076	-0.01265	-0.05273	-0.00672	-0.01258	0.01118	-0.01026	-0.03801
	3PZ	-0.03373	-0.06424	0.03853	0.02696	0.01536	-0.00312	0.00191	0.00479
	4XX	0.00278	-0.00641	-0.00454	-0.00005	-0.00058	0.00076	-0.00032	-0.00094
	4YY	-0.00266	0.00286	0.00814	0.00022	0.00018	-0.0005	0.00023	0.00066
	4ZZ	-0.00113	0.00138	-0.00233	-0.00035	0.00041	-0.00005	-0.00028	-0.00117
	4XY	0.00084	-0.00171	-0.00039	0.0014	0.00086	-0.00028	0.00008	-0.00043
	4XZ	0.00457	0.00246	-0.00393	-0.0002	-0.00002	0.00005	-0.00003	-0.00065
	4YZ	-0.00224	-0.00507	-0.00141	0.00039	-0.00021	0.00035	-0.00011	-0.00016
25H	1S	-0.02745	0.02912	0.07909	0.00714	0.00856	-0.00625	0.0027	0.00705
	2S	-0.01077	0.01485	0.08808	0.00317	0.00221	0.00605	-0.01474	-0.06305
	3PX	0.00057	-0.00149	0.00028	0.00012	-0.00062	0.0002	0.00002	0.00023
	3PY	-0.00061	0.00075	0.00183	0.00027	0.00048	-0.00005	-0.00013	-0.00036
	3PZ	-0.00159	-0.0016	0.00111	0.00087	0.00116	-0.00047	0.00023	0.0007
26H	1S	0.03394	-0.06591	-0.03746	0.01299	-0.00149	0.0037	-0.00131	-0.00504
	2S	0.01944	-0.05818	-0.04642	0.00495	0.0232	-0.00343	-0.00227	-0.01835
	3PX	-0.00103	0.00162	0.00094	-0.00078	0.00014	-0.00011	0.00004	0.0001
	3PY	0.00043	0.00031	-0.00142	0	-0.00022	0.00002	0.00003	-0.00006
	3PZ	-0.00068	-0.00238	0.00144	0.00133	-0.00007	0.00011	-0.00007	-0.0004
27H	1S	-0.03784	-0.0294	0.00417	0.00183	0.00346	-0.00008	-0.00088	-0.00229
	2S	-0.04703	-0.04279	0.01219	0.00306	0.00349	-0.0003	-0.00155	-0.00598

	3PX	0.0002	-0.00206	-0.00049	0.00057	0.00023	-0.00001	-0.00005	-0.00028
	3PY	0.00115	-0.00026	-0.00206	-0.00026	-0.00046	0.00017	0	0.00009
	3PZ	0.00001	-0.00109	0.00096	0.00039	0.00014	0.00001	-0.00005	-0.00013
28C	1S	-0.00857	-0.00129	-0.00256	0.00027	-0.00014	-0.00024	-0.00026	-0.00002
	2S	0.01799	0.00218	0.00505	0.0001	-0.00005	-0.00019	0.00003	-0.00004
	2PX	0.10586	-0.02131	-0.03537	0.00062	0.00338	0.00078	-0.00095	0.00114
	2PY	-0.03313	-0.05942	-0.09894	-0.00275	0.00421	0.00131	-0.00081	0.00133
	2PZ	-0.06935	-0.07575	0.03414	0.00027	-0.00374	0.00157	0.0001	0.00151
	3S	0.0548	0.01183	0.01868	-0.00401	0.00247	0.00355	0.00338	0.00255
	3PX	0.06159	-0.01078	-0.01663	0.00343	0.00069	-0.00248	-0.00366	0.00088
	3PY	-0.01709	-0.03194	-0.05201	-0.00028	0.00129	-0.00044	-0.00076	-0.00008
	3PZ	-0.0302	-0.03442	0.01603	0.00015	0.00015	0.00095	0.0005	-0.00116
	4XX	-0.00075	0.0037	0.00738	0.00056	-0.00062	-0.00034	0.00004	-0.00046
	4YY	-0.00028	-0.00236	-0.00236	-0.00018	0.00032	0.00015	-0.00009	0.00038
	4ZZ	-0.00055	-0.00172	-0.00558	-0.00018	0.00022	-0.00003	-0.00012	0.00012
	4XY	-0.00483	0.00202	0.00372	0.0001	-0.00035	-0.00008	0.00014	-0.00026
	4XZ	0.00349	0.00319	-0.00216	-0.0006	-0.00016	-0.00002	-0.00004	-0.00023
	4YZ	-0.006	-0.0075	0.0021	0.00056	0.00003	0.00005	-0.00003	0.00016
29H	1S	-0.04954	-0.0743	-0.02434	0.00023	0.00115	0.00161	-0.0003	0.00215
	2S	-0.05957	-0.07814	-0.0214	0.00266	0.00223	0.00095	-0.00065	0.00304
	3PX	0.00199	-0.00011	-0.00052	0.00001	0.00007	0.00001	0.00002	-0.00009
	3PY	0.00117	0.00116	-0.00129	-0.00011	0.00009	0.00002	-0.00002	0.00004
	3PZ	0.00013	0.00086	0.00177	0.00018	-0.00003	-0.00007	-0.00001	-0.00006
30H	1S	0.04029	0.03298	-0.05814	-0.00372	0.0032	-0.00001	-0.00022	0.00007
	2S	0.03751	0.03806	-0.06096	-0.00636	0.00231	0.00087	-0.00049	-0.0001
	3PX	0.00171	-0.00035	-0.00061	-0.00007	0.00003	0.00008	0.00004	0.00008
	3PY	-0.00146	-0.002	-0.00057	0.00005	0.00007	0.00003	-0.00002	0.00006
	3PZ	0.0001	-0.00047	-0.0015	0.00004	0.00018	0.00002	0	-0.00002
31H	1S	-0.0454	0.03447	0.06802	0.00214	-0.00455	-0.00142	0.00084	-0.00229
	2S	-0.04368	0.02819	0.06202	0.01011	-0.00699	-0.00777	-0.00577	-0.00383
	3PX	0.00029	0.00061	0.00149	0.00008	-0.0001	-0.00012	-0.00007	0.00002
	3PY	-0.00204	-0.00007	0.0003	-0.00005	-0.00012	-0.00009	-0.00004	-0.00008
	3PZ	-0.00143	-0.00189	0.00049	-0.00002	-0.00005	0.00004	0.00003	0.00009
32N	1S	0.0036	-0.00001	0.01234	-0.00793	-0.00105	0.00147	0.00047	-0.00029
	2S	-0.0082	-0.00208	-0.02776	0.0153	0.00107	-0.00262	-0.00094	-0.00007
	2PX	0.01982	0.01496	0.04737	0.01785	-0.01383	0.0076	-0.00452	0.00156
	2PY	-0.00409	-0.0054	-0.03261	0.04907	-0.015	0.00192	-0.0082	0.00178
	2PZ	-0.13028	0.12337	-0.12089	-0.13035	0.28316	-0.09722	0.00776	-0.06307
	3S	-0.01692	0.01173	-0.04585	0.03777	0.01026	-0.01054	0.00189	0.00867
	3PX	0.00665	0.00292	0.01716	0.00866	-0.00785	0.00488	-0.00506	0.00049
	3PY	-0.00105	-0.00555	-0.01763	0.03128	-0.01231	0.00274	-0.00783	-0.00099
	3PZ	-0.082	0.07702	-0.07801	-0.09322	0.19967	-0.07389	0.00819	-0.05294
	4XX	-0.00017	-0.00037	0.00121	-0.00222	-0.00195	0.00093	0.00014	0.00048
	4YY	-0.00067	0.00111	0.00285	-0.0035	0.00185	-0.00034	0.00034	-0.0003

	4ZZ	0.00134	-0.00153	0.0001	0.00209	-0.00088	0.00027	-0.00026	-0.0007
	4XY	-0.00134	-0.00139	-0.00293	-0.00164	-0.00016	-0.00006	-0.00009	-0.00004
	4XZ	0.001	0.00202	-0.00068	0.00916	0.01298	-0.00393	0.00008	-0.00546
	4YZ	0.00785	-0.00876	0.0081	0.00622	-0.01612	0.00517	-0.00045	0.00213
33N	1S	-0.00861	0.00079	-0.00455	0.00217	0.00043	0.00004	0.00167	0.0016
	2S	0.01732	-0.00136	0.01015	-0.00587	-0.00138	0.00005	-0.00403	-0.00148
	2PX	-0.02944	-0.01616	-0.0142	0.00646	0.01692	-0.00515	0.00195	-0.00951
	2PY	0.0257	-0.00004	-0.00028	-0.00159	0.01232	-0.00038	0.00839	-0.00445
	2PZ	-0.05971	-0.01737	-0.01449	-0.22104	-0.25118	0.08156	-0.00175	0.11796
	3S	0.06578	-0.01035	0.02713	-0.00693	0.00037	-0.0003	-0.01043	-0.03016
	3PX	-0.02845	-0.01303	-0.01444	0.01041	0.01321	-0.01097	0.00092	0.00304
	3PY	0.01748	-0.00491	-0.0123	-0.01039	0.01143	0.00408	0.00208	-0.01033
	3PZ	-0.05236	0.00172	-0.02214	-0.15163	-0.18088	0.06838	-0.00471	0.12108
	4XX	0.00133	-0.00451	-0.00486	-0.00068	-0.0019	0.00046	-0.00001	0.00059
	4YY	-0.00295	0.00352	0.00504	0.00171	-0.00152	0.00085	0.00033	0.00046
	4ZZ	-0.00209	0.00163	-0.00138	-0.00102	0.00322	-0.00105	0.00004	0.00032
	4XY	0.00037	-0.00237	-0.00438	0.00108	-0.00255	0.00006	0.00048	0.00055
	4XZ	-0.00296	0.00795	-0.0071	-0.00623	0.00806	-0.00285	0.00046	-0.00103
	4YZ	-0.00879	0.00149	-0.00376	-0.00164	0.01695	-0.00519	0.00052	0.00177
34N	1S	-0.00025	0.00125	0.00296	0.00059	0.00012	-0.00129	-0.00058	-0.00102
	2S	0.00057	-0.0028	-0.00666	-0.00162	-0.00045	0.00353	0.00079	-0.00014
	2PX	-0.0206	0.00476	0.01053	-0.01983	0.0033	-0.01152	-0.0007	-0.01141
	2PY	-0.00303	0.00628	-0.01296	-0.00777	0.01	-0.00998	-0.0027	-0.00718
	2PZ	0.07979	0.04411	0.01405	0.3093	-0.0593	0.05638	-0.0097	0.08228
	3S	0.00061	-0.00805	-0.01976	0.00235	-0.0006	0.00136	0.01072	0.03286
	3PX	-0.00517	0.00725	0.00661	-0.00741	0.0038	-0.00944	0.00054	-0.01999
	3PY	-0.00366	0.00446	0.00129	-0.00083	0.00992	-0.00905	0.00144	-0.00196
	3PZ	0.06165	0.03157	0.01097	0.24041	-0.04912	0.04153	0.00067	0.11215
	4XX	0.00061	0.00013	0.00038	0.00036	-0.00089	-0.00017	0.00025	-0.0002
	4YY	0.00051	-0.00038	0.00173	-0.00098	-0.0006	-0.00028	-0.00016	-0.00005
	4ZZ	-0.00107	0.00078	-0.00061	0.00062	0.00173	-0.00005	-0.00028	-0.00073
	4XY	0.00091	-0.00078	-0.00025	-0.0009	-0.00203	-0.00035	-0.00001	0.00014
	4XZ	-0.00742	0.00243	-0.00395	-0.00149	0.01316	-0.00304	-0.00055	0.00155
	4YZ	0.00146	0.00583	-0.00256	0.01066	0.00495	-0.00005	-0.00051	-0.00002
35C	1S	0.00075	0.00176	0.00257	-0.00084	-0.00022	0.00025	0.0002	0.00241
	2S	-0.00214	-0.00496	-0.00789	0.00392	0.00051	-0.00039	-0.00011	-0.00609
	2PX	0.00281	-0.06972	-0.09145	0.03149	-0.01911	-0.04961	-0.06612	0.00317
	2PY	0.04615	-0.03934	0.01019	-0.08813	-0.04316	-0.10166	-0.13566	0.02096
	2PZ	0.00597	-0.00808	0.00762	0.08971	-0.04846	-0.15504	-0.22512	0.03446
	3S	-0.00156	-0.0067	-0.0097	-0.00332	-0.00044	0.00094	-0.00371	0.01292
	3PX	0.00554	-0.02236	-0.02208	0.00352	-0.01222	-0.03518	-0.04804	0.00898
	3PY	0.01864	-0.01863	0.00019	-0.02677	-0.03038	-0.07446	-0.0995	0.01271
	3PZ	0.0075	-0.01278	-0.00141	0.04262	-0.02892	-0.1	-0.17292	0.03289
	4XX	0.00154	0.00156	0.00452	-0.00606	-0.00132	-0.00234	-0.00108	0.00076

	4YY	-0.0009	0.00014	-0.00122	0.00356	0.00123	0.00219	0.00048	0.00016
	4ZZ	-0.00032	-0.00072	-0.00164	0.00097	0.00008	0.00032	0.00072	-0.00015
	4XY	0.00047	-0.0037	-0.00484	0.00075	-0.00172	-0.00295	-0.00109	-0.00066
	4XZ	0.00079	-0.00067	0.00075	0.0033	-0.00083	-0.00276	-0.00317	0.00019
	4YZ	-0.00005	0.00177	0.00237	-0.00316	0.00045	0.00123	0.001	0.00011
36C	1S	-0.00159	0.00263	0.0007	0.00123	-0.00329	-0.00574	0.00268	-0.0027
	2S	0.0028	-0.00435	-0.00041	-0.00071	0.00737	0.01114	-0.00545	0.00517
	2PX	0.03045	0.01263	0.07368	-0.05068	0.00762	-0.00071	-0.03802	0.01302
	2PY	-0.01527	-0.00994	-0.02565	0.12221	-0.0176	-0.05942	-0.05162	-0.00249
	2PZ	0.03597	-0.0519	-0.02029	-0.02021	-0.05103	-0.10888	-0.08234	0.00348
	3S	0.01006	-0.01528	-0.00369	-0.02195	0.01691	0.0435	-0.02429	0.02317
	3PX	0.01602	-0.00788	0.01823	-0.02951	0.00524	0.00954	-0.03328	0.01432
	3PY	-0.00276	-0.0061	-0.00923	0.04767	-0.02302	-0.05815	-0.02646	-0.02641
	3PZ	0.01677	-0.02375	-0.00687	0.00464	-0.02744	-0.06789	-0.06414	0.01412
	4XX	0.00163	0.00038	0.00273	-0.0045	-0.00067	0.00064	0.00438	-0.00084
	4YY	-0.00053	-0.00126	-0.00222	0.00462	-0.00162	-0.00585	-0.00956	0.0011
	4ZZ	-0.00122	0.00071	-0.00125	-0.00093	0.0012	0.00363	0.00591	-0.00121
	4XY	0.00121	-0.00369	-0.00393	-0.00247	-0.0019	-0.0019	0.00274	-0.00071
	4XZ	-0.00012	0.00046	0.00115	0.0038	0.00147	0.00406	0.00824	-0.0018
	4YZ	0.00069	0.00101	0.00257	-0.00108	-0.00089	-0.00361	-0.00717	0.00148
37C	1S	0.00271	-0.00536	-0.00346	0.00114	0.00625	0.01172	-0.00572	0.00603
	2S	-0.0049	0.01084	0.008	-0.00699	-0.0139	-0.02432	0.01234	-0.01422
	2PX	-0.02165	-0.02945	-0.08015	0.04802	-0.03627	-0.04343	0.06689	-0.02674
	2PY	0.04119	-0.02211	0.02755	-0.08941	-0.01659	0.01187	0.09625	-0.00691
	2PZ	0.02015	-0.03676	-0.00905	0.06499	0.01345	0.05519	0.1416	-0.03206
	3S	-0.01475	0.02353	0.00587	0.01241	-0.02731	-0.07639	0.03111	-0.00846
	3PX	0.00003	-0.02006	-0.0294	0.00012	-0.00068	0.01571	0.02136	0.0283
	3PY	0.01447	-0.01232	0.00283	-0.00754	-0.00285	0.01603	0.06915	0.03221
	3PZ	0.01454	-0.02399	-0.00538	0.01866	-0.0007	0.02157	0.12036	-0.06443
	4XX	0.00137	-0.00114	0.00055	-0.00787	0.00176	0.00479	0.00283	0.00173
	4YY	-0.00005	-0.00121	-0.00148	0.00909	0.00065	0.00181	0.00385	-0.00044
	4ZZ	-0.00136	0.00119	-0.00074	0.0014	-0.00092	-0.00447	-0.00819	0.00033
	4XY	0.00071	-0.00141	-0.00162	-0.00307	-0.00003	0.00326	0.00688	-0.00065
	4XZ	-0.00082	0.00125	0.00084	0.00286	0.00306	0.00749	0.00693	-0.0005
	4YZ	0.0017	-0.00111	0.00128	-0.00507	-0.0007	-0.00067	0.00056	-0.00036
38C	1S	0.00089	0.00518	0.00889	0.00385	-0.00032	0.00108	0.0019	0.00318
	2S	-0.0031	-0.0115	-0.02135	-0.00673	-0.00028	-0.00154	-0.00624	0.00587
	2PX	0.00612	-0.02167	-0.00279	-0.0627	0.02561	0.0562	0.05224	-0.00591
	2PY	0.02465	-0.01308	0.02083	0.12505	0.05485	0.13776	0.12135	0.00023
	2PZ	0.03415	-0.05022	-0.01856	-0.06121	0.01114	0.12041	0.23263	-0.01593
	3S	0.00253	-0.01327	-0.01188	-0.04448	0.01143	-0.01264	0.00652	-0.11052
	3PX	0.00268	-0.01791	-0.01874	-0.00813	0.01457	0.03266	0.04058	0.04572
	3PY	0.01265	-0.00245	0.01576	0.02042	0.03156	0.06537	0.06987	-0.00618
	3PZ	0.01705	-0.02488	-0.00509	-0.01594	0.00644	0.09256	0.15303	-0.02501

	4XX	-0.00075	0.00315	0.00349	-0.00837	-0.0009	-0.00173	-0.00277	0.00242
	4YY	0.00113	-0.00166	-0.00052	0.00618	0.00174	0.00343	0.00134	0.00087
	4ZZ	-0.00032	-0.00039	-0.00097	0.0014	-0.00082	-0.00118	0.0017	-0.00051
	4XY	-0.00178	0.00108	-0.00167	-0.00133	-0.00249	-0.00452	-0.00161	-0.00163
	4XZ	0.00054	0.00059	0.00149	0	0.00571	0.00922	-0.01218	0.00505
	4YZ	0.00037	0.00041	0.00124	-0.00166	-0.00195	-0.00299	0.00498	-0.00286
39C	1S	-0.00362	-0.00063	-0.00752	-0.0022	-0.00643	-0.01145	0.00555	0.00037
	2S	0.00685	0.00377	0.01805	0.00533	0.01418	0.02378	-0.01307	0.00066
	2PX	0.02719	-0.06694	-0.05	0.0446	0.01812	0.04309	0.02561	-0.01869
	2PY	0.01674	-0.02677	-0.00513	-0.11275	-0.03359	-0.02359	0.10114	-0.0372
	2PZ	0.0243	-0.02222	0.00631	0.0812	0.00833	0.05352	0.14056	-0.0153
	3S	0.01961	-0.01419	0.01691	0.02354	0.02988	0.0755	-0.02219	0.00195
	3PX	-0.00142	-0.01194	-0.01078	0.02409	-0.00523	0.00109	0.03119	-0.02128
	3PY	0.01735	-0.01584	0.00722	-0.04984	0.00624	0.01105	0.0605	-0.06889
	3PZ	0.01707	-0.0251	-0.01377	0.04119	-0.00441	0.03091	0.11608	0.01224
	4XX	-0.00063	0.00011	-0.00063	-0.00582	-0.00036	0.00053	0.00381	0.0002
	4YY	-0.00124	0.00135	-0.00024	0.00412	-0.00122	-0.00539	-0.00918	0.0008
	4ZZ	0.00139	-0.0023	-0.00109	0.00035	0.00011	0.00269	0.00663	-0.0008
	4XY	0.00059	-0.00141	-0.00162	-0.00377	0.00022	0.00127	0.00024	-0.0002
	4XZ	-0.0011	0.00234	0.00155	0.00287	0.00299	0.00688	0.00579	0.0001
	4YZ	-0.00076	0.00118	0.00055	-0.0014	-0.0014	-0.00513	-0.00613	0.00026
40C	1S	0.00235	0.00109	0.00557	0.00289	0.00323	0.00549	-0.00241	-0.00041
	2S	-0.00371	-0.0035	-0.0124	-0.01009	-0.00668	-0.01065	0.00549	0.00002
	2PX	-0.01122	0.05021	0.06019	-0.02435	-0.02144	-0.04845	-0.01899	0.0064
	2PY	0.00761	-0.00609	0.00742	0.10917	-0.00768	-0.04072	-0.06526	0.00488
	2PZ	0.03588	-0.06497	-0.03434	-0.01931	-0.0488	-0.10664	-0.09556	0.00273
	3S	-0.02148	0.00736	-0.01683	0.00223	-0.02222	-0.04007	0.01388	0.0045
	3PX	-0.01142	0.02244	0.01771	-0.0039	-0.02497	-0.04838	-0.00931	0.00885
	3PY	0.01007	-0.01368	-0.00121	0.02995	-0.0138	-0.03372	-0.04402	0.01244
	3PZ	0.01715	-0.02805	-0.01002	0.0079	-0.02445	-0.0668	-0.07316	-0.00662
	4XX	0.00098	0.00091	0.00271	-0.00616	-0.00022	0.00165	0.00567	-0.00136
	4YY	-0.0018	0.00166	-0.0005	0.00684	0.00277	0.00471	0.00165	0.00018
	4ZZ	0.001	-0.00202	-0.00116	0.0022	-0.00151	-0.00478	-0.00792	0.00094
	4XY	0.00054	-0.00263	-0.00283	-0.00392	0.00028	0.00296	0.00759	-0.00226
	4XZ	0.00002	0.00057	0.00086	0.00416	0.00153	0.00502	0.00966	-0.00143
	4YZ	-0.00011	0.00158	0.00177	-0.00535	-0.00003	0.00012	-0.00045	0.00017
41H	1S	0.00912	0.0355	0.06331	-0.04344	0.00028	0.00095	0.00037	0.00439
	2S	0.01061	0.03891	0.07072	-0.05189	0.0006	0.0011	0.00097	0.00998
	3PX	0.00052	0.00038	0.00133	-0.00105	-0.00038	-0.00112	-0.00181	0.00018
	3PY	0.00076	-0.00141	-0.00084	-0.00075	-0.00081	-0.00225	-0.0038	0.0007
	3PZ	0.00011	-0.00034	-0.00013	0.00179	-0.00133	-0.00408	-0.00597	0.00093
42H	1S	0.00638	-0.02619	-0.03643	-0.0333	-0.01511	-0.01553	0.00588	-0.00193
	2S	0.00653	-0.02775	-0.03898	-0.03924	-0.02066	-0.02326	0.01145	-0.01069
	3PX	0.00073	-0.00068	0.00002	-0.00161	-0.00039	-0.00079	-0.00069	-0.00006

	3PY	-0.00004	-0.00087	-0.0013	0.00139	-0.00072	-0.00161	-0.00141	0.0002
	3PZ	0.00057	-0.00044	0.00047	0.00051	-0.00081	-0.0023	-0.00235	0.00012
43H	1S	-0.02345	0.00434	-0.02468	0.09219	0.00526	-0.00193	0.00326	-0.00914
	2S	-0.02069	0.00392	-0.02207	0.10828	0.01869	0.03101	-0.01428	0.04636
	3PX	0.00012	-0.00049	-0.00066	-0.00025	-0.00033	0.00001	0.00099	0.00043
	3PY	-0.00034	-0.00049	-0.00101	0.00186	-0.00027	0.00013	0.0027	-0.00096
	3PZ	0.001	-0.00096	0.00027	-0.00077	0.00012	0.0012	0.00351	-0.00085
44H	1S	0.01404	-0.0339	-0.02454	-0.04738	-0.00443	-0.00119	-0.00349	-0.0088
	2S	0.01251	-0.03836	-0.04762	-0.04526	-0.0243	-0.02509	0.01243	0.04375
	3PX	0	-0.00015	-0.00042	0.00253	0.00013	0.00026	0.00177	0.00072
	3PY	0.00015	0.00001	0.00015	-0.00076	-0.00041	0.00005	0.00233	-0.00102
	3PZ	0.00097	-0.00157	-0.00075	0.00037	0.0001	0.00129	0.0034	-0.00053
45H	1S	-0.0088	0.00783	-0.0018	0.08483	0.01386	0.01603	-0.00394	0.00369
	2S	-0.00992	0.01305	0.00255	0.10067	0.01953	0.02345	-0.00808	0.0017
	3PX	-0.00023	0.0008	0.00093	0.00042	-0.00019	-0.00078	-0.00069	-0.00011
	3PY	0.00044	-0.00055	0.00018	-0.00095	-0.00075	-0.00166	-0.00166	0.00012
	3PZ	0.00055	-0.00102	-0.00058	0.00147	-0.00087	-0.00232	-0.00266	0.00023
46C	1S	-0.00082	-0.00204	-0.00549	0.00606	0.00043	-0.00151	-0.00138	-0.00079
	2S	0.00221	0.00443	0.01203	-0.01258	-0.00055	0.00294	0.0038	0.00106
	2PX	-0.0109	0.02726	0.01008	0.06598	-0.00777	-0.00016	-0.0083	-0.00426
	2PY	-0.04907	0.07159	0.0303	-0.09125	-0.03786	-0.06925	-0.00737	-0.01177
	2PZ	0.06108	-0.04839	0.02681	-0.06834	0.13889	0.27327	-0.18307	0.10869
	3S	-0.00935	0.02009	0.02609	-0.05358	-0.01198	0.0003	-0.01387	0.0118
	3PX	-0.00778	0.00469	-0.00199	0.01402	0.001	0.00948	0.00485	0.01826
	3PY	-0.01211	0.01582	0.00751	-0.0023	-0.01731	-0.0132	0.00269	-0.02352
	3PZ	0.0326	-0.02807	0.01063	-0.03186	0.08752	0.16706	-0.11128	0.09678
	4XX	-0.00166	0.00085	-0.00085	-0.00637	-0.0009	-0.00395	-0.00626	-0.0011
	4YY	0.00087	-0.0001	0.0007	0.00518	0.00091	0.00405	0.00339	0.00592
	4ZZ	0.00018	-0.00037	-0.0004	0.00056	-0.00019	-0.00075	0.00196	-0.00437
	4XY	-0.00096	0.00527	0.00523	-0.00008	-0.00206	-0.00377	-0.00284	0.00131
	4XZ	0.00215	-0.00001	0.00307	0.00058	0.00321	-0.00118	-0.01171	-0.0068
	4YZ	0.00161	-0.00088	0.00107	-0.00048	-0.00008	-0.00247	0.00611	-0.02009
47C	1S	0.00495	-0.01346	-0.01253	-0.00264	0.00171	0.0089	0.01226	-0.00207
	2S	-0.01095	0.02818	0.02591	0.00322	-0.00211	-0.01708	-0.02499	0.00374
	2PX	0.02109	-0.04471	-0.01661	-0.01991	0.03101	0.03787	0.00334	-0.02344
	2PY	0.00187	-0.02858	-0.035	0.06036	-0.01223	-0.01061	0.04192	0.05984
	2PZ	0.11276	-0.07544	0.06164	-0.03997	0.13181	0.10116	-0.15967	-0.30907
	3S	-0.02071	0.05548	0.044	0.0106	-0.02199	-0.06475	-0.08701	0.01925
	3PX	0.00756	-0.02036	-0.01606	0.01002	-0.00126	0.00578	-0.033	-0.01984
	3PY	-0.01573	0.01036	0.00562	0.00637	-0.01288	-0.01298	0.02159	0.07735
	3PZ	0.05808	-0.03468	0.04126	-0.03184	0.07668	0.08251	-0.13026	-0.29357
	4XX	-0.00016	-0.00002	0.00046	-0.00494	0.00024	0.00042	0.00168	-0.00087
	4YY	0.00194	-0.00267	-0.00219	0.00519	0.00096	0.0005	-0.00033	0.00093
	4ZZ	-0.00079	-0.0001	-0.00131	0.00016	-0.00109	0.00009	0.00139	-0.00022

	4XY	-0.00288	0.00303	0.0011	-0.00129	-0.00114	0.0004	-0.00103	0.00156
	4XZ	0.00501	-0.00238	0.00379	-0.00112	0.00011	-0.01004	0.00313	-0.01117
	4YZ	-0.00237	0.00152	-0.00139	0.00283	-0.00491	-0.00493	0.00458	-0.00425
48H	1S	0.01319	-0.01924	-0.01494	0.04747	0.00155	-0.00749	-0.00007	-0.00045
	2S	0.03044	-0.05126	-0.0488	0.06229	0.00739	0.01509	0.03108	-0.03395
	3PX	0.00053	-0.00095	-0.00038	0.00019	0.00049	0.00015	-0.00086	-0.00067
	3PY	-0.00034	-0.00052	-0.00172	-0.00091	-0.00084	-0.00034	0.0012	0.00212
	3PZ	0.00228	-0.00135	0.00183	-0.00133	0.00298	0.0026	-0.00388	-0.0092
49C	1S	-0.00635	0.00633	0.0062	0.00176	-0.00209	-0.00419	-0.00179	0.00053
	2S	0.01444	-0.0149	-0.01657	-0.00169	0.00265	0.00759	0.00184	-0.00221
	2PX	0.00828	0.00419	-0.00482	0.03529	-0.01301	-0.02604	-0.00641	-0.00132
	2PY	-0.07207	0.03971	0.00342	-0.0315	-0.01464	0.02378	0.00084	0.02671
	2PZ	0.20873	-0.12041	0.13524	-0.07138	0.12053	-0.12191	0.01606	-0.16222
	3S	0.01338	-0.00727	0.00055	-0.03887	0.02229	0.03395	0.03515	0.01057
	3PX	0.00317	0.00182	-0.00495	0.0127	-0.01021	-0.02045	-0.03569	0.00236
	3PY	-0.01383	0.00622	-0.00814	0.00266	-0.00294	0.02489	0.00836	0.00144
	3PZ	0.11828	-0.07225	0.07216	-0.03745	0.08551	-0.08917	0.02198	-0.07953
	4XX	-0.00131	0.00245	0.00214	-0.0006	0.00055	-0.00163	-0.00332	0.00096
	4YY	-0.00014	-0.00092	-0.00006	-0.00036	0.0018	-0.00311	0.00627	0.00838
	4ZZ	-0.00137	0.00117	0.00032	0.00021	-0.00295	0.00363	-0.00349	-0.00862
	4XY	-0.00331	0.00204	-0.00012	-0.00425	-0.00005	0.00154	0.00075	-0.00342
	4XZ	0.0039	-0.00147	0.00255	0.00049	-0.00454	-0.01028	0.01196	0.01941
	4YZ	-0.00127	0.00109	-0.0013	0.00264	-0.01061	0.01143	-0.00787	-0.02467
50O	1S	0.00838	-0.00576	-0.01085	0.00778	-0.00135	-0.00175	-0.0017	0.00028
	2S	-0.01747	0.01326	0.02415	-0.01561	0.00125	0.00305	0.00227	0.00143
	2PX	-0.01892	0.03159	0.04507	-0.00634	0.00997	-0.01615	-0.06264	-0.00688
	2PY	0.01718	-0.00111	-0.04946	0.08276	-0.03809	0.031	-0.06786	-0.0618
	2PZ	0.19104	-0.1144	0.10785	-0.05869	0.16991	-0.25779	0.16369	0.32987
	3S	-0.03131	0.01701	0.04143	-0.03071	0.0121	0.01132	0.01635	-0.01199
	3PX	-0.01278	0.02194	0.02924	-0.00545	0.00705	-0.01128	-0.0453	-0.00181
	3PY	0.00934	-0.00074	-0.02943	0.05139	-0.02332	0.0229	-0.04769	-0.05451
	3PZ	0.11802	-0.07081	0.06713	-0.03755	0.11464	-0.17752	0.12247	0.27788
	4XX	0.00047	-0.00074	-0.00158	-0.00027	-0.00066	0.00029	0.00114	0.00085
	4YY	-0.001	0.00139	-0.00381	0.00462	-0.00354	0.00248	-0.00508	-0.00229
	4ZZ	0.00361	-0.00176	0.00282	-0.00135	0.00227	-0.00425	0.00181	0.0033
	4XY	-0.00097	0.00107	0.00233	-0.00172	0.00116	-0.00179	-0.00147	0.00049
	4XZ	-0.00518	0.00314	-0.00253	0.00182	-0.00477	0.00426	-0.00205	-0.00294
	4YZ	0.01212	-0.0069	0.00667	-0.00275	0.00824	-0.01277	0.00674	0.00804
51C	1S	-0.00317	0.00413	0.00235	-0.00815	-0.00217	-0.00741	-0.007	-0.00023
	2S	0.00639	-0.00845	-0.00451	0.01658	0.00475	0.01566	0.01664	0.00051
	2PX	-0.03027	-0.05416	-0.11483	-0.02275	-0.01133	-0.03198	-0.04374	-0.00037
	2PY	0.0271	-0.05429	-0.03664	0.09563	0.0022	0.00299	0.05758	-0.04008
	2PZ	0.03554	-0.03505	0.00561	-0.01034	0.09337	0.19261	-0.16674	0.29012
	3S	0.01737	-0.02318	-0.01564	0.05337	0.00906	0.04465	0.02528	-0.00979

	3PX	-0.0081	-0.01814	-0.04179	-0.00346	-0.00455	-0.00969	-0.0199	-0.00449
	3PY	0.00919	-0.01767	-0.00977	0.04891	-0.00152	-0.00731	0.0308	-0.04374
	3PZ	0.0227	-0.02029	0.00695	-0.00652	0.0631	0.12229	-0.12416	0.25509
	4XX	-0.00168	0.00133	-0.00037	-0.00483	-0.00073	-0.0021	-0.00239	0.00018
	4YY	0.00028	0.00047	0.00101	0.00241	-0.00106	-0.00197	0.00252	-0.00194
	4ZZ	0.00031	-0.00026	0.0003	-0.00077	0.00133	0.00258	-0.00204	0.00167
	4XY	0.00011	0.0041	0.00529	0.00101	0.00003	0.00153	0.00145	0.00011
	4XZ	0.00027	0.00073	0.00129	0.00002	-0.0004	-0.00273	0.00094	-0.00276
	4YZ	0.00274	-0.00217	0.00114	-0.00162	0.00557	0.01089	-0.00763	0.00535
52H	1S	-0.0227	-0.02288	-0.06087	-0.03453	-0.00872	-0.02381	-0.02499	-0.00069
	2S	-0.02565	-0.01568	-0.04418	-0.04848	-0.00619	-0.03121	-0.02232	0.00794
	3PX	0.00075	0.00028	0.00168	0.00073	0.00048	0.00088	0.00122	0.00052
	3PY	-0.00009	-0.00135	-0.00176	0.00098	-0.00015	-0.00024	0.00139	-0.00097
	3PZ	0.00114	-0.0011	0.0002	-0.00067	0.00255	0.00328	-0.00358	0.00823
53H	1S	0.00332	0.05103	0.07192	-0.01529	0.00083	0.00983	0.01366	-0.00174
	2S	-0.00111	0.05548	0.07067	-0.01178	-0.00253	-0.00619	-0.00406	-0.00963
	3PX	-0.00011	0.00102	0.00125	-0.00126	-0.00005	0.00019	0.00083	-0.00033
	3PY	0.00063	0.00077	0.00176	0.0013	-0.00006	-0.00022	0.00112	-0.00123
	3PZ	0.00058	-0.00031	0.00043	-0.00001	0.00206	0.0047	-0.00407	0.00823

3.3.2 Combined coefficients and computational details of HFV index (F) of M1b

Table S7. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of **M1b**

i/j \ k / $\|c_{ki}\|/\|c_{kj}\|$	83	84	85	89	92	93	97	99
46	0.1164	0.1300	0.0727	0.1792	0.2131	0.4420	0.2833	0.1739
47	0.1761	0.1577	0.1378	0.1017	0.1984	0.2064	0.3058	0.5049
49	0.3358	0.1942	0.2124	0.1243	0.1901	0.2196	0.0792	0.2140
51	0.0837	0.1238	0.1777	0.1512	0.1429	0.3178	0.2962	0.4497

Table S8. The calculation details of HFV index (F) of **M1b**

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	ΣP	HFV (F)
α (47)	47-46	83 (1), 92 (1), 93 (1), 97 (1), 99 (-1)	0.31 [a]	0.75	1.01
	47-49	83 (1), 84 (1), 85 (1), 92 (1), 93 (-1), 99 (1)	0.44 [b]		
γ (51)	51-46	92 (1), 93 (1), 97 (1), 99 (1)	0.67 [c]	0.67	1.09

a : $P_{47\text{-}46}$=2*0.1761*0.1164+2*0.1984*0.2131+2*0.2064*0.4420+2*0.3058*0.2833-2*0.5049*0.1739=0.31

b : $P_{47\text{-}49}$=2*0.1761*0.3358+2*0.1577*0.1942+2*0.1378*0.2124+2*0.1984*0.1901-2*0.2064*0.2196+2*0.5049*0.2140=0.44

c : $P_{51\text{-}46}$=2*0.1429*0.2131+2*0.3178*0.4420+2*0.2962*0.2833+2*0.4497*0.1739=0.67

3.4 The occupied π-type molecular orbitals associated with the active sites of M1c

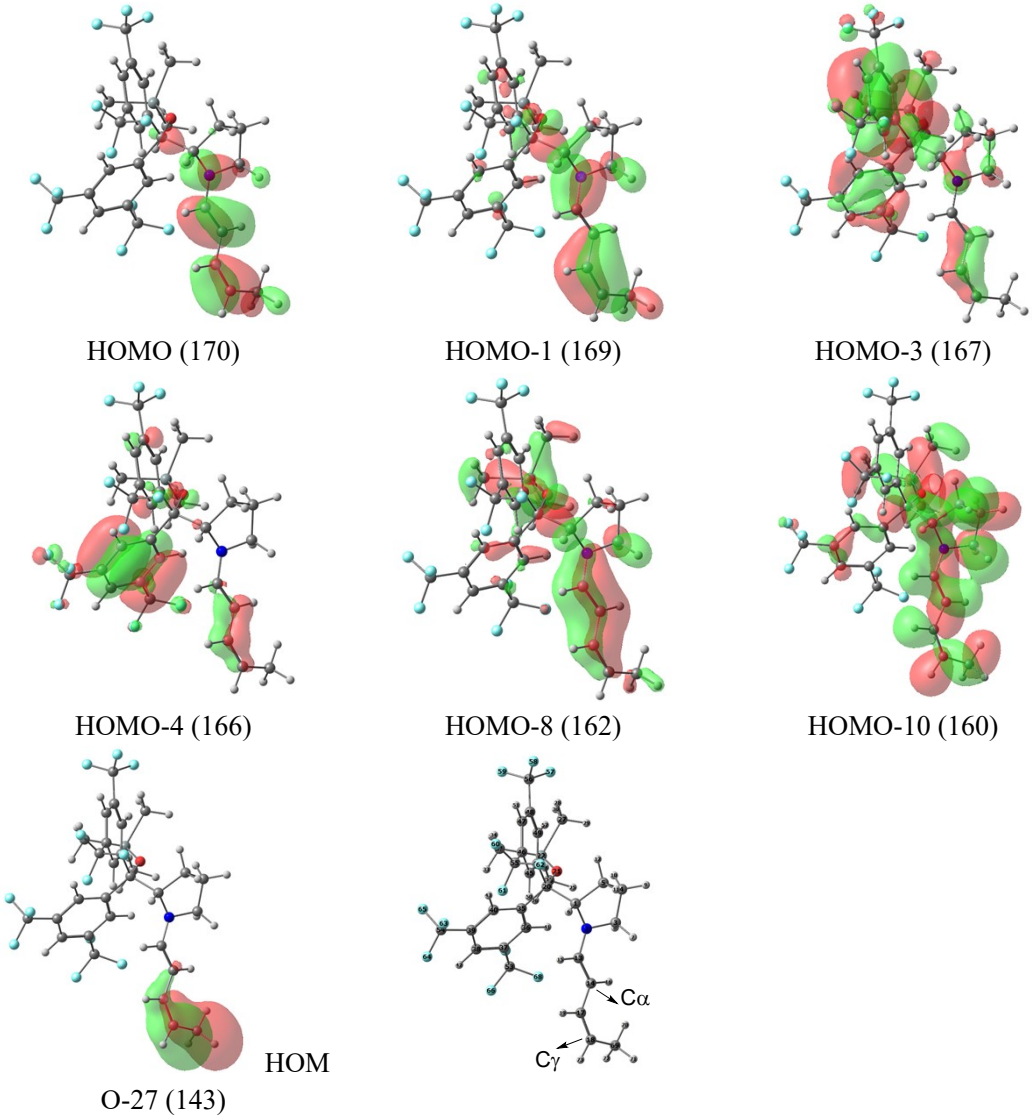


Fig. S7. The occupied π-type molecular orbitals associated with the active sites of **M1c**

3.4.1 Molecular orbital coefficients of M1c

		143	160	162	166	167	169	170
1C	1S	0.00023	0.00319	-0.0006	-0.00685	0.01686	-0.00817	-0.00482
	2S	-0.00028	-0.00388	0.00224	0.01206	-0.02975	0.01976	0.01421
	2PX	-0.01477	0.00591	-0.00033	0.02109	-0.04711	-0.00961	-0.03144
	2PY	0.00146	-0.01554	-0.01708	0.01585	-0.03896	0.00575	0.00307
	2PZ	-0.00605	0.0927	-0.12423	-0.03848	0.07897	-0.1227	-0.02732
	3S	0.00025	-0.02991	0.00432	0.04498	-0.1192	0.03915	0.02049
	3PX	-0.00481	-0.00971	-0.00181	0.00806	-0.00427	-0.01734	-0.02773
	3PY	-0.00266	-0.01188	-0.01314	0.0108	-0.00522	-0.0047	0.01386
	3PZ	-0.00155	0.06079	-0.05347	-0.02908	0.05347	-0.04086	0.0242
	4XX	0.00085	-0.00062	0.00041	-0.00241	0.00404	-0.00098	-0.00036
	4YY	-0.00084	0.00471	-0.00465	-0.00064	0.00083	-0.00592	-0.00434
	4ZZ	0.00014	-0.00348	0.00474	0.0018	-0.00276	0.00649	0.00427
	4XY	0.00066	-0.00283	0.0003	-0.00059	0.00133	0.00061	0.00166
	4XZ	0.00016	-0.00335	-0.00827	0.0008	-0.00196	-0.01526	-0.01632
	4YZ	-0.00017	0.00307	-0.00617	-0.00068	-0.0013	-0.00696	-0.00661
2N	1S	-0.00048	-0.00065	0.00565	0.00296	-0.00205	0.01187	0.0111
	2S	0.00138	0.00113	-0.01046	-0.00667	0.00124	-0.02234	-0.02115
	2PX	0.01673	-0.01071	0.0244	-0.02022	0.04878	0.05843	0.07636
	2PY	-0.00755	0.03764	0.01474	-0.01029	0.01677	-0.00226	-0.00589
	2PZ	-0.00666	0.10893	0.14456	-0.01459	0.05804	0.30219	0.31767
	3S	0.00007	0.01201	-0.03039	-0.01956	0.03666	-0.06558	-0.05749
	3PX	0.00785	-0.01086	0.01857	-0.01531	0.04725	0.03792	0.05582
	3PY	-0.00426	0.0123	0.01501	-0.0007	0.00753	0.00138	-0.01328
	3PZ	-0.00306	0.07534	0.1016	-0.01351	0.04446	0.24195	0.28284
	4XX	0.00033	-0.00058	-0.0034	-0.00109	0.0009	-0.00262	0.00235
	4YY	-0.00029	-0.00141	-0.00182	0.00003	-0.00236	-0.00149	0.0008
	4ZZ	0.00016	0.00106	0.00625	0.00159	-0.00097	0.00736	0.0004
	4XY	0.00075	0.00033	0.0009	0.00036	-0.00011	0.00161	-0.00092
	4XZ	-0.00041	0.00151	-0.00621	-0.002	0.00349	-0.00296	0.00748
	4YZ	0.00042	0.00772	0.00755	-0.00018	0.00098	0.00496	-0.00425
3C	1S	0.00086	-0.00106	0.003	-0.00034	0.00332	-0.00378	-0.00885
	2S	-0.0016	0.0029	-0.00531	0.00132	-0.00815	0.00889	0.01993
	2PX	-0.00713	-0.02042	-0.00052	0.0101	-0.03626	0.00077	-0.00425
	2PY	0.00004	-0.05349	-0.02693	0.00654	-0.01237	-0.00052	0.02327
	2PZ	-0.0143	-0.14398	-0.1135	-0.00358	-0.02083	-0.0869	-0.02262
	3S	-0.00429	-0.00688	-0.01607	0.00449	-0.01928	0.01862	0.05125
	3PX	-0.00282	-0.00826	0.00494	0.00696	-0.02181	0.01043	0.00855
	3PY	-0.00013	-0.03706	-0.0022	0.00935	-0.00904	0.00253	0.00112
	3PZ	-0.00762	-0.06409	-0.05473	-0.00366	-0.00517	-0.02566	0.03799
	4XX	-0.00013	0.00337	0.00266	-0.00005	0.00116	0.00169	0.00148
	4YY	0.00036	0.00136	0.00296	0.0007	-0.00058	0.00511	0.00388
	4ZZ	-0.00002	-0.00541	-0.00423	-0.00002	-0.00049	-0.00649	-0.00635

	4XY	0.0006	0.00213	0.00182	-0.00104	0.00315	0.00396	0.00574
	4XZ	0.00054	0.01251	0.00586	-0.00074	0.00322	0.00653	0.0064
	4YZ	-0.00003	0.00429	0.00737	-0.00045	0.0028	0.01258	0.01287
4C	1S	0.00116	0.00031	-0.00103	-0.00169	0.00152	0.00208	0.0048
	2S	-0.00257	0.0008	0.00557	0.00509	-0.00613	0.00214	-0.00438
	2PX	0.00238	0.00702	-0.01104	-0.00646	0.03061	-0.00582	0.00896
	2PY	-0.0124	0.02854	0.00949	0.00395	0.00057	-0.00834	-0.01807
	2PZ	0.00387	0.17424	0.01975	-0.00953	0.02292	0.00006	-0.00621
	3S	-0.00367	-0.00952	-0.00535	0.00433	-0.00037	-0.03497	-0.05847
	3PX	0.00053	0.00289	-0.01492	-0.00413	0.01784	-0.01014	0.00736
	3PY	-0.00513	0.01818	-0.01226	-0.00594	0.00937	-0.03422	-0.03875
	3PZ	0.00166	0.07851	0.00556	-0.00601	0.01257	-0.00475	-0.00648
	4XX	-0.00014	0.00372	0.00134	0.00022	-0.00135	0.00205	0.00088
	4YY	-0.00012	0.00416	-0.00014	-0.00035	0.00116	-0.00074	-0.00006
	4ZZ	0.00041	-0.00814	-0.00097	0.00035	-0.00058	-0.00016	0.00019
	4XY	-0.00004	0.00305	0.0002	-0.0004	0.00145	-0.0007	-0.00136
	4XZ	0.0006	0.00412	0.00443	0.00016	0.00092	0.00363	0.00151
	4YZ	-0.00032	-0.01019	-0.00057	0.00062	-0.00076	0.00042	0.00178
5C	1S	0.00047	-0.00615	-0.00008	-0.00006	0.00361	0.00332	0.00589
	2S	-0.00092	0.01411	-0.00091	0.00056	-0.00854	-0.00943	-0.01755
	2PX	0.00819	-0.02232	-0.00883	0.00175	-0.04629	0.02997	0.02282
	2PY	-0.00287	-0.03491	-0.02616	0.0004	-0.00459	-0.04155	-0.03238
	2PZ	0.0164	-0.12368	0.04458	0.01054	-0.00265	0.03045	0.01628
	3S	-0.00385	0.02558	0.01057	0.00139	-0.01673	0.00538	-0.00177
	3PX	0.00417	-0.00925	-0.00957	-0.0031	-0.03868	0.00473	-0.01483
	3PY	-0.00319	-0.02426	-0.02476	-0.00209	0.01491	-0.04873	-0.04009
	3PZ	0.00809	-0.06271	0.02611	0.00877	-0.00737	0.02018	0.01513
	4XX	-0.00035	0.0045	-0.00103	-0.00086	0.00043	0.00089	0.00269
	4YY	-0.00045	0.00381	-0.00257	-0.00006	0.00103	-0.00334	-0.0025
	4ZZ	0.00083	-0.00934	0.00308	0.00106	-0.00131	0.00243	-0.00017
	4XY	-0.00009	0.00019	0.00229	0.00065	-0.00011	0.00083	-0.00136
	4XZ	-0.00009	-0.00384	0.00093	0.0006	-0.00039	-0.00052	-0.00177
	4YZ	0.00018	-0.00382	-0.00199	-0.00023	0.00031	-0.00139	-0.00015
6H	1S	-0.00344	0.02671	-0.06597	0.00087	-0.01164	-0.06024	-0.04064
	2S	-0.00186	0.0282	-0.06274	-0.00503	0.0016	-0.08196	-0.1032
	3PX	-0.00021	-0.00066	-0.00006	0.00004	0.00019	-0.001	-0.00095
	3PY	0.00015	-0.00103	0.00208	-0.00016	-0.00016	0.00161	0.0006
	3PZ	-0.00001	0.00062	-0.00046	-0.00057	0.00179	-0.00109	-0.00045
7H	1S	-0.00658	-0.09505	-0.07577	-0.00223	-0.01153	-0.07433	-0.04723
	2S	-0.00257	-0.10013	-0.05911	0.00674	-0.01955	-0.10321	-0.14656
	3PX	-0.00029	-0.00144	-0.00193	-0.0001	-0.00057	-0.00128	-0.00009
	3PY	0.00004	-0.00121	0.00045	0.00037	-0.00029	0.00072	0.00009
	3PZ	0.00009	0.00115	0.00135	0.00014	-0.00014	0.00112	0.00036
8H	1S	0.00828	0.09994	0.06513	-0.00679	0.03432	0.06609	0.05015

	2S	0.00738	0.09684	0.07037	-0.0098	0.04404	0.08924	0.10382
	3PX	0.00017	0.00257	0.00213	0.00011	0.00016	0.00179	0.00051
	3PY	0.00014	0.00083	-0.00023	-0.0001	0.00028	-0.00027	0.0001
	3PZ	0.00006	0.00046	-0.00003	-0.00023	0.00058	0.00025	0.00053
9H	1S	0.00679	0.072	0.00526	-0.00552	0.0115	0.00162	-0.00051
	2S	0.00643	0.07692	-0.00044	-0.00929	0.01586	-0.00825	-0.01106
	3PX	0.00009	-0.00013	0.00047	-0.00003	0.00052	0.00077	0.0009
	3PY	0.00009	0.00292	0.00055	-0.00005	0.00037	0.00012	-0.0002
	3PZ	-0.00016	0.00097	0.00043	0.00012	-0.00008	0.00005	-0.00039
10H	1S	-0.00028	-0.12473	-0.02008	0.00496	-0.01012	-0.00574	0.00643
	2S	0.00049	-0.11936	-0.02812	-0.00132	-0.00123	-0.01584	0.01001
	3PX	-0.00003	0.00131	-0.00066	-0.00023	0.00083	-0.00055	-0.00001
	3PY	-0.00023	-0.00021	-0.00049	-0.0001	0.00029	-0.00067	-0.00068
	3PZ	0.00003	-0.00303	-0.0002	0.00031	-0.00064	0.00032	0.00041
11H	1S	0.01065	-0.0947	0.03088	0.00939	-0.01215	0.01999	0.0018
	2S	0.00945	-0.10281	0.03144	0.00938	-0.00839	0.02493	-0.00103
	3PX	0.00009	-0.00036	-0.0002	0.00016	-0.00097	0.00048	0.00035
	3PY	-0.00013	-0.00034	-0.0011	-0.00007	-0.00014	-0.00113	-0.00071
	3PZ	-0.00027	0.00196	-0.00064	-0.00018	0.00047	-0.00031	0.00018
12H	1S	0.00047	0.03627	-0.0156	-0.00455	-0.01604	0.00888	0.0148
	2S	0.00055	0.03741	-0.01565	-0.00331	0.02307	0.00413	0.03575
	3PX	0.00008	-0.00189	0.00083	0.00001	0.00086	0.00017	0.00033
	3PY	-0.00004	-0.00008	0.00011	-0.00005	0.00091	-0.00062	-0.00058
	3PZ	0.00033	-0.00217	0.00064	0.00025	-0.00193	0.00123	0.00059
13C	1S	-0.00141	-0.00325	-0.00566	0.00147	0.00002	-0.00566	-0.0036
	2S	0.00264	0.01119	0.01348	-0.00954	-0.00169	0.01318	0.0113
	2PX	-0.01258	0.03071	0.09305	0.01529	-0.01486	0.05255	-0.05162
	2PY	0.00343	-0.06634	-0.04958	-0.01271	0.00026	-0.03486	0.02333
	2PZ	0.01994	0.09971	0.22737	0.04855	-0.01682	0.11112	-0.21034
	3S	0.00461	-0.00066	0.01416	0.0174	0.00928	0.01324	-0.00314
	3PX	-0.00137	0.02487	0.04644	0.00349	-0.01034	0.0238	-0.04435
	3PY	-0.00027	-0.0127	-0.02674	-0.00238	0.00412	-0.00912	0.03593
	3PZ	0.00561	0.06427	0.14627	0.02511	-0.01529	0.07612	-0.17423
	4XX	-0.0004	0.00315	-0.00209	-0.0037	0.00351	0.00654	0.01141
	4YY	-0.00047	-0.00353	0.00113	-0.00037	-0.00155	0.00131	0.00061
	4ZZ	0.0004	-0.00061	-0.0001	0.00282	-0.00245	-0.00939	-0.01252
	4XY	0.00115	-0.00787	-0.00127	0.00077	-0.00133	-0.0054	-0.00582
	4XZ	-0.00074	-0.00223	-0.00432	-0.00371	0.00345	0.01117	0.01855
	4YZ	-0.00041	-0.00071	-0.0047	-0.00084	-0.0013	-0.00748	-0.00499
14C	1S	0.00045	-0.01344	0.00068	0.00052	-0.0011	0.00015	-0.00036
	2S	-0.0015	0.02979	-0.00184	-0.0022	0.00295	0.00058	0.00275
	2PX	0.02674	-0.00092	0.05185	0.02182	-0.00773	-0.03823	-0.078
	2PY	-0.01241	0.11485	-0.05108	-0.015	0.01376	0.01484	0.04453
	2PZ	0.02388	0.1071	0.21292	0.09734	-0.06608	-0.1111	-0.27437

	3S	-0.00035	0.075	-0.00034	-0.00672	-0.00484	-0.00147	-0.00162
	3PX	0.01067	-0.0037	0.0279	0.0112	-0.00767	-0.02835	-0.05411
	3PY	-0.00559	0.05065	-0.02588	-0.01339	0.006	0.01135	0.03498
	3PZ	0.01925	0.05494	0.12632	0.06369	-0.04364	-0.08122	-0.22735
	4XX	-0.00008	0.00373	0.00276	-0.00026	0.0003	0.00498	-0.00647
	4YY	-0.00095	-0.00606	-0.00073	-0.00122	0.00008	0.00194	-0.00052
	4ZZ	0.0009	-0.00096	-0.00153	0.0009	-0.00081	-0.00656	0.00712
	4XY	0.00133	-0.00543	0.00068	0.0005	-0.00074	-0.00381	0.00236
	4XZ	-0.00102	0.00074	0.00592	0.00034	0.00035	0.00836	-0.01295
	4YZ	0.00109	0.00303	0.00566	0.00292	-0.00206	-0.00575	0.00037
15H	1S	0.00126	-0.04362	-0.00048	-0.00445	-0.00824	-0.00585	-0.00386
	2S	0.00083	-0.06272	-0.0018	-0.00818	-0.01716	-0.01578	-0.02057
	3PX	-0.00021	0.00133	0.00184	0.0006	-0.00034	0.0008	-0.00196
	3PY	-0.00004	0.00004	-0.00113	0.00017	0.00035	-0.00058	0.00061
	3PZ	0.00051	0.00264	0.00546	0.00065	-0.00041	0.00254	-0.00577
16H	1S	0.00041	-0.06894	0.01018	-0.00111	-0.00281	0.0028	0.00083
	2S	0.00095	-0.07838	0.00668	-0.00413	-0.00164	-0.00023	0.00469
	3PX	0.00049	-0.00171	0.0013	0.00065	-0.0003	-0.00107	-0.00232
	3PY	-0.00029	-0.00091	-0.00066	-0.00038	0.00023	0.00075	0.00172
	3PZ	0.00073	0.00195	0.00485	0.00235	-0.00168	-0.00307	-0.00776
17C	1S	0.00149	0.00019	-0.00005	-0.00017	0.00015	-0.00055	-0.00049
	2S	-0.00332	0.00269	0.00022	0.00013	-0.00053	0.00159	0.00011
	2PX	0.00449	0.03404	0.04748	0.03071	-0.02368	-0.07382	0.04648
	2PY	-0.00133	-0.13745	-0.01286	-0.01973	0.01342	0.04584	-0.02566
	2PZ	0.07678	0.02242	0.14672	0.10135	-0.07151	-0.27673	0.1568
	3S	-0.00753	-0.00325	-0.00151	0.00074	0.00133	0.00321	0.0122
	3PX	0.00686	0.00071	0.02537	0.02088	-0.0122	-0.05604	0.02992
	3PY	-0.00169	-0.02859	-0.00998	-0.01255	0.0065	0.03213	-0.0247
	3PZ	0.03469	0.03153	0.09509	0.06443	-0.04945	-0.18962	0.11537
	4XX	-0.00156	0.00292	0.00032	-0.00035	0.0005	0.00264	-0.0095
	4YY	-0.00004	-0.0038	0.00229	0.00067	-0.00079	-0.00066	-0.00171
	4ZZ	0.00169	0.00032	-0.0025	-0.00051	0.00031	-0.00195	0.01106
	4XY	0.00055	-0.0118	-0.00077	-0.00087	0.00032	0.00014	0.00493
	4XZ	-0.00405	-0.00168	0.00212	-0.00039	0.00026	0.00588	-0.01725
	4YZ	-0.00194	0.0005	-0.00476	-0.00234	0.00161	0.00393	0.00549
18C	1S	-0.00091	-0.00036	0.00094	0.00023	-0.00049	0.0007	0.00025
	2S	0.0017	-0.00214	-0.00183	-0.00054	0.00121	-0.00111	-0.0005
	2PX	0.05347	0.00652	0.01187	0.01575	-0.00946	-0.0617	0.07871
	2PY	-0.01859	0.14153	-0.01984	-0.00845	0.00591	0.03449	-0.04702
	2PZ	0.13829	0.0453	0.06847	0.06179	-0.04515	-0.20639	0.28472
	3S	0.00443	0.00294	-0.00532	0.00063	0.00269	-0.00626	-0.00641
	3PX	0.02724	-0.00778	0.00722	0.01047	-0.00587	-0.04288	0.06503
	3PY	-0.0095	0.02783	-0.00952	-0.00534	0.00603	0.02268	-0.038
	3PZ	0.07392	0.01833	0.03651	0.03899	-0.02731	-0.13946	0.24347

	4XX	-0.00224	-0.00123	0.00314	0.00225	-0.00157	-0.00619	0.00408
	4YY	0.0023	0.00274	-0.00017	-0.0001	0.00005	0.0008	-0.00074
	4ZZ	-0.00039	-0.00055	-0.00278	-0.00199	0.00142	0.00563	-0.00344
	4XY	-0.00152	-0.01144	-0.00004	-0.00077	0.00054	0.00146	-0.00065
	4XZ	-0.00415	0.0007	0.00605	0.00423	-0.00298	-0.01176	0.0081
	4YZ	-0.00791	0.00426	0.00116	0.00098	-0.00071	-0.0026	0.00281
19H	1S	0.00018	-0.08975	0.0107	-0.00118	-0.00106	0.00224	0.00103
	2S	0.00056	-0.10608	0.01142	0.0007	-0.00065	0.00282	0.0019
	3PX	0.00009	0.00193	0.00099	0.0007	-0.00064	-0.00187	0.00108
	3PY	-0.00011	0.00121	-0.00083	-0.00049	0.00031	0.00102	-0.00073
	3PZ	0.00164	0.00095	0.0035	0.0025	-0.00171	-0.00674	0.00416
20C	1S	-0.00106	0.00003	-0.00903	-0.00076	-0.00056	-0.01757	-0.01557
	2S	0.00225	-0.0015	0.01694	0.00142	0.00023	0.03507	0.03298
	2PX	-0.00092	-0.00883	-0.05115	-0.0222	-0.01791	-0.06192	-0.03868
	2PY	-0.00298	0.0503	-0.0411	-0.0217	0.06632	-0.06048	-0.02763
	2PZ	0.00062	-0.06693	0.1189	0.01798	-0.05183	0.12643	0.08155
	3S	0.00442	0.01347	0.04942	0.00026	0.01055	0.1049	0.10426
	3PX	-0.0044	0.00071	-0.0069	0.00027	-0.01017	-0.00263	0.02123
	3PY	0.00156	-0.00981	-0.0076	-0.01038	-0.01415	-0.01787	-0.01211
	3PZ	0.0006	-0.00696	0.0571	-0.01005	-0.0018	0.07486	0.08271
	4XX	0.00016	-0.00061	-0.00166	-0.00199	0.00234	-0.00444	-0.00248
	4YY	-0.00009	0.00666	-0.00511	-0.00162	0.0029	-0.00481	-0.00177
	4ZZ	-0.0003	-0.00682	0.00523	0.00352	-0.00556	0.00615	0.00199
	4XY	0.00031	-0.00147	-0.00196	-0.00111	-0.00989	-0.00074	-0.00063
	4XZ	-0.00027	0.00332	-0.00243	-0.00423	0.01022	-0.0061	-0.00054
	4YZ	0.00025	-0.00408	0.00013	-0.00018	-0.00368	-0.00083	-0.00043
21O	1S	0.0008	-0.00779	0.00433	0.003	-0.00705	0.00721	0.00149
	2S	-0.00172	0.01781	-0.01012	-0.00469	0.01453	-0.01399	-0.00223
	2PX	-0.00337	-0.02155	0.0328	0.05873	0.03424	0.05818	-0.0017
	2PY	0.0028	-0.10244	0.04025	0.03223	-0.10284	0.04533	0.00772
	2PZ	0.00324	0.12589	-0.09845	-0.04025	0.07964	-0.07808	-0.01811
	3S	-0.00328	0.02393	-0.01478	-0.01889	0.02646	-0.03831	-0.00716
	3PX	-0.00193	-0.01569	0.02266	0.04542	0.0299	0.046	-0.00041
	3PY	0.00193	-0.0762	0.0318	0.02068	-0.08352	0.03785	0.01017
	3PZ	0.00199	0.08063	-0.06666	-0.03062	0.04938	-0.05984	-0.01868
	4XX	0.00011	0.00096	-0.00081	0.00032	0.00074	-0.00036	-0.00087
	4YY	0.00015	-0.00011	-0.00236	0.00042	-0.00147	-0.00015	0.00022
	4ZZ	0.00006	-0.00331	0.00445	0.00212	-0.00261	0.0051	0.00254
	4XY	-0.00001	-0.00157	-0.00049	0.00165	-0.00031	0.0001	-0.00145
	4XZ	0.00004	0.00168	-0.00236	-0.00153	0.00107	-0.00181	0.00042
	4YZ	0.00018	0.00592	-0.00328	-0.00104	0.00215	-0.00055	0.0011
22Si	1S	0.00057	0.00013	0.00001	0.00118	-0.00053	0.0014	0.0008
	2S	-0.0026	-0.00165	0.00144	-0.0036	0.00236	-0.00494	-0.00298
	2PX	0.00074	0.01139	-0.03549	0.01891	0.00946	0.0048	0.00026

	2PY	0.00063	0.06565	-0.06579	0.00052	-0.01857	-0.00287	-0.00237
	2PZ	0.00074	0.00293	-0.00271	-0.00566	0.02029	-0.01719	-0.00557
	3S	0.0061	-0.00285	0.00615	0.02058	-0.00619	0.02247	0.0128
	3PX	-0.00179	-0.02769	0.08629	-0.0468	-0.02388	-0.01157	-0.00145
	3PY	-0.00153	-0.15812	0.15966	-0.00114	0.04598	0.00768	0.00629
	3PZ	-0.00162	-0.00819	0.00726	0.01302	-0.05199	0.04355	0.0154
	4S	0.00145	0.01537	-0.0215	-0.01934	-0.00458	-0.01395	-0.00444
	4PX	-0.00073	-0.00659	0.01458	0.02236	-0.00969	0.02153	0.00619
	4PY	-0.00055	-0.03361	0.02526	-0.00885	-0.02673	0.01843	0.01488
	4PZ	0.00146	0.01306	-0.01243	-0.00356	0.00484	-0.00945	-0.00959
	5XX	0.00091	0.0209	-0.02816	0.00561	0.0007	-0.00116	-0.00191
	5YY	-0.00031	-0.00393	0.00888	-0.00852	-0.00307	-0.00498	-0.00124
	5ZZ	-0.00111	-0.01741	0.01881	0.00109	0.00201	0.00352	0.00078
	5XY	-0.00023	-0.0155	0.00953	0.00784	0.01446	0.0017	-0.00079
	5XZ	-0.00061	0.00673	-0.00938	0.00996	-0.00003	0.00808	-0.00044
	5YZ	-0.00128	-0.00156	-0.00615	0.00809	-0.01894	0.01261	0.00198
23C	1S	0.00005	-0.00454	0.01089	-0.00901	-0.00262	-0.00194	0.00104
	2S	-0.00009	0.0093	-0.02193	0.0161	0.00626	0.002	-0.00265
	2PX	-0.0014	0.05757	-0.10485	0.04133	0.0185	0.0155	-0.00129
	2PY	0.00389	0.06007	-0.08673	0.04073	0.00432	0.00255	-0.00392
	2PZ	0.01443	0.00912	-0.0291	0.02112	0.01249	0.00162	-0.00246
	3S	-0.00026	0.01785	-0.04846	0.05533	0.00856	0.01659	-0.00608
	3PX	-0.00054	0.02747	-0.05507	0.0277	0.00673	0.01767	0.00292
	3PY	0.00214	0.03771	-0.04632	0.02607	0.00869	0.00238	-0.00343
	3PZ	0.00654	0.0049	-0.01222	0.00605	-0.00049	0.00686	0.00372
	4XX	0.00028	0.00255	-0.00344	0.0012	0.00011	-0.00014	-0.00021
	4YY	0.00012	-0.00075	0.00142	-0.00103	0.00004	-0.00051	-0.00005
	4ZZ	-0.00034	-0.00204	0.00267	-0.00173	-0.00019	-0.00034	0.0001
	4XY	0.00016	-0.00227	0.00164	0	0.00109	0.0003	0.00022
	4XZ	0.00002	0.00194	-0.0027	0.00098	-0.00037	0.0003	0.00009
	4YZ	-0.00068	0.00048	-0.00045	-0.00044	-0.00065	0.0005	0.00026
24H	1S	-0.00988	-0.01965	0.03313	-0.01882	-0.00628	0.00065	0.00255
	2S	-0.00878	-0.02178	0.04169	-0.02516	-0.01311	0.00554	0.00693
	3PX	-0.00003	0.00165	-0.00279	0.00104	0.00045	0.00025	-0.00014
	3PY	-0.00018	0.00061	-0.00089	0.00043	-0.00014	0.00015	0.00001
	3PZ	-0.00018	-0.00057	0.00094	-0.00033	-0.00003	0.00014	0.00005
25H	1S	0.00546	-0.03427	0.0432	-0.01133	0.00435	-0.00401	-0.00025
	2S	0.00525	-0.03838	0.05461	-0.01133	0.00498	0.00103	0.00402
	3PX	0.00011	0.00098	-0.00203	0.00083	0.00047	0.00018	-0.0001
	3PY	0.00026	0.00018	-0.00045	0.00066	0.00015	0.00005	-0.00009
	3PZ	0.00011	0.00157	-0.0025	0.00086	0.00024	0.00008	-0.00004
26H	1S	0.00138	0.01314	-0.00836	0.00414	-0.00717	-0.00445	-0.0017
	2S	0.00151	0.01062	0.00081	-0.01038	-0.01416	0.00124	0.00582
	3PX	0.00002	0.00131	-0.0023	0.00096	0.00031	0.00022	-0.00001

	3PY	0.00005	0.00106	-0.00154	-0.00023	0.00027	0.00011	0.00004
	3PZ	0.00029	0.0003	-0.00048	0.00005	0.00016	0.00013	0.00003
27C	1S	-0.00003	-0.00785	0.00528	0.00337	0.00774	0.00131	0.00034
	2S	-0.00003	0.0149	-0.01091	-0.00609	-0.0155	-0.00323	-0.00124
	2PX	0.00007	-0.04168	0.0115	0.02273	0.0394	0.00709	0.00101
	2PY	0.00288	0.10567	-0.08775	-0.02418	-0.0567	-0.01177	-0.00198
	2PZ	0.00866	-0.00083	0.00323	-0.00457	-0.00748	-0.00348	-0.00128
	3S	0.00084	0.03731	-0.02087	-0.01825	-0.0387	-0.00338	-0.00098
	3PX	0.00056	-0.01751	0.00379	0.01234	0.03393	-0.00283	-0.00384
	3PY	0.00169	0.05693	-0.04923	-0.02079	-0.03073	-0.01108	0.00056
	3PZ	0.00347	0.00336	0.00145	-0.00069	0.00393	0.00041	0.00234
	4XX	0.00023	0.00246	-0.00383	0.00075	-0.00016	-0.00013	-0.00022
	4YY	0.00013	-0.00105	0.00195	-0.0003	-0.00031	-0.00001	-0.00001
	4ZZ	-0.00034	-0.00218	0.00226	0.00056	0.00116	0.0003	-0.00011
	4XY	0.00002	-0.00209	0.0015	0.00033	0.0013	-0.00002	-0.00009
	4XZ	-0.00006	0.00053	-0.00093	0.00012	0	-0.00009	-0.00009
	4YZ	-0.00034	0.00151	-0.00152	0.00043	-0.00024	0.00066	0.00014
28H	1S	0.00171	0.00086	-0.01653	0.00829	0.00765	0.00104	-0.00044
	2S	0.00095	-0.00663	-0.01378	0.00909	0.00388	0.0039	0.00232
	3PX	-0.00007	-0.00049	0.00058	0.00015	0.00066	0.00002	-0.00002
	3PY	0.00005	0.00237	-0.0016	-0.00071	-0.00146	-0.00026	-0.00006
	3PZ	0.00017	0.00007	0.00012	-0.00018	-0.00035	-0.00011	-0.00009
29H	1S	0.00257	-0.03957	0.0394	0.00141	0.01085	-0.0001	-0.00058
	2S	0.00241	-0.05247	0.04289	-0.00295	0.01375	-0.00175	0.00385
	3PX	0.00001	-0.00186	0.00129	0.00054	0.00096	0.00028	0.00008
	3PY	0.00016	0.00105	-0.00085	-0.00052	-0.001	-0.00026	-0.00004
	3PZ	0.00009	0.0013	-0.0014	-0.00013	-0.00062	-0.00015	-0.00008
30H	1S	-0.00622	-0.02011	0.01755	0.00647	0.01283	0.00506	0.00132
	2S	-0.00589	-0.02376	0.02071	0.00533	0.01958	0.00707	0.00449
	3PX	0.00001	-0.00128	0.00062	0.0006	0.00087	0.00032	0.00012
	3PY	-0.00009	0.00192	-0.0016	-0.00043	-0.00102	-0.00023	-0.00003
	3PZ	-0.00013	-0.00111	0.00093	0.00014	0.00059	0.0001	0.00009
31C	1S	-0.00008	0.00799	-0.01239	0.00421	-0.00931	0.00526	0.00128
	2S	0.00001	-0.01486	0.0225	-0.00975	0.01675	-0.01046	-0.00156
	2PX	-0.00264	0.03508	-0.05385	0.01557	-0.00102	0.0082	0.00184
	2PY	-0.007	0.10417	-0.11086	0.01187	-0.05023	0.01851	0.00175
	2PZ	-0.00527	-0.04725	0.07475	-0.02716	0.06169	-0.03206	-0.00416
	3S	0.00126	-0.0335	0.0609	-0.01804	0.05655	-0.03016	-0.01199
	3PX	-0.00121	0.01623	-0.02913	0.00621	-0.00108	0.00147	0.002
	3PY	-0.00394	0.0526	-0.0596	0.01811	-0.03537	0.02049	0.00323
	3PZ	-0.00261	-0.03337	0.04564	-0.00603	0.03533	-0.01719	-0.0052
	4XX	-0.00035	0.00281	-0.00324	0.00008	0.00023	-0.00005	0.00018
	4YY	-0.00004	0.00081	-0.00018	-0.00044	-0.00042	-0.00036	0.00002
	4ZZ	0.00035	-0.00324	0.00216	0.00055	-0.00159	0.00141	0.00047

	4XY	0.00001	-0.00148	0.00056	0.00066	0.00206	-0.00029	-0.00005
	4XZ	-0.00015	0.00168	-0.00172	0.00009	-0.00041	-0.00007	-0.00011
	4YZ	0.00009	0.00147	-0.00258	0.00086	-0.00099	0.00053	0.00001
32H	1S	0.00486	-0.00538	-0.00862	0.01236	-0.02081	0.01394	0.00218
	2S	0.00397	-0.00435	-0.014	0.02207	-0.02597	0.0184	0.0003
	3PX	-0.00007	0.00083	-0.00109	0.00026	-0.00008	0.00024	0.00007
	3PY	-0.00004	0.00215	-0.00264	0.00057	-0.00167	0.00081	0.00009
	3PZ	0.00014	-0.00105	0.00098	0.00019	0.00046	-0.00016	-0.00011
33H	1S	-0.00237	0.03462	-0.02591	-0.00488	-0.01969	0.00169	-0.00021
	2S	-0.00188	0.03874	-0.03604	-0.00145	-0.0165	-0.00285	-0.00019
	3PX	-0.00013	0.00202	-0.00228	0.00066	-0.00062	0.0002	-0.00008
	3PY	-0.00005	0.00096	-0.00149	0.00106	-0.00035	0.00057	0.0001
	3PZ	-0.00011	-0.00111	0.00164	-0.00046	0.00185	-0.00074	0
34H	1S	-0.00409	0.03179	-0.03802	0.00379	0.00516	-0.0002	0.00023
	2S	-0.00344	0.03956	-0.0517	0.00635	-0.0061	0.00369	-0.00012
	3PX	0.00015	-0.00085	0.00066	0.00015	-0.0004	0.00032	0.00013
	3PY	-0.00006	0.00177	-0.00202	0.00035	-0.00112	0.00035	0.00001
	3PZ	-0.00005	-0.00172	0.00232	-0.00082	0.00061	-0.00056	-0.00007
35C	1S	0.00099	-0.00919	0.00265	0.00191	-0.01926	0.00536	0.00055
	2S	-0.00207	0.02429	-0.00814	-0.00399	0.04141	-0.01045	-0.00315
	2PX	-0.00247	0.03895	-0.01038	0.00297	0.08267	-0.01949	-0.00501
	2PY	0.00197	-0.06245	0.05045	0.00856	-0.09023	0.03531	0.00749
	2PZ	-0.00006	0.01464	0.02318	-0.02698	0.0171	-0.01846	-0.00732
	3S	-0.003	0.03289	0.01137	-0.0153	0.1107	-0.00547	0.03322
	3PX	-0.00357	0.04039	-0.02961	-0.0035	0.06274	-0.04101	-0.02666
	3PY	0.00342	-0.01588	0.00718	-0.00707	-0.03512	-0.00324	-0.02977
	3PZ	-0.00141	0.01169	0.00597	-0.0087	0.00506	-0.01777	-0.00971
	4XX	0.00005	0.00151	-0.00484	0.00558	0.00074	-0.00175	-0.00193
	4YY	0.00012	0.0005	0.00313	-0.00575	-0.00159	0.00074	0.00058
	4ZZ	0.00006	-0.00091	0.00095	-0.00009	-0.00043	0.00175	0.00139
	4XY	-0.00027	-0.00285	0.00291	0.00062	-0.00136	0.00271	0.00111
	4XZ	0.00008	0.00241	0.00142	-0.01033	-0.00104	-0.00069	0.00161
	4YZ	-0.00011	-0.00013	0.00124	-0.01111	-0.00376	-0.00291	-0.0008
36C	1S	-0.00017	-0.00184	-0.00429	0.00019	0.00342	-0.00621	-0.00282
	2S	0.00102	0.00664	0.01369	0.00048	-0.00684	0.01767	0.00313
	2PX	-0.00183	-0.005	-0.00348	-0.08754	-0.04189	-0.00966	0.00628
	2PY	0.00725	-0.00655	-0.05744	0.06314	0.01454	-0.03662	-0.02685
	2PZ	-0.00282	-0.02206	-0.03067	0.21448	0.02736	0.02453	-0.01516
	3S	-0.00349	0.0145	-0.01888	-0.00406	-0.00195	-0.00418	0.01377
	3PX	-0.00076	0.01064	-0.01236	-0.05553	-0.01966	-0.03823	-0.04464
	3PY	0.00118	-0.00472	-0.04546	0.04646	0.01085	-0.03244	-0.01054
	3PZ	-0.00195	-0.01691	-0.03453	0.13659	0.02045	-0.01125	-0.03712
	4XX	-0.00002	0.00158	-0.00227	0.00414	0.00319	0.00045	-0.00038
	4YY	0	-0.0003	0.00269	0.00436	-0.00092	0.00289	-0.0007

	4ZZ	0.00006	-0.0012	0.00009	-0.00848	-0.00218	-0.00418	-0.00112
	4XY	-0.0002	-0.00191	0.0033	-0.00387	-0.00532	0.00179	0.00094
	4XZ	0.00007	0.00092	0.00099	-0.00466	-0.00048	-0.00179	-0.00156
	4YZ	0.00004	-0.00011	-0.00023	0.00485	0.0003	0.00236	0.00135
37C	1S	0.00068	-0.00064	0.0022	-0.00078	-0.00448	0.00324	0.0023
	2S	-0.00144	0.00254	-0.00178	0.00067	0.00946	-0.00755	-0.0086
	2PX	0.00426	0.0063	0.02119	-0.10999	-0.01284	-0.03235	-0.00747
	2PY	-0.00496	-0.00587	0.00841	0.0826	0.00959	0.03545	0.00971
	2PZ	0.00444	0.02041	-0.05339	0.25159	0.08962	0.04178	-0.0082
	3S	-0.00299	-0.00539	-0.01855	0.01022	0.01271	-0.0154	-0.02207
	3PX	0.00252	0.0008	0.03123	-0.07371	-0.02343	-0.00437	-0.01191
	3PY	-0.00234	-0.0075	0.00507	0.05614	0.00322	0.04153	0.02981
	3PZ	0.00291	0.01159	-0.02412	0.15845	0.05183	0.03597	-0.00529
	4XX	0.00002	-0.00084	-0.00042	-0.00251	-0.00208	-0.00096	-0.00071
	4YY	0	0.00164	0.00274	-0.00282	0.00039	0.00176	0.00076
	4ZZ	0.00012	-0.00086	-0.00049	0.00517	0.00025	-0.00007	-0.00101
	4XY	-0.00035	-0.00118	-0.00028	0.00335	0.00032	0.00025	-0.00023
	4XZ	0.0001	0.00005	-0.00132	0.0029	0.00005	0.00008	-0.00073
	4YZ	-0.00009	0.00115	-0.00052	-0.00342	0.00005	0.00002	0.00068
38C	1S	-0.00016	-0.00044	-0.00204	0.00071	-0.00296	-0.00101	-0.00089
	2S	0.00008	0.00012	0.00605	-0.00164	0.00616	0.00405	0.0027
	2PX	-0.00463	-0.02064	0.00206	-0.01131	0.00055	-0.01276	-0.00577
	2PY	0.00635	0.01569	-0.02654	0.01124	0.01322	-0.00387	-0.00169
	2PZ	-0.00263	0.03377	-0.00789	0.02497	0.0342	0.02682	0.01254
	3S	0.00118	0.0095	-0.00464	0.00161	0.02002	-0.01892	-0.0099
	3PX	-0.00176	-0.01131	-0.00879	-0.0001	0.00315	-0.01601	-0.00131
	3PY	0.00196	0.0056	-0.0111	0.01218	0.00379	0.00952	0.0062
	3PZ	-0.00076	0.02401	-0.01054	0.01983	0.02889	0.01202	0.00763
	4XX	-0.00004	-0.00068	-0.00164	0.00762	0.00151	0.00113	0
	4YY	0.00001	-0.00024	0.00128	-0.00673	-0.00184	-0.00176	-0.00027
	4ZZ	0.00014	0.0012	-0.00041	-0.00062	0.00021	-0.00012	-0.0002
	4XY	-0.00057	-0.00069	0.00109	0.00058	-0.00014	0.00117	0.00041
	4XZ	0.00024	0.00164	0.0008	-0.0106	-0.00245	-0.00229	-0.00017
	4YZ	-0.00026	-0.00044	0.00232	-0.0115	-0.00346	-0.00164	0.00056
39C	1S	0.00095	-0.00363	0.00218	0.00109	-0.00016	0.00155	0.00044
	2S	-0.00215	0.00657	-0.00424	0.00086	0.00237	-0.00334	-0.00121
	2PX	0.00259	0.00213	-0.01661	0.0857	0.01518	0.00765	-0.00317
	2PY	-0.00413	-0.01012	0.03232	-0.08577	-0.03097	-0.00327	0.00248
	2PZ	0.00378	0.05385	0.01978	-0.22564	-0.0438	-0.03943	-0.00158
	3S	-0.00421	0.01442	0.00278	-0.02014	-0.03133	0.00842	0.001
	3PX	0	0.00245	-0.01691	0.05913	0.00693	0.0013	-0.00111
	3PY	-0.00235	-0.00319	0.01392	-0.0546	-0.00502	-0.01209	-0.00101
	3PZ	0.00138	0.03092	0.00931	-0.14037	-0.03663	-0.02515	-0.00157
	4XX	0.00003	0.0008	-0.00156	0.00421	0.00397	0.00077	0.0003

	4YY	-0.00012	-0.00185	0.00119	0.00337	-0.00189	0.00194	0.00061
	4ZZ	0.00015	-0.00037	0.00154	-0.00674	-0.00244	-0.00185	-0.00073
	4XY	-0.00035	-0.00093	0.00214	-0.00422	-0.00183	-0.00037	-0.00013
	4XZ	0.00008	-0.00051	0.0006	-0.00531	-0.00152	-0.00213	-0.0008
	4YZ	-0.00012	-0.00046	-0.00089	0.00263	0.00194	-0.00005	0.00004
40C	1S	-0.00053	0.00523	-0.00594	0.00094	-0.00278	-0.003	-0.00125
	2S	0.00133	-0.01103	0.01397	-0.00112	0.00794	0.00708	0.00282
	2PX	-0.00461	-0.0168	-0.01522	0.06798	0.06628	0.00591	0.00127
	2PY	0.00264	0.03805	-0.01894	-0.09313	0.0079	-0.04368	-0.01208
	2PZ	-0.00092	-0.00213	0.06496	-0.24133	-0.07358	-0.04015	-0.00833
	3S	0.00017	-0.03054	0.03012	-0.00387	0.01041	0.01905	0.01953
	3PX	-0.00083	-0.00444	-0.01059	0.04348	0.03106	0.01021	-0.00087
	3PY	0.00222	0.01516	-0.00042	-0.07341	0.03241	-0.03608	-0.01652
	3PZ	0.00012	0.00086	0.04349	-0.17127	-0.06317	-0.02581	-0.00147
	4XX	0.00001	-0.00012	-0.00015	-0.00381	-0.00207	-0.00066	-0.00009
	4YY	-0.00011	0.00114	0.00016	-0.00246	0.001	-0.00061	0.00006
	4ZZ	-0.00004	-0.00076	-0.00059	0.00664	0.00163	0.00097	0.00014
	4XY	-0.00007	-0.00362	0.00121	0.00386	-0.00109	0.0019	0.00067
	4XZ	-0.00001	0	-0.00151	0.00424	0.00168	0.00044	0.00015
	4YZ	-0.00002	0.0003	-0.00058	-0.00372	-0.00098	-0.00034	0.00016
41H	1S	-0.00348	-0.00111	0.03457	0.00745	-0.0095	0.02738	0.00556
	2S	-0.00234	-0.00493	0.01333	0.00904	-0.01551	0.00006	-0.01302
	3PX	-0.00005	-0.00016	0.00068	-0.00181	-0.00112	0.00005	-0.00039
	3PY	-0.00015	0.00008	0.00066	0.00198	0.00069	0.00145	0.00114
	3PZ	0	-0.00149	-0.00253	0.00502	0.00051	-0.00229	-0.00238
42H	1S	0.0061	0.0081	-0.0105	0.00153	-0.00008	-0.00605	-0.00299
	2S	0.00548	0.0105	-0.0157	0.00181	0.00405	-0.01274	-0.00544
	3PX	0.0001	-0.00025	-0.00015	-0.00023	-0.00011	-0.0004	-0.00027
	3PY	-0.00009	0.00018	-0.00024	0.00024	0.00042	0.00002	-0.00011
	3PZ	0.00009	0.00093	-0.0004	0.00062	0.00077	0.00065	0.00041
43H	1S	-0.0015	-0.01109	0.00165	-0.00865	0.01325	-0.00237	0.00096
	2S	-0.00139	-0.0083	-0.00702	0.014	-0.01294	0.00359	0.0044
	3PX	0.00001	0.00015	-0.00071	0.00277	-0.00165	0.00085	0.00017
	3PY	0.0001	0.00071	-0.00001	-0.0022	0.0007	-0.00086	-0.00008
	3PZ	0.00002	0.00022	0.00141	-0.00543	-0.00306	-0.00077	-0.00016
44C	1S	-0.00076	-0.00042	0.00474	0.00403	0.00198	0.00736	0.00393
	2S	0.00185	0.00002	-0.00864	-0.01167	-0.0049	-0.0161	-0.00671
	2PX	-0.00114	-0.00095	0.04419	0.02432	0.02506	0.04464	0.02176
	2PY	0.00019	0.01586	-0.03735	0.0353	-0.17685	0.04205	0.00054
	2PZ	-0.00041	-0.02367	0.05443	-0.03015	0.22912	-0.03316	0.00836
	3S	0.0017	0.00251	-0.03702	0.00017	0.00373	-0.04011	-0.03362
	3PX	-0.00198	-0.01063	0.0309	0.01855	0.00651	0.04541	0.05023
	3PY	-0.00256	0.02372	-0.02116	0.03235	-0.09657	0.04042	0.01756
	3PZ	-0.00189	-0.00657	0.04169	-0.02128	0.15414	-0.01356	0.01593

	4XX	-0.0001	-0.0001	-0.0001	-0.0013	0.00112	-0.00082	0.00031
	4YY	0.0001	0.00017	0.00071	0.00376	-0.00288	0.00133	0.00097
	4ZZ	-0.00005	-0.00055	-0.00061	-0.00276	0.00186	-0.00036	-0.00079
	4XY	-0.00004	-0.00143	-0.00072	-0.0002	-0.00583	0.00197	0.00049
	4XZ	-0.00005	0.00196	-0.00301	-0.00091	0.00731	-0.00546	-0.00296
	4YZ	0.00014	-0.00016	-0.0003	-0.00062	0.00081	-0.00013	-0.00031
45C	1S	0.00001	0.00056	-0.00113	-0.00369	-0.00077	-0.00342	-0.00146
	2S	-0.00014	0.00017	0.00278	0.00834	0.00175	0.00951	0.00631
	2PX	-0.00484	0.00105	-0.01439	-0.02415	-0.00061	-0.01965	-0.00857
	2PY	0.00016	0.00813	-0.00404	0.05325	-0.1078	0.02582	0.0149
	2PZ	-0.00026	-0.00768	0.0074	-0.06499	0.13692	-0.03237	-0.01227
	3S	0.0026	-0.01007	-0.00311	0.01417	-0.00177	-0.00028	-0.01966
	3PX	-0.00138	0.0067	-0.00827	-0.00924	0.01029	-0.01079	-0.01909
	3PY	-0.001	0.01198	0.00182	0.04703	-0.06228	0.0363	0.02815
	3PZ	-0.00136	0.00115	-0.00236	-0.02665	0.10886	-0.01746	-0.00543
	4XX	-0.00001	0.00042	-0.00078	-0.00093	-0.0009	-0.0006	-0.00033
	4YY	0.00005	-0.00077	0.00282	-0.00051	0.01077	-0.00163	0.00046
	4ZZ	0.00006	0.00089	-0.00183	0.00139	-0.01012	0.00254	0.00019
	4XY	-0.00007	-0.00043	-0.00036	-0.00004	0.00279	-0.00271	-0.00122
	4XZ	-0.00005	0.00032	-0.00258	-0.00245	-0.00586	0.00004	-0.00021
	4YZ	0.00013	0.00008	0.00014	0.00066	-0.00271	0.00152	0.00046
46C	1S	-0.00033	-0.00011	0.00091	0.00189	-0.00003	0.00269	0.00113
	2S	0.00084	0.00071	-0.00266	-0.00451	-0.00137	-0.0055	-0.00299
	2PX	0.0045	-0.00073	0.01211	0.01149	0.00064	0.01695	0.00644
	2PY	0.0014	-0.00578	0.03076	0.03353	0.08221	-0.01891	-0.00526
	2PZ	0.00033	0.00507	-0.03285	-0.03402	-0.09524	0.02858	0.00828
	3S	0.00097	-0.00707	0.005	-0.00746	0.00763	-0.00958	0.00668
	3PX	0.00142	0.00284	0.00336	0.01184	0.01372	0.01058	-0.00352
	3PY	0.00147	-0.00387	0.01432	0.01678	0.04424	-0.02117	-0.01278
	3PZ	0.0009	0.00251	-0.01836	-0.03312	-0.06488	0.01231	0.00128
	4XX	-0.00016	0.00012	-0.00025	0.00052	-0.00194	0.00072	0.00061
	4YY	0.00007	0.00025	-0.00077	0.00025	-0.00304	0.00093	0.00017
	4ZZ	0.00006	-0.00033	0.00122	-0.0004	0.00472	-0.0008	-0.00028
	4XY	-0.00012	-0.00057	0.00104	-0.00297	0.00903	-0.00239	-0.00099
	4XZ	-0.00006	0.00067	-0.00155	0.00332	-0.0114	0.00276	0.00118
	4YZ	0.00011	-0.00008	0.00037	0.0003	0.00029	0.00025	0.00016
47C	1S	0.00003	0.00006	0.00008	-0.00004	0	-0.00007	-0.00014
	2S	0.00008	-0.00042	0.00053	0.00081	0.00064	0.00092	0.0009
	2PX	-0.00443	0.00142	-0.009	-0.0006	-0.02026	0.00048	-0.00024
	2PY	-0.00067	-0.01156	0.03775	-0.02454	0.17763	-0.03917	-0.01182
	2PZ	-0.00038	0.01562	-0.04211	0.03618	-0.21828	0.05346	0.01681
	3S	0.00048	0.00417	-0.00556	-0.01144	-0.0089	-0.00982	-0.00769
	3PX	-0.00196	-0.00375	0.0013	0.00657	-0.00549	0.00839	0.00572
	3PY	-0.00022	-0.01018	0.02708	-0.01857	0.11688	-0.02703	-0.00625

	3PZ	-0.00017	0.01	-0.02976	0.02639	-0.16475	0.0415	0.01844
	4XX	-0.0003	0.00002	-0.00046	-0.00077	0.00043	-0.00088	-0.00038
	4YY	0.00014	0.00052	0.00004	0.00394	-0.00225	-0.00008	-0.00052
	4ZZ	0.00012	-0.00046	0.00014	-0.00357	0.00174	0.00063	0.00072
	4XY	-0.00021	0.00035	-0.00169	-0.00072	-0.00327	0.0004	0
	4XZ	-0.00012	-0.00034	0.00094	0.00006	0.00419	-0.00106	-0.00019
	4YZ	0.00014	-0.00014	0.00032	-0.00085	0.00097	0.0002	0.00021
48C	1S	-0.00044	0.00011	0.00144	-0.00054	0.00085	0.0015	0.00133
	2S	0.00106	0.00006	-0.00308	-0.00048	-0.00019	-0.00421	-0.00318
	2PX	0.00356	0.00298	0.01215	0.01218	-0.01298	0.0132	0.0055
	2PY	0.00068	-0.0121	0.01811	-0.05533	0.09067	-0.00609	0.00788
	2PZ	0.0001	0.0141	-0.02293	0.06915	-0.11495	0.01129	-0.00643
	3S	0.00138	-0.00899	0.0082	0.01868	-0.00809	0.01119	0.00449
	3PX	0.00163	0.01379	-0.00608	-0.00047	-0.01795	-0.00092	0.00258
	3PY	-0.00024	-0.01081	0.01165	-0.03377	0.05487	-0.00103	0.01155
	3PZ	-0.0003	-0.00019	-0.0073	0.04502	-0.07299	0.00997	-0.00244
	4XX	-0.00012	-0.00022	0.00071	0.00017	-0.00035	0.00093	0.00049
	4YY	0.00006	-0.00062	0.00207	-0.00091	0.01033	-0.00286	-0.00106
	4ZZ	0.00003	0.00059	-0.0018	0.00063	-0.00934	0.00244	0.00096
	4XY	-0.00014	-0.00027	0.00005	-0.00012	0.0047	-0.0023	-0.00092
	4XZ	-0.0001	0.00003	-0.00196	-0.00081	-0.00756	0.00171	0.00047
	4YZ	0.00009	0.00007	-0.0005	0.00018	-0.00343	0.00099	0.00036
49C	1S	0.00025	0.0003	-0.00307	0.00009	-0.00054	-0.00214	-0.002
	2S	-0.00037	-0.00161	0.00753	-0.00023	0.00106	0.00559	0.00545
	2PX	-0.00271	-0.00131	-0.01918	-0.00367	0.00953	-0.02003	-0.01058
	2PY	-0.00147	-0.00054	-0.00711	-0.01729	-0.08796	0.04141	0.01484
	2PZ	-0.00106	0.00267	0.02969	0.03216	0.12998	-0.03696	-0.01074
	3S	-0.00176	0.01518	0.00366	-0.00863	0.00372	-0.00086	0.00215
	3PX	-0.00003	0.0033	-0.02012	-0.0104	-0.00456	-0.02022	-0.00631
	3PY	0.00018	0.00904	-0.0105	-0.01901	-0.06373	0.02321	0.00313
	3PZ	0.00011	0.01823	0.00753	0.01633	0.09625	-0.03631	-0.0169
	4XX	-0.00001	0.00037	-0.00148	-0.00023	-0.00138	-0.00124	-0.00092
	4YY	0.0001	0.00024	-0.00036	0.00012	-0.00466	0.00206	0.00063
	4ZZ	0.00002	-0.00036	0.00136	-0.00018	0.00599	-0.00084	0.00031
	4XY	-0.00005	-0.00083	0.00103	-0.00277	0.00835	-0.00145	0.00042
	4XZ	-0.00003	0.00052	-0.00238	0.00358	-0.01045	0.00122	-0.00076
	4YZ	0.00005	-0.00037	0.00096	0.00045	0.00087	0.00043	0.00013
50H	1S	0.0021	0.00068	0.01067	0.0127	0.00549	0.0131	0.00639
	2S	0.0018	-0.00099	0.01272	-0.01189	-0.0033	0.00045	-0.00561
	3PX	0.00001	-0.00024	0.0002	0.00023	0.00022	0.00029	0.00042
	3PY	-0.00005	0.00004	-0.00008	0.00081	-0.00282	0.00063	0.00062
	3PZ	-0.00007	-0.00014	-0.00037	-0.0013	0.00334	-0.00121	-0.00081
51H	1S	-0.00332	0.0003	-0.00457	-0.00308	-0.00088	-0.00358	-0.00161
	2S	-0.00297	0.00199	-0.00832	-0.00625	-0.00228	-0.00771	-0.00505

	3PX	0.00008	0.00002	-0.00005	-0.00001	-0.00048	0.00008	0.00003
	3PY	0.00003	-0.00022	0.00085	-0.00054	0.00434	-0.00097	-0.00037
	3PZ	0.00002	0.00036	-0.00096	0.0009	-0.0054	0.00141	0.00047
52H	1S	0.00126	-0.00075	0.00063	-0.00022	-0.00238	0.00207	0.00197
	2S	0.00167	0.01245	-0.00496	-0.00606	0.00464	-0.00064	-0.00211
	3PX	-0.00003	0.00024	-0.00086	-0.00042	0.00011	-0.00088	-0.00024
	3PY	0.00003	-0.00014	-0.00024	-0.00064	-0.00231	0.00071	0.00028
	3PZ	0.00002	0.00043	0.0003	0.0007	0.0034	-0.0012	-0.00034
53C	1S	0.00051	0.00171	0.0022	0.00008	0.00248	-0.00014	-0.00006
	2S	-0.00109	-0.00509	-0.0075	0.00169	-0.00526	-0.00253	-0.00031
	2PX	-0.00226	-0.008	-0.00683	-0.00402	-0.01395	-0.00472	-0.0045
	2PY	-0.0002	-0.00252	-0.00105	0.00676	-0.0045	0.00012	-0.00223
	2PZ	-0.00202	-0.00323	-0.00645	0.01302	0.0012	0.00376	0.00044
	3S	-0.00203	-0.00491	0.00937	-0.0083	-0.01884	0.0214	0.00328
	3PX	0.00172	0.00313	0.01249	-0.00968	-0.00871	0.00163	-0.00539
	3PY	0.00074	-0.00208	0.00225	0.00858	-0.00285	-0.00055	-0.0067
	3PZ	0.00077	-0.00043	-0.00371	0.018	0.00782	0.00977	0.00126
	4XX	-0.00038	-0.00082	-0.00003	-0.00607	-0.00191	-0.00131	0.00051
	4YY	-0.00018	-0.00019	-0.00003	0.00017	0.0005	0.00071	0.00046
	4ZZ	0.00038	0.00086	0.00014	0.00559	0.00188	0.00111	-0.00017
	4XY	-0.00082	-0.00106	-0.00073	0.00112	-0.00066	0.00102	0.00074
	4XZ	0.00016	0.00051	-0.00123	0.00613	0.00172	0.00081	-0.0006
	4YZ	0.00044	0.00055	-0.00049	0.00719	0.00158	0.00095	-0.00039
54C	1S	0.00046	0.00285	-0.00339	-0.0008	0.00372	-0.00228	-0.00062
	2S	-0.00127	-0.00712	0.00902	0.00064	-0.01001	0.00585	0.00179
	2PX	0.00128	0.0061	-0.0076	0.00398	0.00826	-0.00349	-0.00144
	2PY	0.00354	0.01517	-0.01673	-0.0087	0.01613	-0.01131	-0.00253
	2PZ	-0.00095	-0.00262	0.00532	-0.01037	-0.0072	0.00032	0.00069
	3S	-0.00077	-0.01183	0.01257	0.00957	-0.01468	0.01224	0.00303
	3PX	-0.00017	-0.00001	-0.00131	0.00963	0.00776	0.00209	0.00141
	3PY	-0.00144	0.00134	-0.00043	-0.01273	0.0007	-0.00553	-0.00112
	3PZ	0.00024	0.00161	0.00383	-0.02015	-0.00252	-0.00139	0.00271
	4XX	0.00007	0.00023	-0.00035	-0.00055	0.0003	-0.00026	0.00001
	4YY	-0.00025	-0.00108	-0.0001	0.00525	0.00074	0.00089	-0.0001
	4ZZ	0.00016	0.00125	-0.00014	-0.00466	-0.00038	-0.00101	-0.00001
	4XY	-0.00052	-0.00125	0.00149	-0.00219	-0.0015	0.00028	0.00027
	4XZ	0.00007	-0.00084	-0.00081	0.00578	0.00143	0.00088	0.00003
	4YZ	0.00019	-0.00081	-0.0009	0.00539	0.00146	0.00083	0.00006
55C	1S	-0.00025	0.00023	-0.00055	-0.00047	-0.00017	-0.00075	-0.00011
	2S	0.00062	-0.00053	0.00146	0.00079	0.00092	0.00114	0.00005
	2PX	-0.00045	0.00024	-0.00041	0.00062	-0.00207	0.00086	0.0009
	2PY	-0.00143	0.00065	-0.00111	-0.00028	0.00415	-0.0046	-0.00154
	2PZ	-0.00124	0.00084	-0.00294	-0.00374	-0.00565	-0.00047	0.00069
	3S	0.00034	0.00035	0.00182	0.00748	0.00099	0.01024	0.00523

	3PX	0.00029	0.00077	-0.0001	0.00041	-0.01004	0.00246	0.00326
	3PY	0.00051	-0.00031	0.00321	-0.00065	0.01121	-0.00556	-0.00224
	3PZ	0.00048	-0.00049	-0.00319	-0.00313	-0.01	0.001	-0.00082
	4XX	-0.00017	0.00017	-0.00066	-0.00084	-0.00087	-0.00002	0.00005
	4YY	0.00009	0.00022	-0.00094	-0.00108	-0.00361	0.00131	0.00049
	4ZZ	0.00006	-0.00022	0.00146	0.00189	0.00451	-0.00131	-0.00048
	4XY	-0.00008	0.00002	-0.00038	-0.00066	0.00049	-0.00053	-0.00026
	4XZ	0.00003	-0.0001	0.0003	0.00031	0.00155	-0.00058	-0.00028
	4YZ	0.00027	-0.00006	0.00026	0.00024	-0.00009	0.0003	0.00009
56C	1S	-0.00028	-0.00015	-0.00195	-0.00075	-0.00072	-0.00154	-0.00077
	2S	0.00075	0.00114	0.00484	0.00266	0.00068	0.00421	0.00233
	2PX	-0.00164	-0.00067	-0.00792	-0.00218	-0.00212	-0.0054	-0.00253
	2PY	0.00096	0.00021	0.00662	-0.00155	0.008	0.00301	0.00292
	2PZ	0.0011	0.00096	0.0052	0.00592	-0.00416	0.0049	0.00112
	3S	0.00064	-0.008	0.01207	0.00185	0.01014	0.00752	0.00365
	3PX	0.00073	0.00152	-0.00033	0.00159	0.00098	-0.00165	-0.00141
	3PY	-0.00017	-0.0046	0.00608	-0.00568	0.01747	-0.00153	0.00015
	3PZ	-0.00016	-0.00125	0.00163	0.00829	-0.00867	0.00337	-0.00044
	4XX	-0.00004	-0.00024	-0.00003	-0.00096	0.00046	-0.00032	-0.00009
	4YY	0.00006	-0.00035	0.00054	-0.00182	0.0039	-0.00037	0.00034
	4ZZ	0	0.00043	-0.00079	0.00268	-0.00431	0.00039	-0.00037
	4XY	-0.00016	0.0002	-0.00078	0.00105	-0.00207	0	-0.00021
	4XZ	-0.00022	-0.00046	0.00009	-0.00205	0.00283	-0.00055	0.0002
	4YZ	0.00019	-0.0001	0.00075	-0.00039	0.00132	0.00016	0.00019
57F	1S	0.00005	0.00023	-0.00034	0.00082	-0.00112	0.00017	-0.00008
	2S	-0.00006	-0.00003	0.00013	-0.00227	-0.00099	0.00095	0.00088
	2PX	0.00315	0.0024	-0.00184	0.00665	-0.00139	-0.00087	-0.00055
	2PY	-0.00115	-0.00175	-0.00024	-0.00695	0.01085	-0.00178	0.00073
	2PZ	0.00032	-0.00384	0.00049	-0.01512	0.01589	-0.00087	0.00167
	3S	-0.00036	-0.00249	0.00322	-0.00446	0.01501	-0.00399	-0.00105
	3PX	0.00206	0.00151	-0.00106	0.00356	-0.00027	-0.00072	-0.00034
	3PY	-0.00087	-0.00145	0.00046	-0.0054	0.00937	-0.00194	0.00027
	3PZ	0.00018	-0.00272	0.00054	-0.01183	0.01353	-0.00139	0.00114
	4XX	0.00004	0.00026	-0.00044	-0.00014	-0.00157	0.00047	0.00027
	4YY	-0.00004	0.00019	-0.00019	-0.00024	-0.00169	0.00068	0.00034
	4ZZ	0.00004	0.00025	-0.00026	-0.00002	-0.00174	0.00063	0.00028
	4XY	0.00006	0.00004	-0.00022	0.00001	0.0001	-0.00012	-0.00005
	4XZ	-0.00001	-0.00006	-0.00005	-0.00042	0.0002	0.00008	0.00012
	4YZ	0.00002	-0.00007	0.00006	-0.00025	0.00038	0	0.00002
58F	1S	0.00001	0.0001	0.00005	0.00074	-0.00104	0.00037	0.00004
	2S	0.00006	-0.00084	0.00118	-0.00171	0.0064	-0.00163	-0.00054
	2PX	0.00243	0.0037	0.0018	0.01419	-0.02209	0.00736	0.00121
	2PY	0.00147	-0.00004	-0.00394	0.00227	-0.00365	-0.00121	-0.00105
	2PZ	-0.00101	-0.00316	0.00271	-0.01072	0.02586	-0.00496	-0.00033

	3S	-0.00048	0.00108	-0.00379	-0.00498	-0.00213	-0.00105	0.00065
	3PX	0.00173	0.00218	0.00203	0.01077	-0.01485	0.00524	0.00069
	3PY	0.00102	0.00042	-0.00334	0.00274	-0.00529	-0.00039	-0.00071
	3PZ	-0.0006	-0.0025	0.00229	-0.0076	0.01843	-0.00331	-0.00014
	4XX	-0.00001	-0.00028	0.00067	-0.00014	0.00228	-0.00034	-0.00015
	4YY	0.00004	-0.0003	0.00065	-0.00027	0.00254	-0.00054	-0.00022
	4ZZ	0.00005	-0.0001	0.00026	0.00051	0.00033	-0.00016	-0.00022
	4XY	-0.00007	-0.00006	0.00002	-0.00024	0.00043	-0.00016	-0.00008
	4XZ	-0.00002	0.00005	-0.0001	-0.00014	0.00033	-0.00018	-0.00004
	4YZ	-0.00002	-0.00004	0.00001	-0.00001	-0.00015	0.00003	0
59F	1S	0.00003	-0.0002	0.00049	-0.00142	0.00247	-0.00015	0.00028
	2S	-0.00001	0.0001	-0.00079	0.00271	-0.00408	-0.00028	-0.00092
	2PX	0.00104	-0.00344	0.00815	-0.01786	0.02407	0.00135	0.00274
	2PY	-0.00228	0.00324	-0.00897	0.01088	-0.02453	0.00122	-0.00079
	2PZ	-0.00194	0.00315	-0.0104	0.01523	-0.0311	0.00095	-0.00257
	3S	-0.00038	0.00234	-0.00423	0.01029	-0.01965	0.00225	-0.00128
	3PX	0.00068	-0.0024	0.0057	-0.01295	0.01763	0.00062	0.00188
	3PY	-0.00155	0.00235	-0.00646	0.00686	-0.01612	0.00055	-0.00049
	3PZ	-0.0014	0.0027	-0.00794	0.01243	-0.02543	0.00098	-0.00207
	4XX	0.00004	-0.00017	0.00013	-0.00044	0.00045	-0.00012	0
	4YY	0.00007	-0.00032	0.00049	-0.00061	0.00192	-0.00051	-0.00019
	4ZZ	-0.00005	-0.00001	-0.00007	0.00016	-0.00009	-0.00019	-0.00009
	4XY	0	0.0001	-0.00012	0.00048	-0.00066	0.00004	-0.00005
	4XZ	0	0.00002	-0.00015	-0.0002	-0.00007	-0.00003	-0.00005
	4YZ	-0.00003	0.00005	0.00001	-0.00001	0.00021	-0.00001	0.00005
60F	1S	0	-0.00005	0.00046	0.00047	0.00115	-0.00008	0.00004
	2S	0.00001	0.00057	-0.0015	-0.00039	-0.00675	0.00157	0.00094
	2PX	0.00235	-0.00108	0.00656	0.00613	0.01335	-0.00163	-0.00059
	2PY	0.0005	-0.00138	0.00581	0.00435	0.01046	0.00066	0.00019
	2PZ	0.00213	-0.00274	0.01115	0.00525	0.03042	-0.00604	-0.00192
	3S	-0.00028	-0.00076	-0.00228	-0.00441	0.00157	-0.00274	-0.00279
	3PX	0.00164	-0.00058	0.00512	0.00508	0.01046	-0.00102	-0.00011
	3PY	0.00035	-0.00076	0.00373	0.00362	0.00499	0.00158	0.0007
	3PZ	0.0014	-0.00189	0.00778	0.00397	0.02157	-0.00434	-0.00153
	4XX	-0.00007	0.00021	-0.00047	0.00022	-0.00272	0.00075	0.00045
	4YY	0.00005	0.0002	-0.00023	0.00035	-0.00214	0.00075	0.00051
	4ZZ	0.00004	0.00011	0.00015	0.00043	-0.00047	0.00026	0.0003
	4XY	-0.00001	-0.00002	0.00001	-0.00003	0.00015	-0.00009	-0.00004
	4XZ	-0.00002	0.00004	-0.00016	-0.00001	-0.0004	0.0001	0.00002
	4YZ	-0.00001	-0.00001	0.00006	0.00002	0.00026	-0.00001	0
61F	1S	0.00004	-0.00003	0.00042	0.00037	0.00104	-0.00021	-0.00013
	2S	-0.00003	0.00005	-0.0006	-0.0023	0.00172	-0.00059	-0.00071
	2PX	0.00161	0.00042	0.00094	0.00092	-0.00702	0.00393	0.00184
	2PY	0.00219	-0.00074	0.00404	0.00439	0.00653	-0.00096	-0.0002

	2PZ	0.00026	-0.00135	0.00808	0.01091	0.01105	-0.00237	-0.00009
	3S	-0.00035	0.00047	-0.00328	0.00035	-0.01591	0.00365	0.00305
	3PX	0.00099	0.00042	-0.00012	0.00012	-0.00733	0.003	0.00127
	3PY	0.00151	-0.00057	0.00289	0.00258	0.00597	-0.00094	-0.00066
	3PZ	0.00016	-0.00083	0.00612	0.00745	0.00978	-0.00223	-0.00019
	4XX	0.00005	0	0.00015	-0.00073	0.00165	-0.00044	-0.00047
	4YY	-0.00005	0	0.00012	-0.00078	0.00198	-0.00055	-0.00047
	4ZZ	0.00004	0	0.00025	-0.00042	0.0019	-0.00055	-0.00046
	4XY	0.00002	-0.00001	0.00006	0.00008	0.00005	0.0001	0.00009
	4XZ	0	-0.00001	0.00023	0.00031	0.00013	-0.00001	0.00009
	4YZ	0.00001	-0.00001	-0.00007	0.00012	-0.00017	0.00008	0.00001
62F	1S	0.00003	0.00004	-0.00051	-0.00062	-0.00206	0.00077	0.00026
	2S	0	-0.00033	0.00116	0.00194	0.00384	-0.00128	-0.00055
	2PX	-0.00101	-0.00022	-0.00236	-0.00618	0.00169	-0.00079	-0.00073
	2PY	0.00184	0.00181	-0.01077	-0.00856	-0.02644	0.00719	0.00131
	2PZ	0.00182	0.00132	-0.00878	-0.009	-0.02896	0.00949	0.00263
	3S	-0.00044	0.00024	0.00348	0.00227	0.01539	-0.00625	-0.00186
	3PX	-0.0007	-0.00031	-0.00186	-0.0043	0.001	-0.00055	-0.00077
	3PY	0.00122	0.00124	-0.00721	-0.00607	-0.01771	0.0047	0.00084
	3PZ	0.00133	0.00086	-0.00665	-0.00657	-0.02311	0.008	0.0023
	4XX	0.00005	-0.00011	0.00008	0.00016	-0.00011	0.00012	0
	4YY	0.00007	-0.00003	-0.00039	-0.00011	-0.00153	0.00051	0.00012
	4ZZ	-0.00003	-0.00014	0.00026	0.00036	0.00028	0.00004	0.00003
	4XY	-0.00001	-0.00004	0.00001	-0.00024	0.00064	-0.00016	-0.00012
	4XZ	0.00003	0.00003	0.00005	0.00005	-0.00001	0.00002	0.00004
	4YZ	-0.00001	-0.00001	0.00007	0.00009	-0.00023	0.0002	0.0001
63F	1S	-0.00005	0.00003	0.0005	-0.00232	-0.00047	-0.00032	0.00009
	2S	-0.00003	-0.00057	-0.00126	0.00896	0.00237	0.00217	0.00063
	2PX	0.00203	0.00416	0.00991	-0.03757	-0.01362	-0.00397	0.00009
	2PY	-0.00509	0.00066	0.0129	-0.03617	-0.00982	-0.00403	0.00001
	2PZ	-0.00109	-0.003	-0.00658	0.02675	0.00635	0.00357	0.00005
	3S	0.0007	0.00119	-0.0037	0.00706	0.0004	-0.00153	-0.00278
	3PX	0.00122	0.00266	0.00781	-0.02919	-0.01012	-0.00287	0.0006
	3PY	-0.00341	0.00039	0.00865	-0.02282	-0.00637	-0.00213	0.00031
	3PZ	-0.00086	-0.00258	-0.00403	0.01882	0.00467	0.00295	0.00046
	4XX	-0.00014	-0.00033	-0.00035	0.00281	0.00081	0.0008	0.00035
	4YY	0.00001	-0.00029	0.00001	0.00147	0.00049	0.00061	0.00034
	4ZZ	-0.00001	0.00014	0.00007	0.0002	0.00027	0.00031	0.00029
	4XY	0.00001	-0.00008	0.00013	-0.00025	-0.00037	0.00004	-0.00001
	4XZ	0.00003	0.00009	-0.00017	0.0005	0.00022	0.00004	-0.00003
	4YZ	0.00011	-0.0001	-0.00018	0.00114	0.0001	0.00025	0
64F	1S	0	-0.00019	0.00042	-0.00162	-0.00084	-0.00012	0.00001
	2S	-0.0001	-0.00016	-0.00038	0.00261	0.00056	-0.00026	-0.00049
	2PX	0.00205	0.00122	0.00039	-0.00172	-0.00136	-0.00004	-0.00033

	2PY	-0.00199	-0.0087	0.0143	-0.02274	-0.0159	0.00244	0.00135
	2PZ	0.00434	-0.00369	-0.0081	0.03076	0.00823	0.00203	-0.00092
	3S	0.0006	0.00301	-0.00454	0.01281	0.00887	0.00181	0.00101
	3PX	0.00156	0.00107	-0.00026	0.00064	0.00006	0.00034	-0.00002
	3PY	-0.00136	-0.00666	0.01051	-0.01656	-0.01227	0.00163	0.00067
	3PZ	0.00297	-0.00272	-0.00636	0.02499	0.00625	0.00184	-0.00092
	4XX	0.00006	-0.00005	0.00013	-0.00078	-0.00049	-0.00037	-0.00024
	4YY	-0.00011	-0.00041	0.00042	-0.00047	-0.00075	-0.00006	-0.00008
	4ZZ	-0.00005	-0.00029	0.00027	-0.00055	-0.00059	-0.00025	-0.00019
	4XY	-0.00006	-0.00008	0.00009	-0.00028	-0.00012	-0.00006	-0.00007
	4XZ	0.0001	-0.00019	-0.00022	0.00109	0.00014	0.00006	-0.00009
	4YZ	-0.00007	0.00004	0.00003	-0.00009	0.00009	-0.00005	-0.00002
65F	1S	-0.00005	-0.00079	-0.00015	0.00415	0.00055	0.00088	0
	2S	0.00005	0.00167	0.00053	-0.00908	-0.00135	-0.002	-0.00027
	2PX	-0.0047	-0.01237	0.00264	0.02768	-0.00083	0.00618	0.00016
	2PY	-0.00622	-0.02243	-0.00297	0.07392	0.00813	0.01376	0.00073
	2PZ	-0.00073	0.00587	-0.00011	-0.02878	-0.00374	-0.0065	-0.00045
	3S	0.00058	0.00562	0.00041	-0.02793	-0.0029	-0.00593	0.0007
	3PX	-0.0033	-0.00914	0.0016	0.02236	-0.00083	0.00482	-0.00028
	3PY	-0.00419	-0.01561	-0.00181	0.05187	0.00562	0.00987	0.00063
	3PZ	-0.0004	0.00484	0.00004	-0.02465	-0.00335	-0.00563	-0.00034
	4XX	0.00008	0.00007	0.00017	-0.00036	-0.00002	-0.00005	-0.00006
	4YY	-0.00008	-0.00041	-0.00008	0.00212	0.00038	0.00036	-0.00011
	4ZZ	-0.00007	0.00005	0.00012	-0.00067	-0.00025	-0.00022	-0.00017
	4XY	0.00006	-0.00006	0.00024	-0.00039	-0.00033	0.00001	-0.00001
	4XZ	-0.0001	-0.0002	-0.00001	0.00044	-0.00002	0	-0.00008
	4YZ	-0.00011	-0.00023	-0.00028	0.00099	0.00029	-0.00001	-0.00004
66F	1S	-0.00004	-0.00025	-0.00057	0.00134	-0.00019	0.00063	0.00033
	2S	-0.00022	-0.00098	0.00037	-0.00372	-0.00009	-0.00101	-0.00059
	2PX	0.00322	0.00473	0.00613	-0.01851	0.0075	-0.00485	-0.00012
	2PY	-0.00236	-0.00227	0.00194	-0.00468	0.00001	0.00063	0.00222
	2PZ	-0.00258	0.00095	0.00982	-0.03771	-0.00974	-0.00945	-0.0016
	3S	0.00123	0.00535	0.00482	-0.00727	0.00296	-0.00499	-0.00179
	3PX	0.00222	0.00385	0.00367	-0.0126	0.00656	-0.00405	-0.00005
	3PY	-0.002	-0.00248	0.00014	-0.00255	-0.00014	0.00178	0.00247
	3PZ	-0.00164	0.00118	0.00811	-0.02916	-0.00799	-0.00812	-0.00154
	4XX	-0.00016	-0.00085	-0.00057	-0.00034	-0.00027	0.00019	0.00015
	4YY	-0.00001	-0.00045	-0.00042	0.00014	-0.00005	0.00014	0.00001
	4ZZ	-0.0002	-0.00067	-0.0004	-0.0003	-0.0002	0.00019	0.00013
	4XY	-0.0001	-0.00008	-0.00002	0.0001	-0.00019	0.00023	0.00013
	4XZ	-0.00008	0.00007	0.0001	0.0001	-0.00004	0.00004	-0.00002
	4YZ	0.00003	0.00003	-0.00035	0.00117	0.00047	0.00046	0.00011
67F	1S	-0.00008	-0.00006	0.00055	-0.00462	-0.00176	-0.00089	0.00021
	2S	0.00027	0.00087	0.00047	0.01158	0.00358	0.00248	-0.00096

	2PX	0.00065	0.00363	-0.01548	0.07737	0.02918	0.01528	0.00139
	2PY	-0.00632	0.00681	-0.00495	0.03118	0.01426	0.00876	0.00182
	2PZ	0.00937	0.00373	0.00205	0.0363	0.01066	0.00537	-0.00226
	3S	0.00083	-0.00076	-0.00697	0.02691	0.0123	0.00404	-0.00087
	3PX	0.00026	0.00224	-0.01171	0.05353	0.02043	0.01112	0.00238
	3PY	-0.00421	0.00468	-0.0049	0.02464	0.01213	0.0071	0.00189
	3PZ	0.00659	0.002	0.00002	0.02931	0.00917	0.00374	-0.00197
	4XX	-0.00001	0.00029	0.00114	-0.00182	-0.00091	-0.00016	-0.0001
	4YY	-0.00022	0.00038	0.00053	0.0009	0.00008	0.00031	-0.00018
	4ZZ	0.00038	0.00016	0.00058	0.00129	0.00007	0.00013	-0.00032
	4XY	-0.00011	-0.00032	-0.0003	0.00025	-0.00005	-0.00003	0
	4XZ	0	-0.00008	-0.0004	0.00082	0.00022	0.00021	0.00015
	4YZ	-0.00002	0.00008	-0.0002	0.00051	0.00028	0.00011	0.00005
68F	1S	-0.00029	-0.00043	-0.00142	0.00249	0.00104	0.00142	0.00114
	2S	0.00102	0.00268	0.00723	-0.00726	-0.00385	-0.00437	-0.00726
	2PX	0.00321	0.00539	0.01911	-0.04536	-0.01213	-0.00836	-0.0063
	2PY	0.00794	0.00122	0.01871	-0.04034	-0.01179	-0.00736	0.00136
	2PZ	0.01449	0.00849	0.02347	-0.02321	-0.01077	-0.01079	-0.00998
	3S	0.00091	-0.00076	0.00133	-0.01163	-0.00375	-0.00812	0.00072
	3PX	0.00255	0.00319	0.01235	-0.03012	-0.0083	-0.00774	-0.00311
	3PY	0.00586	0.00171	0.0145	-0.03045	-0.00945	-0.00769	-0.00133
	3PZ	0.00845	0.00384	0.01111	-0.01836	-0.00568	-0.00289	-0.00025
	4XX	0.00038	0.001	0.00236	-0.00026	-0.00097	-0.00101	-0.00262
	4YY	0.00072	0.00118	0.00304	-0.00127	-0.00124	-0.00129	-0.00281
	4ZZ	-0.00024	0.00044	0.00049	0.00066	0.0001	-0.00012	-0.00136
	4XY	0.00023	0.00007	0.00017	0.00019	-0.00015	-0.00031	-0.00034
	4XZ	0.00008	-0.00016	-0.00049	0.00104	0.00041	0.00033	0.00092
	4YZ	0	-0.00006	-0.00022	0.00045	0.00012	0.00038	-0.00011
69C	1S	0.00006	0.01012	-0.00069	0.00016	-0.00017	0	-0.00013
	2S	-0.00035	-0.02068	0.00168	-0.00026	0.00026	0.00004	-0.00014
	2PX	0.12098	-0.02738	-0.0116	-0.00907	0.0067	0.02303	-0.01501
	2PY	-0.08385	-0.13717	0.01943	0.00395	-0.00368	-0.01244	0.009
	2PZ	0.39586	-0.03696	-0.05413	-0.03169	0.02235	0.07917	-0.05399
	3S	0.0002	-0.06099	0.0023	-0.00085	0.0022	-0.00049	0.00325
	3PX	0.05363	-0.02221	-0.00288	-0.00332	0.00246	0.00848	-0.00823
	3PY	-0.03654	-0.07383	0.00912	0.00123	-0.00127	-0.00414	0.00521
	3PZ	0.17241	-0.01282	-0.01638	-0.01011	0.0067	0.0265	-0.03533
	4XX	-0.00788	-0.00053	0.00222	0.00162	-0.0011	-0.00496	0.00578
	4YY	-0.00035	0.00315	-0.0005	-0.00038	0.00028	0.00163	-0.00248
	4ZZ	0.00834	-0.00002	-0.00191	-0.00117	0.00085	0.00331	-0.0034
	4XY	0.00281	-0.00652	0.00002	-0.00021	0.00017	0.00012	0.00042
	4XZ	-0.01575	0.00099	0.00449	0.0032	-0.0023	-0.00973	0.01161
	4YZ	0.00231	0.0029	0.00166	0.00161	-0.00118	-0.00557	0.00883
70H	1S	0.01458	0.06832	-0.00382	0.0005	0.00001	0.00078	-0.00042

	2S	0.01208	0.07526	-0.00211	0.00103	-0.00118	0.00122	-0.00295
	3PX	0.00198	-0.00249	-0.00005	-0.00017	0.00009	0.00049	-0.0004
	3PY	-0.00098	0.00015	0.00024	0.00011	-0.00008	-0.00026	0.00021
	3PZ	0.00804	0.00028	-0.0011	-0.00061	0.00045	0.00166	-0.00155
71H	1S	0.21379	-0.01502	-0.0375	-0.02312	0.0165	0.06281	-0.05961
	2S	0.18817	-0.01392	-0.04381	-0.02876	0.02055	0.08235	-0.08441
	3PX	0.00696	-0.00054	-0.00087	-0.00048	0.00034	0.00102	0.00015
	3PY	0.00063	-0.0025	0.00031	0.00015	-0.00013	-0.0007	0.00153
	3PZ	-0.00339	-0.00008	0.00057	0.00031	-0.00021	-0.00076	0.00042
72H	1S	-0.22258	0.01158	0.03592	0.02315	-0.01657	-0.06416	0.05998
	2S	-0.19446	0.01619	0.0415	0.02877	-0.02075	-0.08334	0.08496
	3PX	-0.00769	0.00015	0.00106	0.00054	-0.00039	-0.00118	-0.00007
	3PY	-0.00086	-0.00257	-0.00001	-0.00024	0.00015	0.00085	-0.00158
	3PZ	-0.00008	-0.00044	-0.00007	-0.00003	0.00001	0.00003	0.00004
73H	1S	-0.0011	0.1005	-0.00425	0.00163	-0.0017	0.00101	0.00001
	2S	-0.00169	0.11338	-0.00411	0.00163	-0.00296	0.00164	-0.00034
	3PX	0.00111	0.00225	0.00024	0.00038	-0.00028	-0.00143	0.00214
	3PY	-0.00033	-0.00152	-0.00023	-0.00024	0.00021	0.00082	-0.00127
	3PZ	0.00295	-0.00031	0.00162	0.00141	-0.00104	-0.005	0.00757

3.4.2 Combined coefficients and computational details of HFV index (F) of M1c

Table S9. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of **M1c**

i/j \ k ($\|c_{ki}\|/\|c_{kj}\|$)	143	160	162	166	167	169	170
13	0.0386	0.1839	0.4002	0.0819	0.0400	0.1914	0.3277
14	0.0679	0.2477	0.3530	0.1599	0.1039	0.1841	0.4275
17	0.1307	0.1933	0.2486	0.1692	0.1174	0.4403	0.2372
18	0.2600	0.1972	0.1114	0.1010	0.0698	0.3295	0.4501
69	0.7072	0.2279	0.0838	0.0465	0.0318	0.1110	0.0796

Table S10. The calculation details of HFV index (F) of **M1c**

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	ΣP	HFV (F)
α (14)	14-13	160 (1),162 (1),166 (1),167 (1),169 (-1),170 (1)	0.62 [a]	0.85	0.91
	14-17	143 (1),162 (1),166 (1),167 (1),169 (1),170 (-1)	0.23 [b]		
γ (18)	18-17	143 (1),160 (-1),162 (1),166 (1),167 (1),169 (1),170 (1)	0.60 [c]	0.79	0.97
	18-69	143 (1),162 (-1),166 (-1),167 (-1),169 (-1),170 (-1)	0.19 [d]		

a : $P_{14\text{-}13}$=2*0.2477*0.1839+2*0.3530*0.4002+2*0.1599*0.0819+2*0.1039*0.0400-2*0.1841*0.1914+2*0.4275*0.3277=0.62

b : $P_{14\text{-}17}$=2*0.0679*0.1307+2*0.3530*0.2486+2*0.1599*0.1692+2*0.1039*0.1174+2*0.1841*0.4403-2*0.4275*0.2372=0.23

c : $P_{18\text{-}17}$=2*0.2600*0.1307-2*0.1972*0.1933+2*0.1114*0.2486+2*0.1010*0.1692+2*0.0698*0.1174+2*0.3295*0.4403+2*0.4501*0.2372=0.60

d: $P_{18\text{-}69}$=2*0.2600*0.7072-2*0.1114*0.0838+2*0.1010*0.0465+2*0.0698*0.0318+2*0.3295*0.1110+2*0.4501*0.0796=0.19

3.5 The occupied π-type molecular orbitals associated with the active sites of 1d

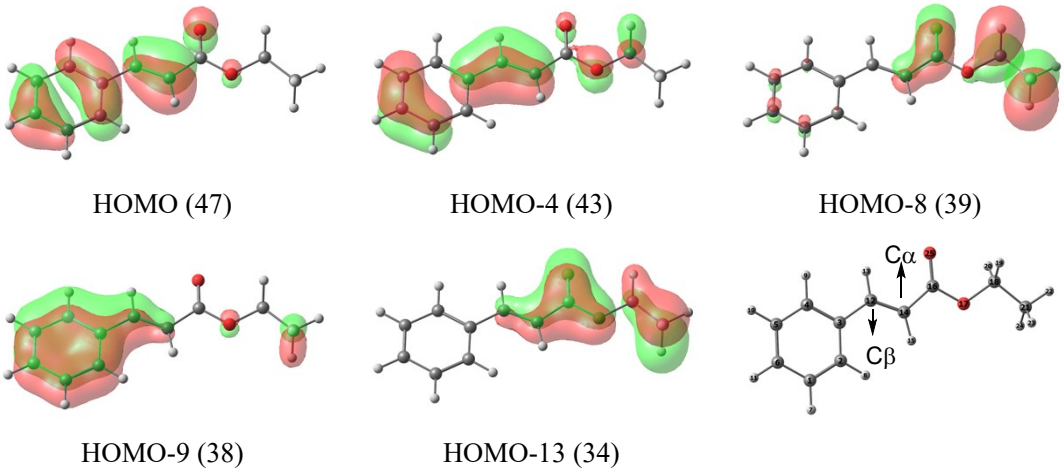


Fig. S8. The occupied π-type molecular orbitals associated with the active sites of **1d**

3.5.1 Molecular orbital coefficients of 1d

		34	38	39	43	47
1C	1S	0.00001	0.00004	0	0	0
	2S	-0.00002	-0.00008	0	-0.00001	0
	2PX	-0.00001	-0.00021	-0.00015	0.00004	-0.00001
	2PY	0.00006	-0.00026	-0.00002	-0.00001	0.00002
	2PZ	0.01354	0.18571	-0.0569	-0.1673	0.09149
	3S	-0.00004	-0.00023	0	-0.00003	-0.00001
	3PX	0.00001	0.00005	-0.00005	0.00004	0
	3PY	0.00002	-0.00003	-0.00001	-0.00002	0
	3PZ	0.00597	0.10374	-0.03486	-0.11549	0.06288
	4XX	0	0.00004	0.00001	0	0
	4YY	0	-0.00005	-0.00001	0	0
	4ZZ	0	0.00001	0	0	0.00001
	4XY	0	0.00001	0	0	0
	4XZ	-0.00041	-0.00306	0.00033	-0.0057	0.01381
	4YZ	-0.00063	-0.0084	0.00251	0.00686	-0.00435
2C	1S	-0.00001	-0.00008	0	-0.00001	0
	2S	0.00001	0.00016	0.00001	0.00002	0.00001
	2PX	-0.00001	0.00027	0.00016	-0.00002	0.00002
	2PY	-0.00001	-0.00005	0.00002	-0.00004	-0.00004
	2PZ	0.02177	0.20989	-0.04746	0.00555	-0.17868
	3S	0.00001	0.00033	-0.00002	0.00005	0.00001
	3PX	0.00001	0.00015	0.00004	0	0.00002
	3PY	0.00002	-0.00002	0.00004	0.00001	0.00001
	3PZ	0.01382	0.12172	-0.02552	0.01195	-0.1283
	4XX	0	-0.00001	0	0	0
	4YY	0	-0.00001	-0.00001	0	0
	4ZZ	0	0	0	0	0
	4XY	0	-0.00002	0.00001	0	0
	4XZ	0.00001	0.00526	-0.00226	-0.00923	0.00432
	4YZ	-0.00132	-0.00817	0.00093	-0.0071	0.01031
3C	1S	0	0.00008	0	0	0
	2S	-0.00001	-0.00018	-0.00001	0	0
	2PX	0.00007	0.00051	-0.00011	-0.00004	0.00002
	2PY	0.00003	0.00008	-0.00002	0.00008	-0.00004
	2PZ	0.04125	0.25753	-0.03218	0.18707	-0.24754
	3S	0	-0.00032	0.00002	0.00002	0.00003
	3PX	0.00002	0.00034	0.00002	-0.00003	0.00003
	3PY	0.00003	0.00002	0.00002	0.00004	-0.00001
	3PZ	0.01841	0.1431	-0.02323	0.1123	-0.17083
	4XX	0	0.00001	0.00001	0	0
	4YY	0	0.00001	-0.00001	0	0
	4ZZ	0	0.00001	0	0	0

	4XY	0	0.00003	0.00001	0	0
	4XZ	-0.00121	0.00413	-0.00326	-0.0107	-0.01241
	4YZ	-0.00027	0.00086	-0.00076	-0.00317	-0.00302
4C	1S	-0.00001	0.00001	-0.00001	0.00001	0
	2S	0.00002	0.00001	0.00001	-0.00002	-0.00001
	2PX	0.00002	0.0006	0.00016	0.00004	0.00004
	2PY	0.00007	0.00079	0	-0.00002	-0.00003
	2PZ	0.02136	0.20971	-0.04798	0.00471	-0.16639
	3S	0.00004	-0.00016	0	-0.00003	-0.00002
	3PX	0.00001	0.00017	0.00005	0	0.00002
	3PY	0.00003	0.00018	-0.00002	-0.00001	-0.00003
	3PZ	0.0125	0.12171	-0.02738	0.00722	-0.12983
	4XX	0	0.00002	0	0	0
	4YY	0	-0.00004	-0.00001	0	0
	4ZZ	0	0	0	0	0
	4XY	0	-0.00003	0	0	0
	4XZ	-0.00064	-0.00001	-0.00134	-0.0116	0.01041
	4YZ	0.00114	0.00967	-0.00196	0.00111	-0.00603
5C	1S	0	0.00002	0	0	0
	2S	-0.00001	-0.00005	0	0.00001	0
	2PX	-0.00004	-0.00055	-0.00014	0.00001	-0.00003
	2PY	-0.00002	-0.0009	-0.00004	-0.00001	0.00002
	2PZ	0.01319	0.18492	-0.05724	-0.16993	0.11127
	3S	-0.00002	0.00001	-0.00001	0.00002	0.00002
	3PX	0	-0.00022	-0.00004	0	-0.00002
	3PY	0	-0.00026	-0.00002	-0.00002	0.00001
	3PZ	0.0062	0.10299	-0.03436	-0.11531	0.08196
	4XX	0	0.00005	0	0	0
	4YY	0	-0.00004	-0.00001	0	0
	4ZZ	0	-0.00001	0	0	0
	4XY	0	-0.00001	0.00001	0	0
	4XZ	-0.00069	-0.00704	0.0016	-0.00117	0.00869
	4YZ	0.00032	0.00556	-0.00198	-0.00894	0.01093
6C	1S	0	0.00005	0	0	0
	2S	-0.00001	-0.00013	-0.00001	0	0
	2PX	0.00009	0.00068	0.00016	0.00004	-0.00005
	2PY	0.00002	0.0009	0	-0.00005	0.00004
	2PZ	0.01102	0.17703	-0.06015	-0.24059	0.25734
	3S	-0.00002	-0.00017	0	0	0
	3PX	0.00002	0.00015	0.00004	0.00003	-0.00003
	3PY	0.00001	0.00029	-0.00001	-0.00004	0.00003
	3PZ	0.00655	0.10178	-0.03489	-0.15368	0.1944
	4XX	0	0.00006	0.00001	0	0
	4YY	0	-0.00004	-0.00001	0	0

	4ZZ	0	0	0	0	0
	4XY	0	0.00001	0.00001	0	0
	4XZ	-0.00064	-0.00838	0.00249	0.00668	-0.00308
	4YZ	-0.00017	-0.00244	0.00075	0.00207	-0.00152
7H	1S	0.00003	-0.0003	-0.00004	0.00001	0
	2S	0.00003	-0.00031	-0.00004	0.00002	0.00001
	3PX	0	0	0	0	0
	3PY	0	0.00001	0	0	0
	3PZ	0.0003	0.00393	-0.0012	-0.00382	0.00255
8H	1S	0	-0.00004	-0.00006	0	0
	2S	-0.00001	-0.00001	-0.00009	-0.00003	-0.00003
	3PX	0	0	0	0	0
	3PY	0	0	0	0	0
	3PZ	0.00051	0.00453	-0.00098	0.00049	-0.00422
9H	1S	-0.00003	-0.00059	-0.00003	0.00001	0
	2S	-0.00003	-0.00054	-0.00005	0.00002	0
	3PX	0	0	0	0	0
	3PY	0	-0.00002	0	0	0
	3PZ	0.00045	0.00447	-0.00101	0.00042	-0.00411
10H	1S	-0.00001	0.00018	-0.00007	-0.00002	0
	2S	-0.00001	0.00019	-0.00007	-0.00002	-0.00001
	3PX	0	-0.00001	0	0	0
	3PY	0	-0.00001	0	0	0
	3PZ	0.00028	0.00391	-0.00122	-0.00392	0.00299
11H	1S	0.00006	0.0006	0.00011	0	0
	2S	0.00006	0.00065	0.00012	0	0
	3PX	0	-0.00002	0	0	0
	3PY	0	0.00001	0	0	0
	3PZ	0.0002	0.00366	-0.00132	-0.0058	0.00686
12C	1S	-0.00001	-0.00006	-0.00002	0	0
	2S	0.00002	0.00011	0.00004	-0.00001	0
	2PX	-0.0001	0.00005	0.00009	0.00002	0
	2PY	-0.00002	-0.00133	0.00008	-0.00008	-0.00001
	2PZ	0.07141	0.14036	0.04243	0.29636	0.18611
	3S	0.00003	0.00026	0.00011	-0.00001	0.00001
	3PX	-0.00003	0.00016	0.00004	-0.00001	0.00001
	3PY	-0.00001	-0.00049	0.00004	-0.00004	-0.00001
	3PZ	0.04001	0.07843	0.03043	0.19843	0.12145
	4XX	0	-0.00008	0	0	0
	4YY	0	0.00008	0	0	-0.00001
	4ZZ	0	0	0	0	0
	4XY	0	0	0	0	0
	4XZ	-0.00291	0.00556	-0.00423	-0.00079	-0.01964
	4YZ	0.00244	0.00433	0.00134	0.00814	0.00526

13H	1S	0.00002	0.00094	-0.00004	0.00003	-0.00002
	2S	0.00001	0.00074	-0.00005	0.00003	-0.00003
	3PX	0	0.00001	0	0	0
	3PY	0	0.00003	0	0	0
	3PZ	0.00179	0.00307	0.00108	0.00652	0.00449
14C	1S	0	0.00004	0.00001	0.00001	-0.00001
	2S	0	-0.00011	-0.00003	-0.00001	0.00002
	2PX	0.00006	0.00002	0.00003	-0.00002	0.00002
	2PY	-0.00008	0.00124	-0.00001	-0.00003	-0.00008
	2PZ	0.12092	0.06954	0.09093	0.22001	0.31198
	3S	-0.00001	-0.00012	-0.00007	-0.00005	0.00004
	3PX	0.00001	0.00011	0	0.00001	-0.00001
	3PY	-0.00002	0.0003	-0.00001	-0.00001	-0.00005
	3PZ	0.06327	0.04163	0.05218	0.14207	0.24243
	4XX	0	-0.00006	0	0	0
	4YY	0	0.00009	0	0	0
	4ZZ	0	0	0	0	0
	4XY	0	-0.00002	0	0	0
	4XZ	-0.00534	0.00484	-0.00316	0.01058	0.00454
	4YZ	-0.00509	-0.0027	-0.00411	-0.00714	-0.0071
15H	1S	-0.00003	0.00086	-0.00002	0.00001	0
	2S	-0.00003	0.00092	-0.00001	0.00002	-0.00002
	3PX	0	0	0	0	0
	3PY	0	-0.00002	0	0	0
	3PZ	0.00269	0.0016	0.00187	0.00506	0.00749
16C	1S	0.00001	0	0	0	0
	2S	-0.00002	0.00001	0	0	0
	2PX	-0.00006	-0.00076	0.00001	0.00001	0
	2PY	0.00002	-0.00058	-0.00006	0.00001	0
	2PZ	0.29339	-0.01366	0.17182	-0.04308	0.01044
	3S	-0.00003	-0.00013	0	0.00002	-0.00002
	3PX	-0.00002	-0.00021	0.00001	0.00002	-0.00001
	3PY	-0.00002	0.0001	0.00001	0	-0.00001
	3PZ	0.15055	-0.01186	0.09097	-0.03211	-0.00064
	4XX	0	-0.00005	-0.00001	0	0
	4YY	0	0.00004	0.00001	0	0
	4ZZ	0	-0.00001	0	0	0
	4XY	-0.00001	0.00003	0	0	0
	4XZ	-0.00588	0.00461	0.00328	0.01372	0.01602
	4YZ	-0.00329	-0.00043	-0.01026	0.00105	0.01204
17O	1S	0	0.00002	-0.00002	0	0
	2S	0.00001	-0.00005	0.00003	0	0.00001
	2PX	0.00005	0.00009	0.00008	0	0.00001
	2PY	-0.00003	0.00008	0.00015	-0.00003	0.00001

	2PZ	0.22979	-0.0668	-0.05	-0.17194	-0.07338
	3S	0.00002	-0.00014	0.00008	0	0.00002
	3PX	0.00003	0.00004	0.00005	0	0.00001
	3PY	-0.00002	0.00006	0.00009	-0.00002	0.00001
	3PZ	0.14813	-0.0448	-0.03586	-0.12586	-0.05465
	4XX	0	0	0	0	0
	4YY	0	0.00001	-0.00001	0	0
	4ZZ	0	0	0	0	0
	4XY	0	-0.00002	0	0	0
	4XZ	0.00763	0.00063	0.0085	-0.0019	0.00158
	4YZ	-0.01357	0.00356	0.00277	0.00652	0.00327
18C	1S	0	-0.00002	0.00001	0	0
	2S	-0.00001	0.00004	-0.00002	0.00001	0
	2PX	-0.00004	-0.00041	-0.00005	0	-0.00001
	2PY	0.00003	0.0007	-0.00007	0	-0.00001
	2PZ	-0.11078	-0.03289	-0.26157	0.09231	0.02783
	3S	-0.00001	0.00004	-0.00001	0.00001	-0.00001
	3PX	-0.00002	-0.00013	-0.00003	0.00001	0
	3PY	0.00002	0.00023	-0.00001	0	-0.00002
	3PZ	-0.03905	-0.01743	-0.11768	0.02576	0.00498
	4XX	0	0	-0.00001	0	0
	4YY	0	0.00001	-0.00001	0	0
	4ZZ	0	-0.00002	0.00002	0	0
	4XY	0	-0.00003	0.00001	0	0
	4XZ	0.01252	-0.0031	-0.00248	-0.00673	-0.00346
	4YZ	-0.0002	0.00335	0.02058	-0.00829	-0.00272
19H	1S	-0.05302	-0.01831	-0.14746	0.06114	0.02016
	2S	-0.03381	-0.01689	-0.12935	0.0646	0.0162
	3PX	0.00151	-0.00055	-0.001	-0.00052	-0.00073
	3PY	-0.00277	-0.00033	-0.00406	0.00174	0.00067
	3PZ	0.00058	0.00012	0.00103	-0.00046	0.00003
20H	1S	0.05303	0.01791	0.14759	-0.06116	-0.02017
	2S	0.03383	0.01649	0.12948	-0.06464	-0.01622
	3PX	-0.00151	0.00053	0.001	0.00052	0.00072
	3PY	0.00276	0.00034	0.00406	-0.00174	-0.00067
	3PZ	0.00059	0.0001	0.00103	-0.00046	0.00002
21C	1S	0	-0.00003	0.00001	0	0
	2S	0	0.00006	-0.00002	0.00001	0
	2PX	-0.00008	0.00032	0.00003	0.00002	0.00001
	2PY	0.00006	-0.00073	0.00004	-0.00001	0
	2PZ	-0.26471	0.08782	0.29401	-0.03318	-0.00449
	3S	-0.00001	0.00014	-0.00005	0.00003	0.00002
	3PX	-0.00004	0.00016	0.00002	0.00001	0.00001
	3PY	0.00003	-0.00035	0.00002	-0.00002	-0.00001

	3PZ	-0.1355	0.04413	0.13371	0.0002	0.00935
	4XX	0	0.00001	0	0	0
	4YY	0.00001	0	-0.00001	0	0
	4ZZ	0	-0.00002	0.00002	0	0
	4XY	0	-0.00002	0.00001	0	0
	4XZ	-0.00505	0.00082	0.0011	0.0003	0.00015
	4YZ	-0.00934	0.00501	0.02131	-0.00457	-0.00116
22H	1S	0.00002	-0.00003	-0.00002	-0.00001	-0.00001
	2S	0.00002	-0.00004	-0.00001	-0.00002	-0.00001
	3PX	0	0	0	0	0
	3PY	0	-0.00001	0	0	0
	3PZ	-0.00474	0.00167	0.00593	-0.00089	-0.00026
23H	1S	-0.13514	0.04847	0.17277	-0.02449	-0.00493
	2S	-0.10013	0.04121	0.16717	-0.03903	-0.01401
	3PX	0.00134	-0.00058	-0.00211	0.00009	-0.00003
	3PY	0.00414	-0.0013	-0.00442	0.00074	0.00026
	3PZ	0.00109	-0.00037	-0.0014	0.00027	0.0001
24H	1S	0.13512	-0.04889	-0.17268	0.02449	0.00493
	2S	0.10011	-0.04161	-0.16707	0.03902	0.01401
	3PX	-0.00134	0.0006	0.0021	-0.00009	0.00003
	3PY	-0.00414	0.00128	0.00442	-0.00074	-0.00026
	3PZ	0.00109	-0.00039	-0.00139	0.00027	0.0001
25O	1S	-0.00001	0.00011	0	0	0
	2S	0.00002	-0.00024	-0.00001	0	0
	2PX	-0.00004	-0.00018	0.00005	0.00003	-0.00001
	2PY	-0.00005	0.00098	0.00005	-0.00002	0
	2PZ	0.24677	-0.01556	0.208	-0.07323	-0.16616
	3S	0.00003	-0.0004	-0.00001	0	-0.00001
	3PX	-0.00002	-0.00009	0.00003	0.00002	-0.00001
	3PY	-0.00003	0.00058	0.00003	-0.00001	0
	3PZ	0.1443	-0.00847	0.13091	-0.04587	-0.12401
	4XX	0	-0.00001	0	0	0
	4YY	0	0.00006	0	0	0
	4ZZ	0	-0.00001	0	0	0
	4XY	0	-0.00002	0	0	0
	4XZ	0.00326	0.00038	0.00367	0.00031	0.00024
	4YZ	0.01846	-0.00104	0.0136	-0.00439	-0.00717

3.5.2 Combined coefficients and computational details of HFV index (F) of 1d

Table S11. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of **1d**

i/j \ k ($\|c_{ki}\|/\|c_{kj}\|$)	34	38	39	43	47
3	0.0665	0.4677	0.0554	0.3102	0.3951
12	0.1205	0.2555	0.0728	0.5065	0.2929
14	0.2010	0.1290	0.1459	0.3723	0.5187
16	0.4851	0.0297	0.2706	0.0787	0.0297

Table S12. The calculation details of HFV index (F) of **1d**

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	ΣP	HFV (F)
α (14)	14-12	34 (1),38 (1),43 (1),47 (1)	0.79 [a]	1.06	0.70
	14-16	34 (1),39 (1)	0.27 [b]		
β (12)	12-3	38 (1),43 (1),47 (-1)	0.33 [c]	1.12	0.64
	12-14	34 (1),38 (1),43 (1),47 (1)	0.79 [d]		

a : $P_{14\text{-}12}$=2*0.2010*0.1205+2*0.1290*0.2555+2*0.3723*0.5065+2*0.5187*0.2929=0.79
b : $P_{14\text{-}16}$=2*0.2010*0.4851+2*0.1459*0.2706=0.27
c : $P_{12\text{-}3}$=2*0.2555*0.4677-2*0.5065*0.3102-2*0.2929*0.3951=0.33
d: $P_{12\text{-}14}$=2*0.2010*0.1205+2*0.1290*0.2555+2*0.3723*0.5065+2*0.5187*0.2929=0.79

3.6 The occupied π-type molecular orbitals associated with the active sites of 1e

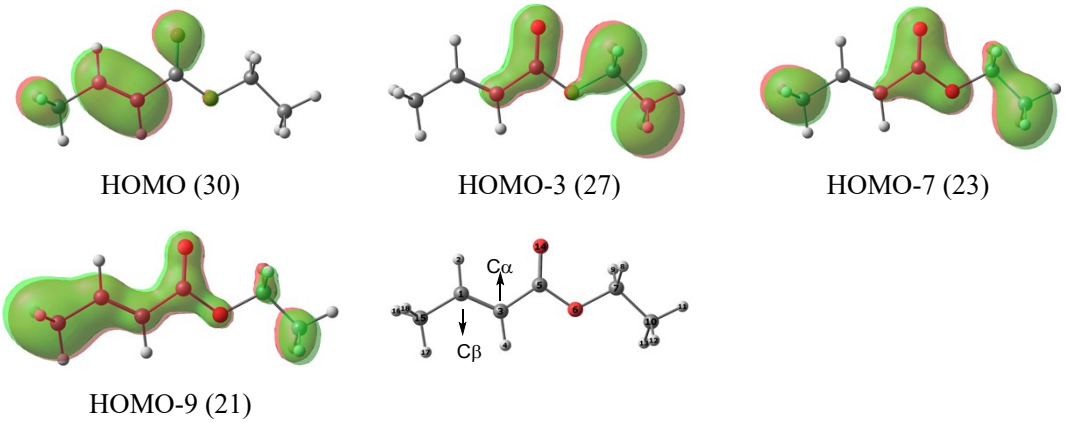


Fig. S9. The occupied π-type molecular orbitals associated with the active sites of **1e**

3.6.1 Molecular orbital coefficients of 1e

		21	23	27	30
1C	1S	0.00001	0.00005	0	-0.00001
	2S	-0.00002	-0.00011	-0.00001	0.00003
	2PX	-0.00069	0.00037	0.00005	0.00002
	2PY	-0.00001	0.0003	0.00014	-0.00003
	2PZ	0.15892	-0.03049	0.03972	0.34592
	3S	-0.00018	-0.00008	-0.00001	0.00003
	3PX	-0.00033	0.00008	0.00001	-0.00019
	3PY	0.00005	0.00005	0.00005	0.00002
	3PZ	0.08358	-0.01446	0.0279	0.23047
	4XX	0	0.00001	-0.00001	0.00001
	4YY	0.00001	0	0.00001	0
	4ZZ	0	0	0	-0.00001
	4XY	0	-0.00003	-0.00001	0
	4XZ	-0.00563	0.00768	0.00471	0.01846
	4YZ	-0.00601	0.00199	-0.00055	-0.00651
2H	1S	0.00003	0.00011	0.00011	0
	2S	0	0.00013	0.0001	-0.00018
	3PX	-0.00001	0.00001	0	-0.00001
	3PY	0	0	0	0
	3PZ	0.00329	-0.00035	0.00103	0.00806
3C	1S	-0.00003	-0.0001	0.00001	-0.00005
	2S	0.00005	0.0002	-0.00001	0.00011
	2PX	0.00041	-0.00006	-0.00001	0.00034
	2PY	-0.00074	-0.00005	-0.00015	0.00018
	2PZ	0.10758	0.06468	0.08998	0.38299
	3S	0.00028	0.00036	-0.00004	0.00048
	3PX	-0.00003	0.0001	-0.00002	0.00015
	3PY	-0.00014	0	-0.00005	0.00017
	3PZ	0.05488	0.03408	0.05247	0.28197
	4XX	-0.00001	-0.00002	-0.00001	0
	4YY	0.00003	0.00001	0.00001	-0.00002
	4ZZ	0	-0.00001	0	0.00001
	4XY	0.00001	-0.00002	-0.00001	0.00001
	4XZ	-0.00211	0.00711	0.00266	-0.01217
	4YZ	0.00424	0.00383	0.0045	0.00774
4H	1S	0.00049	0.00012	0.00009	-0.00014
	2S	0.00041	0.00005	0.00011	-0.00014
	3PX	0	0	0	0.00001
	3PY	0.00002	0.00001	0	0
	3PZ	0.00239	0.00139	0.00183	0.00908
5C	1S	-0.00009	0.00007	0.00001	-0.00002
	2S	0.00021	-0.00017	-0.00001	0.00006

	2PX	0.00008	0.00013	0.00008	-0.00012
	2PY	0.00031	-0.00017	0.00008	-0.00006
	2PZ	0.13452	0.26152	0.17697	-0.02976
	3S	0.00013	-0.00023	-0.00002	0.00007
	3PX	0.00013	0.00009	0.00002	0.00024
	3PY	-0.00011	0.00015	-0.00002	-0.00013
	3PZ	0.0663	0.13652	0.09347	-0.02964
	4XX	-0.00003	0.00004	-0.00001	-0.00001
	4YY	0	-0.00001	0.00001	0
	4ZZ	-0.00001	0.00001	0	0.00001
	4XY	0.00004	0.00001	0	0.00012
	4XZ	0.0001	0.0069	-0.00457	-0.01549
	4YZ	0.00137	0.00415	0.01003	-0.0204
6O	1S	0.00009	0.00004	0	0.00003
	2S	-0.00019	-0.00008	0.00001	-0.00005
	2PX	0.0003	0.00015	-0.00004	0.00029
	2PY	0.00026	0.00044	-0.00007	-0.00048
	2PZ	0.08158	0.22621	-0.04851	-0.04894
	3S	-0.00048	-0.00013	0.00001	-0.00029
	3PX	0.00017	0.00006	-0.00003	0.00023
	3PY	0.00014	0.00026	-0.00005	-0.0004
	3PZ	0.05189	0.1465	-0.0348	-0.0331
	4XX	0.00001	-0.00002	0	0.00002
	4YY	0.00003	0.00003	0	-0.00001
	4ZZ	0	0	0	0.00001
	4XY	0	0.00001	0	0.00001
	4XZ	-0.00465	-0.00825	-0.00824	-0.00041
	4YZ	0.00439	0.01212	-0.00393	-0.00344
7C	1S	-0.00001	0.00003	0	0.00002
	2S	0.00002	-0.00007	-0.00001	-0.00004
	2PX	-0.00022	-0.00041	0.00008	-0.00007
	2PY	-0.00016	0.00025	-0.00002	-0.00005
	2PZ	-0.06772	-0.08503	-0.26825	0.0348
	3S	0.00007	-0.00007	0	-0.00015
	3PX	-0.0001	-0.00017	0.00003	-0.00016
	3PY	-0.00007	0.0001	-0.00002	0.00006
	3PZ	-0.02592	-0.02797	-0.12049	0.01356
	4XX	0.00001	0.00002	-0.00001	0
	4YY	0	-0.00001	-0.00001	0.00001
	4ZZ	-0.00001	0	0.00001	0
	4XY	0.00001	0.00001	0	0
	4XZ	-0.00481	-0.01196	0.00545	0.00235
	4YZ	-0.00141	-0.00078	-0.02052	0.00289
8H	1S	-0.03228	-0.04062	-0.15136	0.02137

	2S	-0.02181	-0.02477	-0.13284	0.00979
	3PX	-0.00074	-0.00183	0.0004	0.00094
	3PY	0.00143	0.00204	0.00427	-0.00068
	3PZ	0.00034	0.00046	0.00105	0.00008
9H	1S	0.03219	0.04072	0.15139	-0.02141
	2S	0.0217	0.02488	0.13288	-0.0097
	3PX	0.00073	0.00181	-0.0004	-0.00095
	3PY	-0.00143	-0.00203	-0.00427	0.00068
	3PZ	0.00034	0.00046	0.00105	0.00007
10C	1S	-0.00001	0	0	0.00001
	2S	0.00002	0.00001	0	-0.00003
	2PX	-0.00022	0.00032	-0.00008	0.00008
	2PY	-0.00032	-0.00042	0.00003	0.00003
	2PZ	-0.11094	-0.25005	0.29982	-0.0095
	3S	0.00001	0.00002	-0.00001	0.00008
	3PX	-0.00007	0.00016	-0.00004	-0.00004
	3PY	-0.00014	-0.00018	0.00002	0.00004
	3PZ	-0.05587	-0.12868	0.13614	0.00546
	4XX	-0.00001	-0.00001	-0.00001	0.00001
	4YY	0	0	-0.00001	0
	4ZZ	0.00001	0.00001	0.00001	-0.00001
	4XY	-0.00001	0.00002	0	0
	4XZ	0.00187	0.0031	0.00209	-0.00049
	4YZ	0.00368	0.00989	-0.02171	0.00145
11H	1S	-0.0002	0.00009	-0.00006	0.00007
	2S	-0.00018	0.00007	-0.00005	0.00012
	3PX	0.00001	0	0	0
	3PY	0	-0.00001	0	0
	3PZ	-0.00198	-0.00449	0.00606	-0.00038
12H	1S	-0.05548	-0.12851	0.17628	-0.00789
	2S	-0.04039	-0.09604	0.1708	-0.01541
	3PX	-0.00024	-0.00074	0.00146	-0.00003
	3PY	-0.00185	-0.00402	0.00477	-0.0003
	3PZ	0.00046	0.00102	-0.00143	0.00011
13H	1S	0.05572	0.12875	-0.17623	0.00782
	2S	0.04057	0.09623	-0.17074	0.01535
	3PX	0.00023	0.00075	-0.00147	0.00004
	3PY	0.00185	0.00402	-0.00478	0.0003
	3PZ	0.00047	0.00103	-0.00142	0.00011
14O	1S	0.0001	-0.00005	0.00001	0
	2S	-0.00023	0.0001	-0.00002	-0.00001
	2PX	0.00015	0.00019	0.00003	0.00133
	2PY	-0.00059	0.00032	-0.00014	-0.00004
	2PZ	0.10664	0.22572	0.21481	-0.25142

	3S	-0.00035	0.00012	-0.00003	0.00006
	3PX	0.00008	0.00011	0.00001	0.00092
	3PY	-0.00034	0.0002	-0.00008	-0.00005
	3PZ	0.062	0.13228	0.13532	-0.18005
	4XX	-0.00001	0.00001	0	-0.00001
	4YY	0.00004	-0.00002	0.00001	0
	4ZZ	-0.00001	0	0	0
	4XY	-0.00001	-0.00001	0	-0.00005
	4XZ	-0.00051	-0.00023	-0.00167	-0.0014
	4YZ	-0.00832	-0.01696	-0.01445	0.01203
15C	1S	0.00002	0.00001	0.00001	-0.00001
	2S	-0.00003	-0.00002	-0.00002	0.00003
	2PX	0.00023	-0.0007	-0.00008	0.00005
	2PY	0.00066	0.00022	-0.0001	0
	2PZ	0.37593	-0.20233	-0.0426	-0.1165
	3S	-0.00005	-0.0001	-0.00005	-0.00004
	3PX	0.00011	-0.00032	-0.00004	0.00001
	3PY	0.00028	0.0001	-0.00004	-0.00008
	3PZ	0.16529	-0.09259	-0.02314	-0.03988
	4XX	0.00001	0	0	0
	4YY	-0.00004	-0.00001	0.00001	0.00001
	4ZZ	0.00003	0.00001	0	-0.00002
	4XY	0.00003	-0.00002	0	-0.00001
	4XZ	-0.01192	0.00816	0.00332	0.01882
	4YZ	0.01095	-0.00556	-0.00086	0.00076
16H	1S	-0.19213	0.10688	0.02555	0.09255
	2S	-0.16152	0.09194	0.0242	0.12165
	3PX	-0.00656	0.00336	0.00053	0.0008
	3PY	0.00227	-0.00127	-0.00034	-0.00188
	3PZ	-0.00156	0.00083	0.00016	0.00055
17H	1S	-0.00056	-0.00012	0.00008	0.00009
	2S	-0.00045	-0.00008	0.00008	0.00006
	3PX	0.00001	-0.00001	0	0
	3PY	-0.00002	0	0	0
	3PZ	0.00709	-0.00374	-0.00072	-0.00252
18H	1S	0.19233	-0.10644	-0.02557	-0.09266
	2S	0.1617	-0.09154	-0.0242	-0.12178
	3PX	0.00656	-0.00337	-0.00053	-0.00079
	3PY	-0.00223	0.00127	0.00033	0.00188
	3PZ	-0.00158	0.00081	0.00016	0.00056

3.6.2 Combined coefficients and computational details of HFV index (F) of 1e

Table S13. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of **1e**

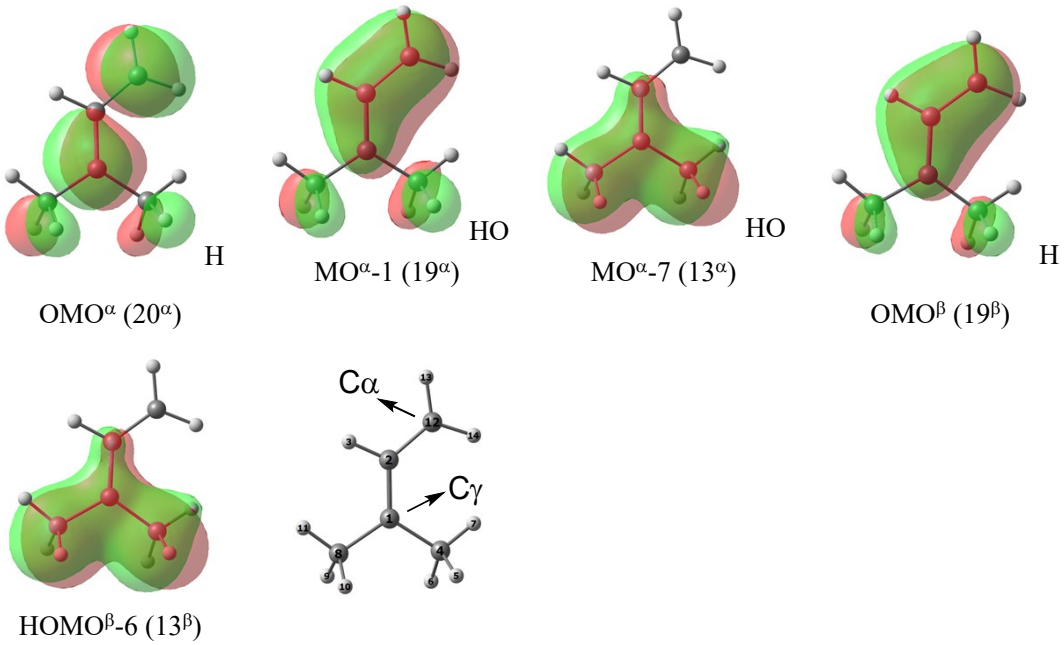
i/j \ k ($\|c_{ki}\|/\|c_{kj}\|$)	21	23	27	30
1	0.2765	0.0507	0.0674	0.5526
3	0.1859	0.1075	0.1441	0.6319
5	0.2307	0.4314	0.2769	0.0653
15	0.6323	0.3256	0.0671	0.1654

Table S14. The calculation details of HFV index (F) of **1e**

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	$\sum P$	HFV (F)
α (3)	3-1	21 (1),27 (-1),30 (1)	0.78 [a]	1.04	0.72
	3-5	21 (1),23 (1),27 (1),	0.26 [b]		
β (1)	1-3	21 (1),27 (-1),30 (1)	0.78 [c]	0.95	0.81
	1-15	21 (1), 30 (-1)	0.17 [d]		

a : $P_{3\text{-}1}$=2*0.1859*0.2765-2*0.1441*0.0674+2*0.6319*0.5526=0.78
b : $P_{3\text{-}5}$=2*0.1859*0.2307+2*0.1075*0.4314+2*0.1441*0.2769=0.26
c : $P_{1\text{-}3}$=2*0.1859*0.2765-2*0.1441*0.0674+2*0.6319*0.5526=0.78
d: $P_{1\text{-}15}$=2*0.2765*0.6323-2*0.5526*0.1654=0.17

3.7 The occupied π-type molecular orbitals associated with the active sites of III



OMO$^{\alpha}$ (20$^{\alpha}$) MO$^{\alpha}$-1 (19$^{\alpha}$) MO$^{\alpha}$-7 (13$^{\alpha}$) OMO$^{\beta}$ (19$^{\beta}$)

HOMO$^{\beta}$-6 (13$^{\beta}$)

Fig. S10. The occupied π-type molecular orbitals associated with the active sites of **III**

3.7.1 Molecular orbital coefficients of III

			13^{α}	19^{α}	20^{α}	13^{β}	19^{β}
1	C	1S	0.00007	0.00017	0.00137	0.00026	0.00028
2S			-0.00074	0.0005	-0.00177	-0.00152	0.00007
2PX			-0.00182	-0.00441	-0.00321	-0.00291	-0.00418
2PY			0.00596	0.00048	0.00237	0.00558	0.00185
2PZ			0.22377	0.21157	0.44317	0.15873	0.18377
3S			0.00429	-0.00669	-0.00923	0.00656	-0.00518
3PX			-0.00425	0.01373	-0.01169	-0.00541	0.0148
3PY			0.002	0.00053	0.00104	0.00104	0.00046
3PZ			0.12052	0.13561	0.36741	0.08159	0.10931
4XX			-0.00049	0.00008	0.00074	-0.00082	-0.00015
4YY			-0.00019	0.00031	0.00036	-0.0001	0.00028
4ZZ			0.0006	-0.00019	-0.00051	0.00073	0.00006
4XY			-0.00009	-0.00026	0.0002	-0.00019	-0.00015
4XZ			0.0052	-0.0165	-0.00636	0.00614	-0.01707
4YZ			0.00242	-0.00811	-0.00511	0.00327	-0.00798
2	C	1S	0.00027	0.00017	-0.00046	0.00068	0.00009
2S			-0.00007	-0.00111	0.00172	-0.00083	-0.00095
2PX			-0.00468	0.00559	0.0035	-0.00383	0.0057
2PY			0.00542	-0.00185	-0.00013	0.00398	-0.00331
2PZ			0.08575	0.34785	0.0562	0.07624	0.43275
3S			-0.00528	0.01002	-0.00408	-0.00772	0.01019
3PX			-0.00303	0.00802	-0.00195	-0.00389	0.00816
3PY			-0.00095	0.00533	-0.00364	-0.00208	0.00441
3PZ			0.04026	0.2264	0.06137	0.04059	0.31574
4XX			0.00017	0.00003	-0.00007	0.00022	-0.0001
4YY			-0.00019	-0.00015	0.00053	-0.00014	0.00005
4ZZ			0.00016	0.00011	-0.00047	0.00021	0.00008
4XY			0.00009	0.00071	-0.00015	0.00016	0.00065
4XZ			0.00517	-0.00359	0.03074	0.00388	-0.00299
4YZ			0.00355	0.00913	0.00143	0.00303	0.00897
3	H	1S	-0.00384	-0.00067	0.00195	-0.00326	0.0004
2S			-0.00416	0.00125	0.00202	-0.00367	0.00245
3PX			-0.00007	-0.00004	0.00009	-0.00003	-0.00003
3PY			-0.00017	-0.00006	-0.00002	-0.00017	-0.00007
3PZ			0.00192	0.00805	0.00129	0.00167	0.0099
4	C	1S	0.00056	-0.00087	0.00009	-0.0003	-0.0007
2S			-0.0013	0.0012	0.00165	0.00035	0.00084
2PX			-0.0047	-0.00881	0.00232	-0.0081	-0.00681
2PY			-0.0083	0.00165	-0.00344	-0.007	-0.00023
2PZ			0.28177	-0.10459	-0.05936	0.29802	-0.08415
3S			-0.00062	0.00645	-0.00803	0.00259	0.00601
3PX			0.00096	-0.02248	0.00983	0.00006	-0.02337

3PY	-0.00257	0.00519	-0.00784	-0.00227	0.00436
3PZ	0.1179	-0.03609	-0.03157	0.13285	-0.01853
4XX	-0.00602	0.00332	0.00381	-0.00645	0.00265
4YY	-0.00003	0.00023	0.00065	-0.00014	0.00021
4ZZ	0.00613	-0.00385	-0.00403	0.00652	-0.00313
4XY	0.0008	-0.00066	-0.00021	0.0008	-0.00047
4XZ	0.00914	-0.00687	-0.00773	0.01003	-0.00612
4YZ	0.00054	-0.00956	-0.01935	0.00147	-0.00882
5 H 1S	0.15462	-0.0835	-0.08461	0.16344	-0.06897
2S	0.12808	-0.09932	-0.14009	0.13711	-0.08832
3PX	-0.00276	0.00093	0.0002	-0.00299	0.00084
3PY	-0.00405	0.00043	-0.0019	-0.00437	0.00028
3PZ	-0.00252	0.00122	0.00088	-0.00283	0.00105
6 H 1S	-0.12067	0.05907	0.06479	-0.1287	0.0494
2S	-0.10269	0.08279	0.10437	-0.11179	0.07716
3PX	0.00461	-0.00198	-0.00087	0.00481	-0.00171
3PY	0.00286	-0.00063	0.00125	0.00309	-0.00059
3PZ	0.00092	-0.00053	-0.00037	0.00086	-0.00046
7 H 1S	-0.03797	0.02296	0.0202	-0.03799	0.01785
2S	-0.03019	0.00793	0.04617	-0.03057	0.00231
3PX	-0.00197	0.00102	0.00055	-0.00198	0.00082
3PY	0.00116	0.00025	-0.0001	0.00114	0.00038
3PZ	0.00479	-0.00168	-0.00198	0.00506	-0.00146
8 C 1S	-0.00035	0.00011	-0.00005	-0.00039	0.0004
2S	0.00112	-0.00012	-0.00047	0.00135	-0.00055
2PX	-0.00197	0.00236	-0.00092	-0.00276	0.00342
2PY	0.00078	0.00038	-0.00017	-0.00412	-0.00059
2PZ	0.27802	-0.09303	-0.06995	0.28901	-0.07795
3S	0.00018	-0.00646	0.00592	-0.00043	-0.00906
3PX	-0.001	0.00413	-0.00179	-0.00129	0.00515
3PY	-0.00036	-0.00121	0.00403	-0.00279	-0.00202
3PZ	0.1164	-0.0341	-0.00482	0.12779	-0.021
4XX	-0.00018	0.0003	0.00034	-0.00028	0.00026
4YY	0.00047	-0.00045	0.00021	0.00069	-0.00036
4ZZ	-0.00004	-0.00009	-0.0006	-0.00011	-0.00004
4XY	0.00001	0.00009	-0.00024	0.00012	0.00015
4XZ	0.00745	-0.01202	-0.02199	0.00847	-0.0111
4YZ	0.00879	-0.00048	0.00421	0.00888	-0.00029
9 H 1S	-0.13943	0.06903	0.08582	-0.14529	0.05908
2S	-0.11636	0.08617	0.15168	-0.12384	0.07852
3PX	0.00517	-0.00117	0.00027	0.00549	-0.00098
3PY	0.00085	-0.00079	-0.00169	0.00075	-0.00071
3PZ	-0.001	0.00043	0.00059	-0.0012	0.00035
10 H 1S	0.13928	-0.06699	-0.08674	0.14331	-0.05692

2S	0.1171	-0.08588	-0.15494	0.1233	-0.07755
3PX	-0.00527	0.0013	-0.00015	-0.00559	0.00113
3PY	-0.00104	0.00086	0.00186	-0.0011	0.00073
3PZ	-0.00101	0.00035	0.00053	-0.00116	0.00028
11 H 1S	0.00274	-0.00192	-0.00023	0.0061	-0.00134
2S	0.00166	-0.00151	0.00162	0.00433	-0.0006
3PX	0.00002	-0.00006	-0.00008	0.00003	-0.00006
3PY	0.00018	-0.00001	-0.00006	0.00027	-0.00001
3PZ	0.00518	-0.0018	-0.002	0.00537	-0.00148
12 C 1S	-0.00059	0.0008	0.00125	-0.00066	0.00073
2S	0.00138	-0.00152	-0.003	0.00144	-0.00149
2PX	0.00426	-0.00113	-0.00587	0.00099	-0.00088
2PY	-0.00595	-0.01143	0.00416	-0.00715	-0.00774
2PZ	0.03631	0.34758	-0.39727	0.0256	0.2568
3S	0.00113	-0.00562	-0.00526	0.00126	-0.00637
3PX	0.00237	0.00049	-0.00341	0.00137	0.00049
3PY	-0.00221	-0.00982	0.00723	-0.0021	-0.00768
3PZ	0.02126	0.24566	-0.37946	0.0158	0.17946
4XX	0.00039	0.00047	0.00036	0.00043	0.00048
4YY	-0.00045	-0.0001	0.00013	-0.00041	0.00001
4ZZ	-0.00004	-0.00027	-0.0001	-0.0001	-0.0004
4XY	-0.00005	0.00017	0.00037	0.00009	0.00006
4XZ	0.00291	0.01258	0.00168	0.00259	0.01511
4YZ	-0.00071	-0.00583	0.0012	-0.00057	-0.00653
13 H 1S	0.00058	0.00417	0.00223	0.00286	0.00302
2S	0.00063	0.00468	0.00509	0.00271	0.004
3PX	0.00008	0.00014	-0.0001	0.00014	0.00009
3PY	-0.00006	-0.00007	0.00011	-0.00002	-0.00005
3PZ	0.00056	0.00744	-0.01039	0.00047	0.00646
14 H 1S	-0.00411	-0.00405	-0.00095	-0.00479	-0.00272
2S	-0.00225	0.00065	-0.00244	-0.00316	0.00232
3PX	0	0.00013	0.00001	-0.00006	0.00015
3PY	-0.00005	-0.00001	0.00049	-0.00002	-0.00005
3PZ	0.00087	0.00742	-0.01014	0.00078	0.00649

3.7.2 Combined coefficients and computational details of HFV index (F) of III

Table S15. Combined coefficients $|c_{ki}|/|c_{kj}|$ after normalization of the i and j atoms in the k_{th} occupied π-type molecular orbital of **III**

i/j \ k ($\|c_{ki}\|/\|c_{kj}\|$)	13^{α}	19^{α}	20^{α}	13^{β}	19^{β}
1	0.4051	0.3595	0.6611	0.2840	0.3083
2	0.1519	0.5916	0.1022	0.1383	0.7676
4	0.4871	0.1628	0.0830	0.5187	0.1297
8	0.4804	0.1426	0.0849	0.5021	0.1178
12	0.0684	0.6069	0.6308	0.0496	0.4496

Table S16. The calculation details of HFV index (F) of **III**

Active site	π Bond	π-Type molecular orbitals with δ_k in parentheses	π Bond order (P)	ΣP	HFV (F)
α (12)	12-2	19^{α} (1), 20^{α} (-1), 19^{β} (1)	0.64 [a]	0.64	1.12
γ (1)	1-2	13^{α} (1), 19^{α} (1), 20^{α} (1), 13^{β} (1), 19^{β} (1)	0.62 [b]	1.00	0.76
	1-4	13^{α} (1), 19^{α} (-1), 20^{α} (-1), 13^{β} (1), 19^{β} (-1)	0.19 [c]		
	1-8	13^{α} (1), 19^{α} (-1), 20^{α} (-1), 13^{β} (1), 19^{β} (-1)	0.19 [d]		

a : $P_{12\text{-}2}$=0.6069*0.5916-0.6308*0.1022+0.4496*0.7676=0.64

b : $P_{1\text{-}2}$=0.4051*0.1519+0.3595*0.5916+0.6611*0.1022+0.2840*0.1383+0.3083*0.7676=0.62

c : $P_{1\text{-}4}$=0.4051*0.4871-0.3595*0.1628-0.6611*0.0830+0.2840*0.5187-0.3083*0.1297=0.19

d: $P_{1\text{-}8}$=0.4051*0.4804-0.3595*0.1426-0.6611*0.0849+0.2840*0.5021-0.3083*0.1178=0.19

Part 4: Absolute SPE, GFEC, and GFE of the optimized structures

Table S17. The SPE calculated at B3LYP-D3/6-311++G(2df, 2pd)(SDD for Cs)/$SMD_{solvent}$ level, GFEC calculated at B3LYP-D3/6-31G(d, p)(Lan2LDZ for Cs)/$SMD_{solvent}$ level, and GFE = SPE + GFEC of the stationary points involved in the reaction models

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
NHC	-708.22622	0.244637	-707.981583
$CsHCO_3$	-284.77811	-0.006847	-284.784953
HCO_3^-	-264.647046	0.00053	-264.646516
H_2CO_3	-265.12229	0.013171	-265.109121
Cl^-	-460.3975	-0.015023	-460.41252
HCl	-460.84277	-0.011271	-460.854039
$CsHCO_3$-THF	-517.33423	0.094035	-517.24019
$CsHCO_3$-2THF	-749.89183	0.201932	-749.689894
CH_3OH-$CsCO_3^-$	-400.0407	0.028574	-400.01213
NHC+1a	-1552.908459	0.35669	-1552.551769
2a	-682.87351	0.07833	-682.795175
TS1	-1552.8959	0.359597	-1552.536339
M1	-1552.9091	0.363391	-1552.545755
TS2	-1837.6927	0.378966	-1837.313707
TS2'	-2070.2454	0.478793	-2069.766577
TS2''	-2302.8028	0.585588	-2302.217173
TS2'''	-1817.5474	0.381264	-1817.166098
M2	-1552.9143	0.361593	-1552.552714
TS3	-1817.5766	0.382231	-1817.194415
TS3'	-1552.9094	0.361961	-1552.547434
M3	-1092.0552	0.352746	-1091.702434
M3'	-1552.9358	0.362826	-1552.572927
ε-TS4	-1774.9362	0.455158	-1774.481032
TS4'	-2235.7893	0.459418	-2235.329879
M4	-1774.9412	0.457803	-1774.483438
M04	-2175.0226	0.512668	-2174.509908
TS5	-2175.0131	0.507348	-2174.505798
M5	-1890.2354	0.496366	-1889.739033
M05	-2155.4153	0.533117	-2154.882229
TS6	-2155.4114	0.531522	-2154.879867
M6	-1890.7449	0.509149	-1890.235767
TS7	-1890.741	0.508732	-1890.232218
3a	-1182.5309	0.240041	-1182.290902
M1b	-1169.520894	0.384693	-1169.136201
M1b+2b	-3456.458726	0.735669	-3455.723057
TSb	-3456.447768	0.739866	-3455.707902
TSb'	-3456.438689	0.74099	-3455.697699

M2b	-3456.461666	0.743365	-3455.718301
M1c	-2741.212907	0.460141	-2740.752766
M1c+2c	-3386.503163	0.616206	-3385.886957
TSc	-3386.481361	0.618768	-3385.858938
TSc'	-3386.475499	0.616561	-3385.858938
M2c	-3386.511647	0.618746	-3385.892901
1d	-577.083665	0.16587	-576.917795
1d+B•	-908.10473	0.303205	-907.801525
TSd	-908.099522	0.304737	-907.794785
TSd'	-908.099487	0.305755	-907.793732
M1d	-908.123763	0.306504	-907.817259
1e	-385.271931	0.116232	-385.155699
1e+B•	-716.289499	0.252703	-716.036796
TSe	-716.274997	0.254359	-716.020638
TSe'	-716.280221	0.255035	-716.025186
M1e	-716.298905	0.257018	-716.041887
II+III	-3485.456168	0.722356	-3484.733812
III	-195.983577	0.092226	-195.891351
***(S)*-^{os}TSf**	-3485.45834	0.724773	-3484.733567
***(S)*-^{os}TSf'**	-3485.455636	0.724501	-3484.731135
IV	-3485.556094	0.732361	-3484.823733

Table S18. Absolute SPE, GFEC, and GFE of the optimized structures obtained at the B3LYP-D3/6-311++G(2df, 2pd)/SMD$_{THF}$//B3LYP/6-31G(d, p)/SMD$_{THF}$ (L2).

	SPE (a.u.)	**GFEC (a.u.)**	**GFE (a.u.)**
M3	-1092.055095	0.351727	-1091.703368
ε-TS4	-1774.932482	0.453449	-1774.479033

Table S19. Absolute SPE, GFEC, and GFE of the optimized structures obtained at the M06-2X/6-311++G(2df, 2pd)/SMD$_{THF}$//M06-2X/6-31G(d, p)/SMD$_{THF}$ (L3).

	SPE (a.u.)	**GFEC (a.u.)**	**GFE (a.u.)**
M3	-1091.54525	0.355696	-1091.189554
ε-TS4	-1774.161409	0.46189	-1773.699519

Table S20. Absolute SPE, GFEC, and GFE of the optimized structures obtained at the ωB97X-D/6-311++G(2df, 2pd)/SMD$_{THF}$//ωB97X-D/6-31G(d, p)/SMD$_{THF}$ (L4).

	SPE (a.u.)	**GFEC (a.u.)**	**GFE (a.u.)**
M3	-1091.635364	0.357574	-1091.27779
ε-TS4	-1774.277013	0.462997	-1773.814016

Table S21. Absolute SPE, GFEC, and GFE of the different conformers of **ε-TS4**.

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
ε-TS4$_{\Phi = -60°}$	-1774.931842	0.455034	-1774.476808
ε-TS4$_{\Phi = 171°}$	-1774.93019	0.455696	-1774.474494
ε-TS4$_{\Phi = -161°}$	-1774.931055	0.456418	-1774.474637
ε-TS4$_{\Phi = 78°}$	-1774.930048	0.457047	-1774.473001

Part 5: Cartesian coordinates of all the stationary points

NHC

Zero-point correction= 0.287528
Thermal correction to Energy= 0.303082
Thermal correction to Enthalpy= 0.304026
Thermal correction to Gibbs Free Energy= 0.244637
Sum of electronic and zero-point Energies= -707.734978
Sum of electronic and thermal Energies= -707.719424
Sum of electronic and thermal Enthalpies= -707.718480
Sum of electronic and thermal Free Energies= -707.777869

Cartesian coordinates

C	3.878352	0.132291	-1.172658
C	2.438369	-0.182961	0.675794
C	3.806828	-0.369252	1.252578
C	4.699028	0.250193	0.137232
H	4.092846	-0.794798	-1.714159
H	4.020899	0.976206	-1.849271
H	3.934418	0.116784	2.222151
H	4.010282	-1.438494	1.383715
H	4.872786	1.307068	0.359746
H	5.669186	-0.243190	0.056790
N	2.504172	0.096220	-0.667082
N	1.202446	-0.240851	1.078296
N	0.502897	0.017950	-0.117441
C	1.263281	0.227966	-1.222430
C	-0.929670	0.019303	-0.067043
C	-1.610301	1.239897	0.035178
C	-1.604990	-1.211659	-0.106458
C	-3.009394	1.208038	0.077785
C	-3.000825	-1.195074	-0.054666
C	-3.719720	0.004258	0.033714
H	-3.553940	2.146225	0.152020
H	-3.540341	-2.138812	-0.089494
C	-0.855569	2.543724	0.094032
H	-0.095318	2.524532	0.882484
H	-0.330859	2.740079	-0.846998
H	-1.532379	3.379489	0.289208
C	-5.227536	-0.013540	0.101372
H	-5.573321	-0.373053	1.078553
H	-5.649240	0.983818	-0.052803
H	-5.652353	-0.683515	-0.654065
C	-0.836387	-2.503876	-0.210946

H	-0.198949	-2.511425	-1.102180
H	-0.176049	-2.639609	0.652401
H	-1.513066	-3.360387	-0.265411

Vibrational frequencies

54.9620	60.4099	63.3360
65.1132	145.5954	150.6983
162.4600	169.9849	201.1837
230.2547	238.4518	239.2160
262.2903	285.2001	341.0896
368.6918	380.0748	512.5174
517.7449	527.5326	561.4798
565.6051	582.2082	610.8719
636.9311	670.7577	691.8183
734.2736	762.7849	772.5771

$CsHCO_3$

Zero-point correction= 0.026809
Thermal correction to Energy= 0.032722
Thermal correction to Enthalpy= 0.033667
Thermal correction to Gibbs Free Energy= -0.006847
Sum of electronic and zero-point Energies= -284.350996
Sum of electronic and thermal Energies= -284.345083
Sum of electronic and thermal Enthalpies= -284.344138
Sum of electronic and thermal Free Energies= -284.384652

Cartesian coordinates

C	-2.186600	0.038482	-0.000113
O	-1.673959	-1.111682	-0.000314
O	-1.640693	1.161686	-0.000284
Cs	1.313577	-0.006001	0.000038
O	-3.595429	0.070499	0.000374
H	-3.846501	-0.864864	0.000375

Vibrational frequencies

25.6681	74.0802	99.7716
545.9308	557.5490	639.7374
815.7054	891.5015	1208.4465
1345.0049	1784.5957	3779.8733

HCO_3^-

Zero-point correction= 0.026308
Thermal correction to Energy= 0.029839
Thermal correction to Enthalpy= 0.030783

Thermal correction to Gibbs Free Energy= 0.000530
Sum of electronic and zero-point Energies= -264.487782
Sum of electronic and thermal Energies= -264.484251
Sum of electronic and thermal Enthalpies= -264.483307
Sum of electronic and thermal Free Energies= -264.513560

Cartesian coordinates

C	-0.150205	0.064265	0.000115
O	0.068386	1.299167	-0.000029
O	1.034792	-0.747755	-0.000003
O	-1.208426	-0.588628	-0.000052
H	1.743218	-0.087871	-0.000014

Vibrational frequencies

523.9329	543.3730	637.0283
819.0375	893.7573	1187.0496
1342.4811	1821.3688	3779.8826

H_2CO_3

Zero-point correction= 0.039118
Thermal correction to Energy= 0.042910
Thermal correction to Enthalpy= 0.043854
Thermal correction to Gibbs Free Energy= 0.013171
Sum of electronic and zero-point Energies= -264.974277
Sum of electronic and thermal Energies= -264.970485
Sum of electronic and thermal Enthalpies= -264.969541
Sum of electronic and thermal Free Energies= -265.000224

Cartesian coordinates

C	0.053089	-0.128825	-0.000006
O	0.716444	-1.136862	-0.000076
O	0.541772	1.130235	0.000015
O	-1.285182	-0.128196	0.000057
H	1.512220	1.065033	-0.000036
H	-1.615032	0.786497	0.000107

Vibrational frequencies

451.9648	545.5470	548.0016
614.1027	778.8671	996.7891
1174.6172	1259.5765	1433.3825
1889.5812	3736.5079	3741.8096

Cl^-

Zero-point correction= 0.000000

Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and zero-point Energies= -460.349322
Sum of electronic and thermal Energies= -460.347906
Sum of electronic and thermal Enthalpies= -460.346962
Sum of electronic and thermal Free Energies= -460.364345

Cartesian coordinates

Cl	0.000000	0.000000	0.000000

HCl

Zero-point correction= 0.006625
Thermal correction to Energy= 0.008985
Thermal correction to Enthalpy= 0.009930
Thermal correction to Gibbs Free Energy= -0.011271
Sum of electronic and zero-point Energies= -460.799253
Sum of electronic and thermal Energies= -460.796893
Sum of electronic and thermal Enthalpies= -460.795948
Sum of electronic and thermal Free Energies= -460.817149

Cartesian coordinates

H	0.000000	0.000000	-1.220089
Cl	0.000000	0.000000	0.071770

Vibrational frequencies
2907.9813

$CsHCO_3$-THF

Zero-point correction= 0.144229
Thermal correction to Energy= 0.157364
Thermal correction to Enthalpy= 0.158308
Thermal correction to Gibbs Free Energy= 0.094035
Sum of electronic and zero-point Energies= -516.712722
Sum of electronic and thermal Energies= -516.699587
Sum of electronic and thermal Enthalpies= -516.698643
Sum of electronic and thermal Free Energies= -516.762916

Cartesian coordinates

C	-3.901775	0.359004	0.201894
O	-5.275499	0.653809	0.316104
O	-3.181064	1.304485	-0.212136
O	-3.591848	-0.805607	0.529078
Cs	-0.491888	-0.438748	-0.171094

H	-5.336991	1.576675	0.028960
O	2.693571	0.009914	-0.440459
C	3.578821	-0.949509	0.172477
C	3.285532	1.323252	-0.379522
C	4.912308	-0.228370	0.379464
H	3.152442	-1.273608	1.134249
H	3.655544	-1.826083	-0.480833
C	4.447983	1.217324	0.608428
H	3.640961	1.607969	-1.380823
H	2.517183	2.042269	-0.072157
H	5.524486	-0.291158	-0.527371
H	5.487259	-0.641258	1.212708
H	5.226433	1.962032	0.422167
H	4.088033	1.343308	1.636149

Vibrational frequencies

4.5893	9.7131	18.8838
34.8548	46.5429	48.3543
62.1451	84.7002	90.2314
99.6583	265.5480	545.6433
559.1397	583.0441	639.9477
674.5919	815.2259	854.2903
887.4327	891.1782	904.7916
917.7547	933.1092	977.1286
1036.6040	1080.0262	1171.8268
1189.1054	1192.2861	1208.6806

$CsHCO_3$-2THF

Zero-point correction= 0.262434
Thermal correction to Energy= 0.282445
Thermal correction to Enthalpy= 0.283390
Thermal correction to Gibbs Free Energy= 0.201932
Sum of electronic and zero-point Energies= -749.046686
Sum of electronic and thermal Energies= -749.026675
Sum of electronic and thermal Enthalpies= -749.025731
Sum of electronic and thermal Free Energies= -749.107188

Cartesian coordinates

C	-0.507590	3.698101	0.211281
O	-0.622917	5.074085	0.484374
O	-0.811689	3.356156	-0.961911
O	-0.118271	3.004598	1.173985
Cs	0.007826	0.365053	-0.527259
H	-0.930097	5.447059	-0.355091

O	-2.470188	-1.599813	0.120825
C	-3.202626	-1.507216	1.360072
C	-3.269305	-2.281413	-0.867082
C	-4.649270	-1.874678	1.027114
H	-2.770685	-2.208649	2.088967
H	-3.093062	-0.491659	1.756885
C	-4.459203	-2.882671	-0.116015
H	-3.602449	-1.556325	-1.624350
H	-2.647385	-3.034277	-1.365001
H	-5.194794	-0.993166	0.671962
H	-5.185119	-2.285943	1.886904
H	-5.341968	-2.993194	-0.751673
H	-4.199878	-3.869038	0.285110
O	2.847584	-1.113624	-0.007172
C	3.692402	-0.467941	0.969898
C	3.557491	-2.210695	-0.613218
C	4.918601	-1.368131	1.141083
H	3.976109	0.526440	0.596518
H	3.123124	-0.334410	1.897010
C	5.029129	-2.017754	-0.246308
H	3.170201	-3.161032	-0.216025
H	3.371931	-2.192311	-1.693198
H	4.730535	-2.131506	1.904422
H	5.810332	-0.806409	1.432292
H	5.587179	-2.958155	-0.245023
H	5.511694	-1.332146	-0.952247

Vibrational frequencies

13.2017	18.5141	21.6367
25.6688	31.6058	33.5783
46.1790	48.4040	50.3358
51.3938	60.7599	62.7865
71.2736	93.2829	101.8542
109.2927	115.0035	264.3250
265.8652	555.4498	560.9066
584.5450	585.4378	644.6637
678.7930	679.7985	819.2471
853.2542	853.4559	883.7848

CH_3OH-$CsCO_3^-$

Zero-point correction= 0.066370

Thermal correction to Energy= 0.075605

Thermal correction to Enthalpy= 0.076549

Thermal correction to Gibbs Free Energy= 0.028574

Sum of electronic and zero-point Energies= -399.501516
Sum of electronic and thermal Energies= -399.492282
Sum of electronic and thermal Enthalpies= -399.491338
Sum of electronic and thermal Free Energies= -399.539312

Cartesian coordinates

C	-4.038558	-1.323575	0.367032
H	-4.453241	-2.273079	-0.028404
H	-2.958720	-1.469399	0.537133
H	-4.516424	-1.194667	1.369540
O	-4.274223	-0.269834	-0.510439
H	-3.473551	0.409530	-0.336543
C	-1.226444	0.905020	0.046420
O	-0.255803	1.732501	0.252578
O	-2.455227	1.368795	-0.001024
O	-1.009457	-0.365248	-0.111249
Cs	2.017266	-0.230741	-0.019298

Vibrational frequencies

55.1820	75.7854	94.1098
111.3005	126.8261	141.2200
182.1378	207.5934	302.8454
673.8758	696.1075	855.1441
1057.5793	1106.0293	1164.4802
1197.7532	1203.6006	1365.2171
1479.3797	1501.1210	1511.3909
1534.5029	1673.7328	2104.4562
2803.4315	2908.4244	2999.7879

NHC+1a

Zero-point correction= 0.417948
Thermal correction to Energy= 0.444445
Thermal correction to Enthalpy= 0.445389
Thermal correction to Gibbs Free Energy= 0.356690
Sum of electronic and zero-point Energies= -1552.138497
Sum of electronic and thermal Energies= -1552.112000
Sum of electronic and thermal Enthalpies= -1552.111056
Sum of electronic and thermal Free Energies= -1552.199755

Cartesian coordinates

C	-1.195401	1.994819	-0.753424
C	0.818059	2.349198	0.428714
C	-0.051298	3.495891	0.841861
C	-1.455830	2.988906	0.403066

H	-1.176068	2.492148	-1.728861
H	-1.910548	1.174150	-0.788404
H	0.009520	3.717520	1.909322
H	0.238804	4.400272	0.294419
H	-1.922656	2.451082	1.233513
H	-2.121183	3.800905	0.104282
N	0.150407	1.510957	-0.431581
N	2.034623	1.935860	0.628379
N	2.079256	0.776365	-0.169038
C	0.939475	0.477344	-0.848671
C	3.308491	0.039638	-0.216381
C	4.053132	0.037636	-1.409361
C	3.753463	-0.629155	0.935872
C	5.246274	-0.690172	-1.438189
C	4.958288	-1.337460	0.857471
C	5.712588	-1.388400	-0.318574
H	5.831663	-0.702055	-2.354547
H	5.314151	-1.861391	1.741334
C	3.598788	0.814156	-2.619856
H	2.673628	0.404406	-3.036482
H	3.393239	1.859203	-2.362046
H	4.364518	0.799002	-3.399928
C	6.989765	-2.188957	-0.389882
H	6.809024	-3.177731	-0.830455
H	7.739376	-1.690999	-1.013597
H	7.421856	-2.346667	0.602815
C	2.985170	-0.568605	2.231177
H	3.058473	0.428456	2.679336
H	1.918542	-0.767694	2.095491
H	3.380632	-1.292383	2.949288
C	-4.290713	0.026622	0.863684
C	-3.068376	-0.268408	1.453333
C	-2.130750	-1.054927	0.765704
C	-2.432611	-1.546185	-0.511457
C	-3.658723	-1.249116	-1.100345
C	-4.593973	-0.457206	-0.419911
H	-5.018854	0.636007	1.391493
H	-2.815894	0.105508	2.440108
H	-1.697081	-2.141803	-1.044922
H	-3.893446	-1.625699	-2.091698
C	-0.806388	-1.328865	1.360858
O	-0.449584	-0.909232	2.451486
H	-0.133271	-1.952230	0.741250
C	-5.911530	-0.133971	-1.054088

H	-6.323200	0.809567	-0.696237
H	-5.856291	-0.125477	-2.142379
Cl	-7.185040	-1.410541	-0.639348

Vibrational frequencies

11.4950	12.6583	32.6812
35.7410	44.1802	49.0285
57.0576	58.8234	73.6008
75.3497	92.2634	107.7508
134.1607	152.5673	161.1111
163.3311	185.5740	195.0396
215.2551	227.3755	229.5412
242.0552	264.6692	273.7191
289.8418	339.7723	342.0106
356.2919	361.1745	385.8061

2a

Zero-point correction= 0.115149
Thermal correction to Energy= 0.124952
Thermal correction to Enthalpy= 0.125896
Thermal correction to Gibbs Free Energy= 0.078330
Sum of electronic and zero-point Energies= -682.519178
Sum of electronic and thermal Energies= -682.509376
Sum of electronic and thermal Enthalpies= -682.508431
Sum of electronic and thermal Free Energies= -682.555997

Cartesian coordinates

C	0.736751	0.809891	-0.000059
O	1.052564	1.985149	-0.000113
C	-0.657911	0.317543	0.000045
C	-1.682588	1.282043	0.000042
C	-0.991690	-1.049191	0.000083
C	-3.015373	0.889163	0.000095
H	-1.412370	2.332559	-0.000005
C	-2.329932	-1.435758	0.000134
H	-0.222558	-1.811408	0.000071
C	-3.340823	-0.471694	0.000145
H	-3.801240	1.638197	0.000095
H	-2.583843	-2.491117	0.000165
H	-4.382329	-0.779478	0.000183
C	1.884944	-0.238404	-0.000072
F	3.082170	0.356543	-0.000740
F	1.812754	-1.032952	1.091876
F	1.811917	-1.033758	-1.091369

Vibrational frequencies

30.8785	52.2094	142.1109
145.7335	238.0625	271.5474
315.8484	392.1102	408.4063
439.0737	479.5915	515.4782
599.2645	629.4449	674.4144
693.0187	725.5372	750.3147
812.7155	862.1626	950.4173
956.3121	997.4929	1014.3448
1023.5307	1057.9449	1123.9867
1156.3604	1191.1307	1200.0053

TS1

Zero-point correction= 0.418224
Thermal correction to Energy= 0.443576
Thermal correction to Enthalpy= 0.444520
Thermal correction to Gibbs Free Energy= 0.359597
Sum of electronic and zero-point Energies= -1552.128020
Sum of electronic and thermal Energies= -1552.102669
Sum of electronic and thermal Enthalpies= -1552.101725
Sum of electronic and thermal Free Energies= -1552.186647

Cartesian coordinates

C	-4.057365	0.467873	0.589151
C	-2.808004	0.698415	1.163188
C	-1.709685	-0.087832	0.805793
C	-1.881021	-1.122751	-0.122046
C	-3.126769	-1.356699	-0.695038
C	-4.229340	-0.559290	-0.348102
H	-4.908973	1.081284	0.873114
H	-2.664356	1.478560	1.904058
H	-1.028027	-1.739431	-0.396910
H	-3.254219	-2.162505	-1.413465
C	-0.365361	0.156335	1.462123
O	-0.245843	0.996996	2.385801
H	0.266108	-0.755176	1.450621
C	-5.569677	-0.815805	-0.955807
H	-6.196117	0.075670	-0.980744
H	-5.501746	-1.248365	-1.953785
Cl	-6.549462	-2.055821	0.029493
C	-0.506898	3.292004	-0.115188
C	1.734445	2.822170	-0.751242
C	1.594034	4.291507	-0.997453

C	0.297493	4.616734	-0.195090
H	-1.255034	3.199646	-0.907273
H	-0.980644	3.124987	0.852768
H	2.460176	4.862936	-0.659041
H	1.464401	4.479954	-2.069232
H	0.571207	4.930123	0.816092
H	-0.283268	5.418011	-0.654557
N	0.547185	2.295957	-0.312225
N	2.659555	1.904831	-0.817156
N	1.968560	0.759151	-0.390472
C	0.677925	0.973110	-0.074560
C	2.672421	-0.479778	-0.231877
C	2.738662	-1.366505	-1.317345
C	3.262770	-0.755379	1.009457
C	3.410250	-2.576153	-1.125924
C	3.923633	-1.981411	1.152101
C	4.004431	-2.900884	0.101285
H	3.474005	-3.280546	-1.951931
H	4.386912	-2.219289	2.106160
C	2.106088	-1.013524	-2.639170
H	1.019594	-0.906632	-2.546387
H	2.487419	-0.058079	-3.015819
H	2.308261	-1.783524	-3.387724
C	4.719643	-4.218633	0.271860
H	5.552173	-4.310485	-0.435375
H	5.121805	-4.331085	1.282500
H	4.045088	-5.061349	0.081091
C	3.190827	0.239698	2.140787
H	3.649265	1.191383	1.847995
H	2.156227	0.463707	2.426839
H	3.719244	-0.135584	3.020773

Vibrational frequencies

-186.5173	15.1717	24.0417
30.7036	35.3202	50.8432
54.6923	64.8433	69.2265
79.0997	89.6714	121.1212
126.9634	140.8436	157.3463
168.6054	182.8031	199.4157
214.8009	224.7500	232.8067
247.6196	253.9115	287.4458
329.1569	340.2808	350.0327
376.1183	391.6625	411.1733

M1

Zero-point correction= 0.420073
Thermal correction to Energy= 0.445169
Thermal correction to Enthalpy= 0.446113
Thermal correction to Gibbs Free Energy= 0.363391
Sum of electronic and zero-point Energies= -1552.137302
Sum of electronic and thermal Energies= -1552.112207
Sum of electronic and thermal Enthalpies= -1552.111263
Sum of electronic and thermal Free Energies= -1552.193984

Cartesian coordinates

C	3.785342	-0.650991	-1.500334
C	2.522173	-0.129805	-1.781673
C	1.413019	-0.519898	-1.031429
C	1.578796	-1.450399	0.002655
C	2.837955	-1.970067	0.289864
C	3.956370	-1.576972	-0.462801
H	4.646263	-0.344367	-2.089906
H	2.354342	0.576253	-2.589102
H	0.713402	-1.776182	0.577016
H	2.961077	-2.690258	1.095101
C	0.028354	0.065822	-1.392220
O	-0.017813	0.894592	-2.438893
H	-0.662484	-0.814177	-1.424402
C	5.306444	-2.139028	-0.160924
H	5.259331	-3.141844	0.263062
H	5.967268	-2.133643	-1.027372
Cl	6.208716	-1.130910	1.124031
C	1.217086	2.882522	-0.199278
C	-0.829856	2.715316	1.005922
C	-0.295245	4.054613	1.401534
C	0.794998	4.288049	0.309810
H	2.108297	2.493756	0.299398
H	1.337019	2.805896	-1.280586
H	-1.067412	4.825869	1.408712
H	0.139675	4.001385	2.405592
H	0.358443	4.852263	-0.518469
H	1.647029	4.850458	0.694088
N	0.053460	2.079540	0.179621
N	-1.909575	2.003635	1.189632
N	-1.665010	0.862027	0.422981
C	-0.478455	0.907079	-0.207871
C	-2.669525	-0.156151	0.306076
C	-3.494973	-0.150454	-0.828893

C	-2.782540	-1.105467	1.331153
C	-4.453464	-1.163887	-0.925711
C	-3.760681	-2.093647	1.188587
C	-4.601315	-2.138285	0.069165
H	-5.101662	-1.189047	-1.797863
H	-3.865384	-2.845890	1.966440
C	-3.346051	0.909351	-1.891135
H	-3.526955	1.904563	-1.466449
H	-2.331586	0.925496	-2.314410
H	-4.064754	0.750425	-2.699153
C	-5.666802	-3.199945	-0.048037
H	-6.596734	-2.873095	0.434264
H	-5.901187	-3.418052	-1.094224
H	-5.359516	-4.131498	0.437033
C	-1.873559	-1.055460	2.532622
H	-0.818645	-1.097059	2.238064
H	-2.009588	-0.121967	3.089709
H	-2.072447	-1.890739	3.207963

Vibrational frequencies

19.5770	29.0249	38.4944
42.9306	53.2836	68.5545
80.5914	82.2633	95.3167
117.4087	130.8648	135.8912
159.4851	168.9373	181.3258
187.9455	212.2574	217.2076
229.3319	240.2981	256.2348
265.6872	289.4437	309.4433
339.4272	346.0061	356.8130
380.7570	402.4984	423.9611

TS2

Zero-point correction= 0.444879
Thermal correction to Energy= 0.475781
Thermal correction to Enthalpy= 0.476725
Thermal correction to Gibbs Free Energy= 0.378966
Sum of electronic and zero-point Energies= -1836.481332
Sum of electronic and thermal Energies= -1836.450430
Sum of electronic and thermal Enthalpies= -1836.449486
Sum of electronic and thermal Free Energies= -1836.547245

Cartesian coordinates

C	-1.136367	0.175431	0.115045
O	-0.287844	-0.289893	1.133615

H	-0.634688	-0.245915	-0.942313
C	1.073277	-1.584003	-1.515223
O	0.088677	-0.842979	-1.995502
O	1.094812	-1.833941	-0.226269
H	0.322372	-0.982340	0.617711
O	1.969964	-2.031823	-2.283425
Cs	4.109528	-2.384619	-0.023855
C	-2.537696	-0.387106	0.193171
C	-3.244919	-0.699336	-0.976651
C	-3.138651	-0.645987	1.434388
C	-4.539816	-1.212876	-0.909190
H	-2.766228	-0.546249	-1.939721
C	-4.431451	-1.156316	1.504097
H	-2.573122	-0.441156	2.338063
C	-5.151623	-1.437631	0.331147
H	-5.077911	-1.452277	-1.823179
H	-4.893537	-1.341680	2.471134
C	-6.538778	-1.985106	0.407150
H	-7.069300	-1.658518	1.301690
H	-7.129727	-1.755237	-0.479394
Cl	-6.552565	-3.846465	0.511335
C	-1.072589	1.628422	-0.017900
N	-2.041674	2.516235	-0.366895
N	0.051154	2.392077	0.054952
C	-3.488532	2.513570	-0.637950
C	-1.470557	3.755224	-0.508057
N	-0.196465	3.729839	-0.251791
C	1.413367	2.022271	0.337301
C	-3.815596	4.027853	-0.596177
H	-3.666925	2.065582	-1.618785
H	-4.020297	1.935844	0.116068
C	-2.488064	4.767277	-0.925455
C	2.285159	1.831772	-0.744210
C	1.841570	1.973905	1.673407
H	-4.140764	4.296545	0.412745
H	-4.616959	4.281641	-1.291732
H	-2.379110	5.715926	-0.396427
H	-2.390612	4.965579	-1.998715
C	3.632326	1.578495	-0.451062
C	1.791899	1.875768	-2.166571
C	3.191303	1.706468	1.913406
C	0.867327	2.171905	2.802816
C	4.102268	1.515068	0.864517
H	4.326045	1.431790	-1.275874

H	1.128467	1.020148	-2.357630
H	1.234813	2.797660	-2.365722
H	2.630366	1.828298	-2.867177
H	3.543763	1.661517	2.941496
H	0.279466	3.086858	2.668393
H	0.171746	1.326462	2.822217
H	1.384687	2.235563	3.763849
C	5.562957	1.266447	1.158163
H	5.693293	0.535134	1.963719
H	6.098063	0.907282	0.273716
H	6.058804	2.188397	1.487002

Vibrational frequencies

-432.8085	17.2917	18.5914
28.9559	35.8845	42.6592
47.7422	53.4261	69.3083
69.5673	81.0051	87.9537
92.0052	97.2781	113.4613
129.9103	132.1261	148.3701
156.2669	160.6720	183.3009
192.0998	207.4282	214.9359
228.5187	236.4135	247.9165
249.9562	268.4902	278.8153

TS2'

Zero-point correction= 0.561390
Thermal correction to Energy= 0.600158
Thermal correction to Enthalpy= 0.601102
Thermal correction to Gibbs Free Energy= 0.478793
Sum of electronic and zero-point Energies= -2068.754251
Sum of electronic and thermal Energies= -2068.715483
Sum of electronic and thermal Enthalpies= -2068.714539
Sum of electronic and thermal Free Energies= -2068.836848

Cartesian coordinates

C	2.241008	-0.094059	0.057142
O	1.248464	-0.143978	1.050329
H	1.615280	0.086987	-1.003674
C	-0.454795	0.795333	-1.583235
O	0.714766	0.387700	-2.053287
O	-0.643519	0.795019	-0.285220
H	0.407330	0.246205	0.549336
O	-1.362525	1.169773	-2.378393
Cs	-3.716698	1.061518	-0.423225

C	3.174470	1.095066	0.216636
C	3.524706	1.879322	-0.892348
C	3.637553	1.485155	1.484115
C	4.348028	2.996624	-0.746203
H	3.122143	1.620921	-1.867395
C	4.460907	2.597700	1.631827
H	3.339755	0.908821	2.354840
C	4.831732	3.366187	0.515500
H	4.606728	3.595727	-1.616217
H	4.819596	2.880274	2.619096
C	5.718893	4.558283	0.670864
H	6.403741	4.465800	1.513192
H	6.276243	4.784950	-0.237292
Cl	4.762977	6.116711	1.027335
C	2.896628	-1.389533	-0.111593
N	4.147902	-1.673340	-0.567849
N	2.310736	-2.615195	0.005346
C	5.375322	-0.949829	-0.941474
C	4.256713	-3.030980	-0.728007
N	3.166048	-3.646569	-0.382803
C	0.977798	-2.993653	0.409332
C	6.412495	-2.100794	-0.994438
H	5.227844	-0.465444	-1.910712
H	5.619136	-0.191707	-0.199496
C	5.606040	-3.403751	-1.253287
C	0.015658	-3.213196	-0.587375
C	0.720568	-3.233967	1.769907
H	6.919545	-2.172183	-0.028254
H	7.167774	-1.920737	-1.760981
H	6.026333	-4.276470	-0.749585
H	5.537981	-3.632981	-2.322765
C	-1.243444	-3.678372	-0.181384
C	0.308525	-2.948441	-2.042128
C	-0.548548	-3.697931	2.120964
C	1.763781	-2.960867	2.820455
C	-1.544260	-3.926838	1.160508
H	-2.001425	-3.856743	-0.940560
H	0.466395	-1.874465	-2.217482
H	1.207608	-3.480931	-2.372485
H	-0.526481	-3.279262	-2.666334
H	-0.764588	-3.887802	3.170048
H	2.717951	-3.444217	2.583430
H	1.943084	-1.882162	2.885580
H	1.435142	-3.318378	3.799974

C	-2.901188	-4.445571	1.573702
H	-3.375674	-3.783389	2.307526
H	-3.573480	-4.535535	0.715502
H	-2.822534	-5.434011	2.042111
O	-6.930572	1.262702	0.088969
C	-7.931494	1.487600	-0.923786
C	-7.569678	0.977213	1.349736
C	-9.252735	0.995254	-0.332024
H	-7.976434	2.561584	-1.157766
H	-7.635791	0.952569	-1.833297
C	-9.054556	1.296026	1.160934
H	-7.418175	-0.083723	1.597364
H	-7.094229	1.580931	2.131396
H	-9.366093	-0.082941	-0.493054
H	-10.119842	1.499703	-0.766989
H	-9.696328	0.699679	1.815166
H	-9.247245	2.355481	1.364342

Vibrational frequencies

-474.0829	9.6687	12.9705
14.0726	17.4290	23.7302
28.2872	31.0699	37.8242
40.3134	42.0511	44.0600
49.1381	54.1727	56.2533
61.2031	64.4221	69.9280
73.2055	86.5455	92.1998
98.8985	115.3637	128.6826
136.3569	146.5387	154.3294
173.5664	181.9723	196.1513

TS2''

Zero-point correction= 0.679659
Thermal correction to Energy= 0.725211
Thermal correction to Enthalpy= 0.726155
Thermal correction to Gibbs Free Energy= 0.585588
Sum of electronic and zero-point Energies= -2301.103759
Sum of electronic and thermal Energies= -2301.058207
Sum of electronic and thermal Enthalpies= -2301.057263
Sum of electronic and thermal Free Energies= -2301.197830

Cartesian coordinates

C	2.730910	-0.201010	-0.043028
O	1.785353	0.054647	0.965143
H	2.060559	-0.251753	-1.097273

C	-0.010996	0.363320	-1.750056
O	1.128861	-0.183210	-2.149569
O	-0.126331	0.728005	-0.496389
H	0.940850	0.354860	0.412432
O	-0.961035	0.515841	-2.568733
Cs	-3.222399	0.541651	-0.493450
C	3.730683	0.931291	-0.213049
C	4.061641	1.403802	-1.491197
C	4.287731	1.577376	0.903237
C	4.958898	2.460778	-1.653177
H	3.590856	0.949056	-2.357974
C	5.185980	2.628503	0.743976
H	4.006654	1.248632	1.899249
C	5.540666	3.078822	-0.538823
H	5.204431	2.813930	-2.652027
H	5.620624	3.108266	1.618092
C	6.522521	4.192337	-0.710287
H	7.257667	4.228447	0.093099
H	7.028648	4.156781	-1.674228
Cl	5.716435	5.870368	-0.672286
C	3.315834	-1.532296	0.094956
N	4.531735	-1.991043	-0.314315
N	2.683666	-2.654118	0.543232
C	5.763745	-1.456050	-0.919313
C	4.574719	-3.347818	-0.120050
N	3.475318	-3.795439	0.408085
C	1.349940	-2.844809	1.058201
C	6.745899	-2.641208	-0.732698
H	5.576571	-1.221715	-1.970850
H	6.085329	-0.551937	-0.405456
C	5.870237	-3.918293	-0.602147
C	0.346539	-3.260078	0.170467
C	1.126485	-2.713828	2.439428
H	7.315050	-2.494061	0.189323
H	7.453050	-2.705017	-1.561267
H	6.289006	-4.657398	0.083551
H	5.717705	-4.407533	-1.570942
C	-0.919440	-3.536213	0.707259
C	0.599124	-3.384180	-1.310671
C	-0.151889	-2.999528	2.922693
C	2.215908	-2.239115	3.363672
C	-1.188361	-3.412413	2.073267
H	-1.708678	-3.865045	0.034937
H	0.780949	-2.395743	-1.757438

H	1.469798	-4.015606	-1.519117
H	-0.265911	-3.831799	-1.808566
H	-0.342132	-2.901411	3.989238
H	3.139303	-2.814697	3.236698
H	2.444246	-1.189901	3.146906
H	1.904220	-2.319638	4.408497
C	-2.558493	-3.717746	2.630746
H	-3.014848	-2.825484	3.076760
H	-3.234246	-4.086668	1.853538
H	-2.508402	-4.476806	3.420111
O	-4.464901	2.350670	1.890486
C	-4.155025	2.204904	3.292111
C	-4.817297	3.719291	1.611900
C	-4.151390	3.617118	3.886437
H	-4.924757	1.574850	3.760075
H	-3.189464	1.695039	3.392750
C	-5.135152	4.354094	2.964990
H	-3.970109	4.227239	1.126253
H	-5.663069	3.723636	0.915512
H	-3.153511	4.063089	3.809547
H	-4.448793	3.626567	4.938674
H	-4.999444	5.439139	2.961851
H	-6.169689	4.136139	3.254454
O	-6.139435	-0.363406	-1.628640
C	-7.031549	-1.451288	-1.315305
C	-6.541869	0.253722	-2.868962
C	-8.235240	-1.295681	-2.245693
H	-6.514449	-2.406621	-1.490140
H	-7.292869	-1.394402	-0.252577
C	-7.585700	-0.675475	-3.491706
H	-6.967764	1.245088	-2.656336
H	-5.656213	0.390417	-3.499990
H	-8.966225	-0.603670	-1.811918
H	-8.738066	-2.246549	-2.442454
H	-8.292016	-0.139917	-4.131944
H	-7.097819	-1.451032	-4.092874

Vibrational frequencies

-542.9801	7.5428	11.2288
12.0117	14.0019	15.8210
20.7005	22.4577	28.2721
31.9887	35.4730	37.3518
42.9635	44.2690	49.1167
53.0229	54.9506	56.1412

61.8562	64.5196	68.5515
68.8146	72.6633	77.0267
80.9383	90.2705	108.7164
109.0862	110.7490	116.0724

TS2'''

Zero-point correction= 0.442460
Thermal correction to Energy= 0.471243
Thermal correction to Enthalpy= 0.472187
Thermal correction to Gibbs Free Energy= 0.381264
Sum of electronic and zero-point Energies= -1816.636101
Sum of electronic and thermal Energies= -1816.607318
Sum of electronic and thermal Enthalpies= -1816.606374
Sum of electronic and thermal Free Energies= -1816.697297

Cartesian coordinates

C	-3.693564	-1.630164	1.268011
C	-2.344196	-1.295722	1.314203
C	-1.698828	-0.739695	0.197230
C	-2.438859	-0.600875	-0.992540
C	-3.788364	-0.934134	-1.041526
C	-4.438710	-1.449495	0.091210
H	-4.182585	-2.039235	2.149717
H	-1.746278	-1.458388	2.204942
H	-1.940374	-0.241483	-1.889121
H	-4.344550	-0.813134	-1.968529
C	-0.221331	-0.450000	0.261607
O	0.462873	-1.065613	1.280203
H	0.242261	-1.011190	-0.801968
C	-5.882715	-1.798456	0.043162
H	-6.223306	-2.074397	-0.954406
H	-6.161041	-2.568755	0.761555
C	-2.016336	2.420527	-0.358311
C	0.247624	3.100658	-0.510696
C	-0.526466	4.336564	-0.839929
C	-1.931195	3.965411	-0.289529
H	-2.455895	2.066419	-1.293841
H	-2.563801	1.977200	0.472471
H	-0.105702	5.233953	-0.382951
H	-0.547248	4.485750	-1.925660
H	-2.008202	4.284415	0.753762
H	-2.739397	4.437014	-0.851075
N	-0.597504	2.039316	-0.303755
N	1.490637	2.777316	-0.320924

N	1.428688	1.423323	0.016430
C	0.147471	0.942836	0.031507
C	2.665342	0.730715	0.247472
C	3.426904	0.338642	-0.863024
C	3.104893	0.544450	1.566385
C	4.650211	-0.295407	-0.619755
C	4.331659	-0.095627	1.756879
C	5.112303	-0.531193	0.678484
H	5.249966	-0.618467	-1.467026
H	4.684739	-0.261169	2.772041
C	2.933465	0.558546	-2.269222
H	2.083110	-0.106699	-2.459885
H	2.611907	1.593330	-2.426827
H	3.719249	0.329700	-2.994693
C	6.409159	-1.266218	0.912957
H	6.238892	-2.349760	0.946406
H	7.129974	-1.077109	0.110985
H	6.869515	-0.978169	1.863410
C	2.254144	0.976848	2.728269
H	1.948296	2.025661	2.636260
H	1.351797	0.352761	2.725313
H	2.786943	0.856589	3.675926
C	1.677590	-2.689368	-1.256565
O	0.839860	-1.793374	-1.731839
O	1.760886	-2.819861	0.075841
O	2.366999	-3.414988	-1.987857
H	1.200384	-2.085398	0.605749
Cl	-6.981032	-0.336558	0.503925

Vibrational frequencies

-905.5524	19.5976	23.2874
32.8518	37.7808	45.8216
53.1937	60.0626	73.6878
79.4579	103.1103	113.7348
131.5156	135.1914	150.4052
155.6828	167.3858	177.9634
183.5995	199.8941	207.0704
225.3021	235.0553	241.1515
250.8374	253.7244	269.1843
282.3170	286.7705	319.7285

M2

Zero-point correction= 0.418976

Thermal correction to Energy= 0.444809

Thermal correction to Enthalpy= 0.445753
Thermal correction to Gibbs Free Energy= 0.361593
Sum of electronic and zero-point Energies= -1552.144895
Sum of electronic and thermal Energies= -1552.119063
Sum of electronic and thermal Enthalpies= -1552.118119
Sum of electronic and thermal Free Energies= -1552.202279

Cartesian coordinates

C	-1.330071	2.647167	-0.163353
C	0.972766	2.865780	0.264703
C	0.474536	4.278470	0.236939
C	-1.060712	4.080904	0.346763
H	-1.468918	2.603471	-1.250644
H	-2.193851	2.182967	0.309972
H	0.887803	4.894366	1.038885
H	0.755119	4.740220	-0.715930
H	-1.366948	4.150535	1.394481
H	-1.621431	4.824536	-0.221828
N	-0.077602	1.975551	0.198327
N	2.132724	2.299362	0.197909
N	1.828950	0.929533	0.060042
C	0.450942	0.703117	-0.001369
C	2.898873	-0.011390	0.066763
C	3.824869	0.013633	-0.993071
C	3.020942	-0.923756	1.130294
C	4.884609	-0.897563	-0.964624
C	4.089749	-1.824824	1.105793
C	5.030015	-1.829014	0.070070
H	5.607085	-0.887373	-1.777292
H	4.192957	-2.536303	1.921771
C	3.677915	0.989178	-2.133386
H	2.653061	0.996946	-2.520693
H	3.896342	2.012887	-1.812010
H	4.353990	0.734487	-2.953758
C	6.157066	-2.832548	0.052603
H	5.859804	-3.746520	-0.477501
H	7.040405	-2.434933	-0.456760
H	6.449245	-3.126290	1.065684
C	2.031580	-0.931138	2.264427
H	1.840679	0.083421	2.629713
H	1.069154	-1.343482	1.941233
H	2.398463	-1.534841	3.098510
C	-0.191844	-0.480721	-0.296059
O	0.572017	-1.558448	-0.765632

H	1.155189	-1.248413	-1.473406
C	-1.594344	-0.771433	-0.096248
C	-2.234211	-1.752885	-0.894386
C	-2.365632	-0.171447	0.930903
C	-3.576488	-2.054438	-0.722810
H	-1.654461	-2.264522	-1.654759
C	-3.712311	-0.472100	1.089139
H	-1.885389	0.500704	1.634666
C	-4.347159	-1.413343	0.263459
H	-4.044926	-2.796448	-1.365452
H	-4.278107	0.007931	1.884235
C	-5.788361	-1.724627	0.428421
H	-6.150466	-1.552221	1.441462
H	-6.049794	-2.730532	0.101722
Cl	-6.887414	-0.612721	-0.633002

Vibrational frequencies

20.0443	27.9588	35.9686
42.8577	48.4741	60.9455
78.6680	91.9898	105.9002
121.8185	129.2216	131.3421
151.1736	152.7046	180.9586
188.0118	190.9989	224.1022
232.2472	237.5749	248.2262
259.2872	282.2248	286.9469
318.6552	337.2995	345.8413
357.5594	368.8287	388.2658

TS3

Zero-point correction= 0.446411
Thermal correction to Energy= 0.476081
Thermal correction to Enthalpy= 0.477025
Thermal correction to Gibbs Free Energy= 0.382231
Sum of electronic and zero-point Energies= -1816.663097
Sum of electronic and thermal Energies= -1816.633427
Sum of electronic and thermal Enthalpies= -1816.632483
Sum of electronic and thermal Free Energies= -1816.727277

Cartesian coordinates

C	-1.482013	2.544462	-1.344773
C	0.772231	3.110872	-0.946310
C	0.236952	4.283184	-1.708166
C	-1.296832	4.056063	-1.612332
H	-1.537223	1.950890	-2.263641

H	-2.356092	2.321575	-0.734595
H	0.557816	5.243386	-1.298225
H	0.591550	4.225616	-2.742968
H	-1.700899	4.621661	-0.767839
H	-1.822734	4.370506	-2.515006
N	-0.230684	2.221023	-0.646683
N	1.950195	2.660519	-0.637904
N	1.693745	1.384586	-0.122634
C	0.349470	1.074440	-0.146445
C	2.779978	0.636316	0.434140
C	3.721562	0.063538	-0.434027
C	2.883858	0.523629	1.830450
C	4.788861	-0.639222	0.136445
C	3.961590	-0.196440	2.350638
C	4.924859	-0.782586	1.520513
H	5.525052	-1.095050	-0.521124
H	4.054552	-0.297325	3.429489
C	3.566575	0.148676	-1.930856
H	4.486202	-0.167581	-2.431358
H	2.756234	-0.511151	-2.264650
H	3.330432	1.165461	-2.257273
C	6.096817	-1.524880	2.115204
H	6.843765	-0.825997	2.512907
H	5.783549	-2.166422	2.945768
H	6.595242	-2.152032	1.370287
C	1.857615	1.149126	2.739227
H	2.176438	1.096871	3.783441
H	1.689429	2.201455	2.485460
H	0.892381	0.637291	2.653398
C	-0.237977	-0.159980	0.179229
O	0.593973	-1.251296	0.154972
H	0.846531	-1.481292	-0.844222
C	-1.599762	-0.321987	0.545942
C	-2.224515	-1.605078	0.424177
C	-2.386140	0.726667	1.128251
C	-3.534091	-1.797726	0.789700
H	-1.655349	-2.418328	-0.010701
C	-3.689868	0.519208	1.508136
H	-1.921300	1.686318	1.331559
C	-4.317332	-0.750034	1.355916
H	-3.994129	-2.772246	0.643221
H	-4.253572	1.330988	1.962254
C	-5.666996	-0.951512	1.728207
H	-6.128166	-0.238701	2.402350

C	0.689571	-3.263770	-2.220838
O	0.267302	-3.846308	-1.019519
O	1.013143	-2.021409	-2.154368
O	0.704831	-3.997421	-3.206339
H	0.314654	-3.165338	-0.325836
H	-6.029586	-1.969068	1.820744
Cl	-7.102237	-0.445923	0.037328

Vibrational frequencies

-188.6802	13.0185	21.6548
25.4881	32.5204	42.2792
50.5100	59.6948	61.3577
67.5004	71.0256	90.9976
94.0860	115.1629	126.7458
136.5881	138.3343	145.2787
175.2744	181.9695	188.1607
196.0954	207.4285	233.1405
239.4587	255.9889	272.1537
286.2399	291.8043	298.4024

TS3'

Zero-point correction= 0.418740
Thermal correction to Energy= 0.444006
Thermal correction to Enthalpy= 0.444950
Thermal correction to Gibbs Free Energy= 0.361961
Sum of electronic and zero-point Energies= -1552.137622
Sum of electronic and thermal Energies= -1552.112355
Sum of electronic and thermal Enthalpies= -1552.111411
Sum of electronic and thermal Free Energies= -1552.194400

Cartesian coordinates

C	-1.320648	2.699677	-0.288615
C	0.954178	2.889826	0.317291
C	0.448620	4.297163	0.362145
C	-1.090183	4.083703	0.358586
H	-1.390079	2.744327	-1.380217
H	-2.195536	2.181395	0.098547
H	0.805266	4.847610	1.234949
H	0.786520	4.830361	-0.532996
H	-1.460680	4.063323	1.387152
H	-1.619555	4.870146	-0.180643
N	-0.069980	2.008824	0.070490
N	2.115500	2.304576	0.331630
N	1.816748	0.968574	0.074905

C	0.473006	0.764625	-0.108235
C	2.874320	0.000789	0.085152
C	3.781733	-0.002644	-0.986004
C	2.973913	-0.890111	1.163847
C	4.813918	-0.943856	-0.956895
C	4.021313	-1.815542	1.143022
C	4.944862	-1.861511	0.092594
H	5.528047	-0.965300	-1.776029
H	4.117771	-2.515435	1.969054
C	3.644763	0.972125	-2.128415
H	2.649433	0.918538	-2.586229
H	3.779767	2.003862	-1.788040
H	4.384563	0.766804	-2.905567
C	6.041815	-2.896826	0.074750
H	5.710956	-3.802804	-0.448632
H	6.931997	-2.528309	-0.444121
H	6.331328	-3.193280	1.087454
C	1.988888	-0.850492	2.303218
H	1.859914	0.169200	2.681572
H	1.001854	-1.207708	1.987508
H	2.325533	-1.481669	3.129015
C	-0.166218	-0.443118	-0.477975
O	0.608062	-1.396871	-1.125942
H	1.112845	-0.978440	-1.839660
C	-1.488969	-0.792973	-0.160020
C	-2.125620	-1.890215	-0.837405
C	-2.236342	-0.152485	0.890478
C	-3.419268	-2.236321	-0.562307
H	-1.565884	-2.419727	-1.599351
C	-3.525765	-0.513474	1.166844
H	-1.749020	0.590342	1.512928
C	-4.184381	-1.561873	0.445757
H	-3.892749	-3.039305	-1.121579
H	-4.063819	-0.017750	1.970740
C	-5.507218	-1.898128	0.704501
H	-6.017119	-1.487992	1.566778
H	-5.944022	-2.782709	0.259181
Cl	-7.100471	-0.536141	-0.719255

Vibrational frequencies

-77.0411	13.9376	21.1605
38.7888	50.0697	54.4865
64.6200	83.5795	100.0484
117.4499	136.8281	140.8895

149.3508	164.7685	168.2871
186.7421	193.9236	199.8733
224.6143	236.8957	252.8183
265.6619	286.9581	288.3954
298.4164	312.9297	343.0490
355.7697	368.8470	381.5168

M3

Zero-point correction= 0.405688
Thermal correction to Energy= 0.429131
Thermal correction to Enthalpy= 0.430076
Thermal correction to Gibbs Free Energy= 0.352746
Sum of electronic and zero-point Energies= -1091.328916
Sum of electronic and thermal Energies= -1091.305473
Sum of electronic and thermal Enthalpies= -1091.304529
Sum of electronic and thermal Free Energies= -1091.381858

Cartesian coordinates

C	2.124022	2.695025	0.460889
C	-0.068919	2.934969	-0.430436
C	0.539391	4.290694	-0.598514
C	2.052137	3.987843	-0.389952
H	2.150889	2.889849	1.535945
H	2.948076	2.036401	0.190290
H	0.320752	4.735125	-1.570940
H	0.146858	4.959901	0.175026
H	2.523170	3.805164	-1.359285
H	2.575406	4.812464	0.094993
N	0.831644	2.069892	0.135080
N	-1.227044	2.358346	-0.614429
N	-1.030881	1.077891	-0.123541
C	0.215474	0.892852	0.341314
C	-2.085219	0.102054	-0.195024
C	-3.029904	0.072340	0.838903
C	-2.120174	-0.763455	-1.295680
C	-4.055483	-0.870571	0.740061
C	-3.166520	-1.689196	-1.346567
C	-4.137174	-1.758646	-0.340190
H	-4.803317	-0.916936	1.527442
H	-3.220683	-2.372888	-2.189577
C	-2.910079	1.007286	2.011593
H	-1.967541	0.809805	2.533989
H	-2.901857	2.054424	1.689069
H	-3.738282	0.870137	2.710810

C	-5.236036	-2.790261	-0.401850
H	-4.932303	-3.711119	0.111771
H	-6.148385	-2.432509	0.085030
H	-5.478097	-3.057583	-1.434884
C	-1.065275	-0.703703	-2.370508
H	-0.944246	0.314390	-2.756647
H	-0.091460	-1.022880	-1.981251
H	-1.323627	-1.357963	-3.206366
C	0.710348	-0.318664	1.093417
O	0.004804	-0.629568	2.087147
C	1.892469	-0.935891	0.630560
C	2.461642	-2.022811	1.384509
C	2.571621	-0.575331	-0.586768
C	3.598646	-2.657045	0.991784
H	1.951049	-2.319459	2.296424
C	3.709436	-1.205326	-0.992928
H	2.157143	0.206708	-1.219112
C	4.314774	-2.289324	-0.226616
H	4.003385	-3.468056	1.593810
H	4.187789	-0.909771	-1.924081
C	5.461142	-2.916069	-0.620192
H	5.978420	-2.630545	-1.531878
H	5.894485	-3.721666	-0.034350

Vibrational frequencies

22.7708	42.3915	48.1417
60.3891	67.4569	71.9662
98.3131	98.8996	127.1366
140.4817	161.7827	167.6375
182.3790	195.9988	214.9275
230.1102	234.3548	242.2216
251.8885	265.8553	287.4867
292.2979	327.4077	339.4978
374.7864	384.3854	417.5706
433.0253	457.4596	487.0702

M3'

Zero-point correction= 0.418528
Thermal correction to Energy= 0.444073
Thermal correction to Enthalpy= 0.445017
Thermal correction to Gibbs Free Energy= 0.362826
Sum of electronic and zero-point Energies= -1552.164393
Sum of electronic and thermal Energies= -1552.138848
Sum of electronic and thermal Enthalpies= -1552.137904

Sum of electronic and thermal Free Energies= -1552.220095

Cartesian coordinates

C	-2.529478	2.648019	-0.707221
C	-0.398362	3.264202	0.140861
C	-1.167450	4.545637	0.131507
C	-2.628711	4.035804	-0.029064
H	-2.541668	2.700820	-1.798953
H	-3.285565	1.941063	-0.369517
H	-1.014803	5.136378	1.036382
H	-0.849268	5.149637	-0.725279
H	-3.085042	3.920742	0.957533
H	-3.244109	4.719914	-0.613997
N	-1.182648	2.223278	-0.282911
N	0.830178	2.875494	0.363144
N	0.809643	1.530549	0.053257
C	-0.409902	1.119506	-0.351045
C	1.966453	0.705559	0.287513
C	2.951041	0.637020	-0.706443
C	2.043570	0.002966	1.497280
C	4.054404	-0.180228	-0.455442
C	3.169210	-0.800186	1.698379
C	4.176418	-0.909907	0.733128
H	4.829939	-0.259349	-1.212789
H	3.253017	-1.361055	2.625256
C	2.796451	1.383323	-2.004507
H	3.707952	1.318043	-2.602954
H	1.972512	0.951609	-2.582909
H	2.568402	2.441549	-1.838488
C	5.346787	-1.836423	0.942953
H	5.144873	-2.809071	0.477474
H	6.260372	-1.440474	0.488602
H	5.536945	-2.013579	2.005545
C	0.949210	0.096943	2.529414
H	1.239969	-0.412902	3.450537
H	0.716884	1.139159	2.774863
H	0.026982	-0.371049	2.165793
C	-0.742282	-0.225785	-0.813445
O	0.151374	-0.688017	-1.704531
H	0.471146	-1.637200	-1.478860
C	-1.860928	-0.903374	-0.376736
C	-2.230195	-2.171470	-0.981027
C	-2.691908	-0.428942	0.718014
C	-3.330785	-2.849383	-0.581222

H	-1.603156	-2.563177	-1.772883
C	-3.786637	-1.114489	1.123017
H	-2.406138	0.472346	1.251040
C	-4.191963	-2.364721	0.491278
H	-3.597635	-3.784585	-1.066075
H	-4.380276	-0.747177	1.955796
C	-5.302274	-3.038333	0.884526
H	-5.936063	-2.667925	1.684875
H	-5.593144	-3.971174	0.410713
Cl	1.194157	-3.320477	-1.032364

Vibrational frequencies

30.3223	40.0046	48.7058
51.4905	61.3325	70.6973
80.6742	86.8085	105.4288
108.8750	127.4425	135.1077
143.9382	153.6747	172.1416
193.5119	214.6832	221.7806
238.6072	239.1150	253.3097
263.5750	283.4247	292.3701
293.1318	340.4449	350.7184
374.1454	384.7930	415.6094

ε-TS4

Zero-point correction= 0.522397
Thermal correction to Energy= 0.556182
Thermal correction to Enthalpy= 0.557126
Thermal correction to Gibbs Free Energy= 0.455034
Sum of electronic and zero-point Energies= -1773.856514
Sum of electronic and thermal Energies= -1773.822730
Sum of electronic and thermal Enthalpies= -1773.821785
Sum of electronic and thermal Free Energies= -1773.923878

Cartesian coordinates

C	0.648336	2.647858	-0.498167
C	2.874563	2.806412	0.330617
C	2.340000	4.197287	0.451738
C	0.808545	3.959089	0.308057
H	0.618122	2.810121	-1.578344
H	-0.206242	2.043290	-0.198477
H	2.615691	4.675174	1.393125
H	2.735115	4.808380	-0.367212
H	0.365757	3.826477	1.298679
H	0.305189	4.791183	-0.184793

N	1.917925	1.965244	-0.174354
N	4.003982	2.173981	0.524585
N	3.732413	0.885930	0.105676
C	2.470009	0.750865	-0.322244
C	4.735513	-0.143086	0.202871
C	5.642820	-0.277709	-0.855003
C	4.760993	-0.944676	1.352160
C	6.618300	-1.270862	-0.734384
C	5.754021	-1.925028	1.420182
C	6.685243	-2.103742	0.388946
H	7.335589	-1.400907	-1.540333
H	5.801046	-2.562643	2.299038
C	5.539346	0.598920	-2.074087
H	4.586183	0.414773	-2.582342
H	5.573988	1.661050	-1.808028
H	6.351976	0.393302	-2.774241
C	7.719214	-3.197850	0.476729
H	8.083833	-3.322074	1.501210
H	7.290609	-4.158822	0.166045
H	8.575770	-2.995023	-0.172431
C	3.758855	-0.756397	2.462104
H	3.739062	0.281920	2.810925
H	2.745231	-1.006288	2.128287
H	3.997360	-1.397530	3.313548
C	1.854845	-0.476155	-0.962494
O	2.484573	-0.963257	-1.910497
C	0.571156	-0.878810	-0.458882
C	-0.251703	-1.731924	-1.241926
C	0.062579	-0.415839	0.787672
C	-1.530636	-2.038590	-0.843890
H	0.138334	-2.100295	-2.185999
C	-1.207295	-0.739849	1.196030
H	0.684634	0.194737	1.436546
C	-2.075161	-1.526225	0.376875
H	-2.167056	-2.647445	-1.476998
H	-1.581509	-0.366950	2.144455
C	-3.453285	-1.667453	0.669594
H	-3.790162	-1.407430	1.669492
H	-3.976384	-2.508353	0.224030
C	-4.406418	-0.318540	-0.640686
C	-5.814792	-0.568050	-0.122134
C	-6.322383	-0.063073	1.085766
C	-6.647095	-1.367631	-0.918211
C	-7.629867	-0.350598	1.479439

H	-5.701542	0.554652	1.723492
C	-7.950291	-1.662658	-0.520042
H	-6.246345	-1.743504	-1.853685
C	-8.449406	-1.153638	0.681811
H	-8.008382	0.052533	2.415072
H	-8.579747	-2.285224	-1.150596
H	-9.465641	-1.378819	0.993210
C	-3.770303	1.017409	-0.164749
F	-4.553691	2.066172	-0.545983
F	-2.561097	1.215679	-0.729971
F	-3.595852	1.157901	1.179557
O	-4.111972	-0.631353	-1.820704

Vibrational frequencies

-179.4986	14.4626	23.5150
24.5982	30.4806	40.9920
43.6609	55.3277	61.5258
70.3618	80.1812	87.8031
92.3138	107.2997	125.0842
130.7828	141.2616	147.8949
154.5491	168.0339	174.8062
179.7113	191.5662	198.1758
219.1446	237.7376	238.7983
253.2946	266.2868	275.2007

TS4'

Zero-point correction= 0.531373
Thermal correction to Energy= 0.567351
Thermal correction to Enthalpy= 0.568296
Thermal correction to Gibbs Free Energy= 0.459418
Sum of electronic and zero-point Energies= -2234.670899
Sum of electronic and thermal Energies= -2234.634920
Sum of electronic and thermal Enthalpies= -2234.633976
Sum of electronic and thermal Free Energies= -2234.742853

Cartesian coordinates

C	0.359335	2.866787	-0.709416
C	2.590187	3.210354	0.040925
C	2.004103	4.584096	-0.004731
C	0.481072	4.273381	-0.077337
H	0.320811	2.889067	-1.801390
H	-0.472991	2.277307	-0.329129
H	2.283319	5.186573	0.861307
H	2.357056	5.098539	-0.905150

H	0.064492	4.249066	0.933074
H	-0.065592	5.016797	-0.657886
N	1.655479	2.274157	-0.313713
N	3.749520	2.652513	0.289645
N	3.525034	1.313281	0.058427
C	2.256938	1.074537	-0.308035
C	4.554493	0.331590	0.295285
C	5.481050	0.082763	-0.725067
C	4.563745	-0.332492	1.529080
C	6.462128	-0.877963	-0.470655
C	5.564181	-1.287170	1.729260
C	6.516412	-1.573073	0.743881
H	7.193830	-1.095657	-1.243851
H	5.597131	-1.820287	2.675496
C	5.385334	0.787911	-2.051377
H	6.241680	0.546444	-2.685095
H	4.473511	0.474686	-2.572526
H	5.342447	1.875270	-1.930355
C	7.558669	-2.638446	0.972449
H	8.472822	-2.434375	0.407120
H	7.818621	-2.724223	2.031689
H	7.184009	-3.616891	0.646968
C	3.526741	-0.041035	2.583189
H	3.769524	-0.550427	3.518253
H	3.453431	1.032971	2.786772
H	2.535743	-0.384160	2.262771
C	1.704481	-0.257818	-0.697267
O	2.418732	-0.903454	-1.513024
C	0.436887	-0.636917	-0.178703
C	-0.316579	-1.650848	-0.837754
C	-0.139833	0.007253	0.957129
C	-1.597634	-1.938455	-0.439518
H	0.117303	-2.147773	-1.699106
C	-1.411636	-0.301424	1.364563
H	0.438589	0.734421	1.519335
C	-2.204953	-1.252674	0.656347
H	-2.191826	-2.660251	-0.987833
H	-1.843883	0.204174	2.221889
C	-3.602002	-1.397073	0.904702
H	-3.970157	-0.994553	1.845366
H	-4.036696	-2.359144	0.646461
C	-4.518602	-0.438662	-0.519905
C	-5.961088	-0.615603	-0.025988
C	-6.514838	0.055268	1.074924

C	-6.759714	-1.524685	-0.730771
C	-7.838603	-0.176036	1.452864
H	-5.918411	0.762974	1.638689
C	-8.079581	-1.763756	-0.348241
H	-6.319218	-2.028324	-1.584694
C	-8.626259	-1.088273	0.745907
H	-8.254663	0.356845	2.303854
H	-8.684329	-2.472888	-0.907553
H	-9.655284	-1.269202	1.044067
C	-3.989375	1.015885	-0.328420
F	-3.862102	1.440682	0.963904
F	-4.821079	1.906640	-0.931530
F	-2.774769	1.176503	-0.897997
O	-4.203205	-0.933462	-1.643749
H	2.583917	-2.372389	-1.247624
Cl	2.867150	-3.673993	-0.915916

Vibrational frequencies

-306.6613	13.9067	16.9684
21.8325	26.2530	29.1039
35.9773	47.5426	48.1379
52.3110	57.6184	65.8118
75.2779	78.5089	95.2928
101.8088	119.9281	134.1744
144.5292	150.1190	161.8300
176.3423	181.8662	190.7535
205.2916	209.7724	227.9318
232.8480	247.3378	251.2925

M4

Zero-point correction= 0.524153
Thermal correction to Energy= 0.557856
Thermal correction to Enthalpy= 0.558800
Thermal correction to Gibbs Free Energy= 0.457803
Sum of electronic and zero-point Energies= -1773.861047
Sum of electronic and thermal Energies= -1773.827344
Sum of electronic and thermal Enthalpies= -1773.826400
Sum of electronic and thermal Free Energies= -1773.927397

Cartesian coordinates

C	0.630482	2.571218	-0.516112
C	2.838803	2.779822	0.350739
C	2.266746	4.154926	0.474093
C	0.744975	3.880272	0.300966

H	0.614003	2.739787	-1.595446
H	-0.212919	1.943288	-0.233185
H	2.514481	4.630440	1.424368
H	2.662899	4.781657	-0.332500
H	0.287018	3.731242	1.282093
H	0.230711	4.702290	-0.197231
N	1.914722	1.917908	-0.177705
N	3.982315	2.175938	0.560613
N	3.758136	0.888252	0.122262
C	2.508225	0.724335	-0.329662
C	4.788926	-0.113389	0.228397
C	5.716111	-0.212969	-0.817184
C	4.819744	-0.920926	1.372570
C	6.716860	-1.178199	-0.688675
C	5.840933	-1.872322	1.448900
C	6.791392	-2.016904	0.431035
H	7.451481	-1.280178	-1.483050
H	5.893958	-2.512851	2.325006
C	5.612203	0.677092	-2.026579
H	4.673332	0.482294	-2.556950
H	5.620511	1.735945	-1.745656
H	6.440302	0.498148	-2.715649
C	7.861754	-3.074946	0.523217
H	7.535771	-3.997619	0.026984
H	8.785863	-2.752324	0.034172
H	8.090144	-3.325244	1.563304
C	3.799146	-0.769565	2.471468
H	3.736190	0.267279	2.819315
H	2.798853	-1.059210	2.129010
H	4.053444	-1.400351	3.325988
C	1.934476	-0.514815	-0.987008
O	2.596572	-1.023031	-1.885939
C	0.604735	-0.910828	-0.547741
C	-0.229233	-1.621883	-1.436258
C	0.104481	-0.532878	0.717455
C	-1.544877	-1.883618	-1.095535
H	0.162828	-1.906085	-2.407863
C	-1.203068	-0.827715	1.061753
H	0.738497	-0.008221	1.425850
C	-2.063032	-1.473668	0.153399
H	-2.220898	-2.349231	-1.802049
H	-1.589686	-0.515422	2.026919
C	-3.515192	-1.576444	0.420836
H	-3.733851	-1.449612	1.483766

H	-3.921876	-2.533663	0.086037
C	-4.358369	-0.509165	-0.504191
C	-5.835455	-0.638004	-0.001076
C	-6.263681	-0.366909	1.306949
C	-6.775672	-1.089220	-0.931273
C	-7.600725	-0.545010	1.670941
H	-5.555637	-0.004513	2.045260
C	-8.112312	-1.274003	-0.571761
H	-6.412160	-1.283204	-1.935735
C	-8.531070	-1.002410	0.733348
H	-7.916124	-0.326680	2.688438
H	-8.829144	-1.627124	-1.309508
H	-9.570598	-1.143478	1.017734
C	-3.853397	0.924993	-0.120909
F	-4.708546	1.892539	-0.540500
F	-2.654919	1.212037	-0.694433
F	-3.672137	1.145259	1.225267
O	-4.191152	-0.712190	-1.787967

Vibrational frequencies

17.8295	26.3481	27.4542
33.2527	48.5517	52.3209
58.3016	64.7226	74.4243
80.7151	88.1387	103.5097
108.1629	119.6101	124.3287
146.2339	153.9987	160.2028
168.2756	173.8911	177.9514
196.3178	204.5318	228.7453
238.7571	244.9652	249.7667
260.0695	270.5457	281.5144

M04

Zero-point correction= 0.593477
Thermal correction to Energy= 0.637499
Thermal correction to Enthalpy= 0.638443
Thermal correction to Gibbs Free Energy= 0.512668
Sum of electronic and zero-point Energies= -2173.398294
Sum of electronic and thermal Energies= -2173.354273
Sum of electronic and thermal Enthalpies= -2173.353328
Sum of electronic and thermal Free Energies= -2173.479103

Cartesian coordinates

C	1.301896	1.914294	-1.138070
C	3.573352	2.077442	-0.459518

C	3.115894	3.491664	-0.536077
C	1.813663	3.358683	-1.380186
H	0.863198	1.439956	-2.017509
H	0.616538	1.862070	-0.281439
H	2.826590	3.806171	0.481001
H	3.861953	4.162768	-0.965011
H	1.067674	4.076326	-1.034925
H	2.028813	3.509616	-2.442943
N	2.552508	1.221412	-0.772462
N	4.661218	1.414930	-0.145754
N	4.294107	0.094600	-0.274913
C	3.006353	-0.029717	-0.635243
C	5.276592	-0.941913	-0.073595
C	6.164930	-1.208522	-1.129826
C	5.323385	-1.613188	1.153071
C	7.145980	-2.175434	-0.915992
C	6.328737	-2.578235	1.313115
C	7.246528	-2.866363	0.301047
H	7.845070	-2.400868	-1.717720
H	6.389972	-3.112285	2.257979
C	6.027211	-0.505842	-2.454709
H	6.832590	-0.792414	-3.135370
H	5.072309	-0.775015	-2.920757
H	6.045388	0.582761	-2.340040
C	8.332254	-3.895933	0.497297
H	9.324947	-3.432108	0.453662
H	8.239271	-4.402251	1.462134
H	8.300735	-4.657565	-0.290354
C	4.318245	-1.352305	2.243273
H	3.423385	-1.968321	2.085092
H	4.730499	-1.624307	3.219170
H	3.978171	-0.312794	2.267982
C	2.322318	-1.331900	-0.978535
O	2.973011	-2.120115	-1.662866
C	0.953194	-1.540768	-0.516707
C	0.217891	-2.616261	-1.066425
C	0.351267	-0.713943	0.455274
C	-1.079461	-2.857845	-0.653362
H	0.687156	-3.239147	-1.821808
C	-0.959024	-0.960590	0.850394
H	0.893576	0.101369	0.928290
C	-1.691716	-2.035853	0.321260
H	-1.675090	-3.648532	-1.093999
H	-1.409993	-0.293538	1.578567

C	-3.104436	-2.299659	0.722366
H	-3.359253	-1.736194	1.623967
H	-3.241310	-3.364413	0.935225
C	-4.166908	-2.037118	-0.471140
C	-5.576218	-2.340562	0.150709
C	-6.113679	-1.717990	1.287837
C	-6.324753	-3.339697	-0.478049
C	-7.369200	-2.089276	1.778067
H	-5.559119	-0.933260	1.792504
C	-7.578307	-3.716895	0.008117
H	-5.875506	-3.796006	-1.355388
C	-8.106935	-3.091823	1.141141
H	-7.771170	-1.595841	2.660113
H	-8.145027	-4.496797	-0.495994
H	-9.082225	-3.381461	1.524454
C	-4.128027	-0.505422	-0.769063
F	-4.168650	0.310370	0.344723
F	-5.160325	-0.100173	-1.552823
F	-2.995739	-0.142719	-1.429094
O	-3.900266	-2.707442	-1.571619
C	1.629364	0.605341	3.367752
H	0.581145	0.937417	3.333441
H	1.637212	-0.496357	3.356342
H	2.053205	0.913588	4.345278
O	2.350839	1.114446	2.276551
H	1.969137	2.097012	2.126228
C	0.248142	3.401464	1.463356
O	-0.247923	4.475369	0.969998
O	1.474571	3.416592	1.954096
O	-0.402476	2.275535	1.458997
Cs	-2.577373	3.067208	-0.549423

Vibrational frequencies

19.7069	22.8296	25.8993
32.1404	36.4252	39.2951
40.2070	49.5659	55.9846
58.9950	60.3362	65.6942
67.8288	77.3586	79.8714
84.8761	92.6272	95.4779
100.1733	105.6835	110.0937
119.4801	125.2037	128.7237
147.1896	153.8414	163.9670
166.1507	170.5340	179.3785

TS5

Zero-point correction= 0.588962
Thermal correction to Energy= 0.632867
Thermal correction to Enthalpy= 0.633811
Thermal correction to Gibbs Free Energy= 0.507348
Sum of electronic and zero-point Energies= -2173.392538
Sum of electronic and thermal Energies= -2173.348634
Sum of electronic and thermal Enthalpies= -2173.347690
Sum of electronic and thermal Free Energies= -2173.474153

Cartesian coordinates

C	-1.113635	1.090851	1.886894
C	-3.465761	1.366468	1.954082
C	-2.972677	2.423335	2.883604
C	-1.443550	2.423211	2.606138
H	-0.737384	0.307326	2.551891
H	-0.420665	1.239222	1.067377
H	-3.437465	3.390365	2.680565
H	-3.216638	2.147022	3.913534
H	-1.178544	3.235106	1.925164
H	-0.867777	2.506890	3.532933
N	-2.439861	0.667710	1.387064
N	-4.629217	0.889362	1.589984
N	-4.312754	-0.153274	0.741131
C	-2.968374	-0.290373	0.599784
C	-5.405598	-0.934851	0.220053
C	-5.730593	-2.141828	0.859108
C	-6.178782	-0.396779	-0.820627
C	-6.837043	-2.856690	0.376566
C	-7.273643	-1.152902	-1.267900
C	-7.611990	-2.387453	-0.695060
H	-7.100487	-3.792530	0.858704
H	-7.877703	-0.760348	-2.079636
C	-4.931438	-2.667046	2.027062
H	-5.455038	-3.501973	2.505096
H	-3.949491	-3.021475	1.701855
H	-4.774140	-1.892058	2.783277
C	-8.770101	-3.192156	-1.222107
H	-9.286814	-3.724052	-0.408330
H	-9.498780	-2.563940	-1.735487
H	-8.427548	-3.946406	-1.936564
C	-5.875393	0.948753	-1.418405
H	-6.456891	1.102847	-2.335484
H	-6.144597	1.758598	-0.720318

H	-4.802166	1.051794	-1.640973
C	-2.292847	-1.370081	-0.205351
O	-2.987683	-2.306093	-0.580271
C	-0.809437	-1.395696	-0.365629
C	-0.179649	-2.633106	-0.094208
C	-0.036580	-0.326684	-0.846840
C	1.191485	-2.786980	-0.258056
H	-0.785567	-3.463129	0.268789
C	1.329793	-0.511662	-1.053939
H	-0.482598	0.624927	-1.112399
C	1.975519	-1.727879	-0.767871
H	1.681765	-3.714502	0.000854
H	1.903903	0.307611	-1.460766
C	3.444473	-1.911207	-0.978622
H	3.831041	-1.120722	-1.624938
H	3.631205	-2.864827	-1.476986
C	4.311541	-2.033107	0.386110
C	5.795306	-2.297656	-0.089421
C	6.543910	-1.468512	-0.929389
C	6.362894	-3.498004	0.358697
C	7.840428	-1.834994	-1.315789
H	6.132099	-0.523857	-1.287268
C	7.656042	-3.870989	-0.024011
H	5.751708	-4.102942	1.011349
C	8.402208	-3.039019	-0.861577
H	8.410440	-1.176440	-1.966871
H	8.084580	-4.801428	0.334851
H	9.407616	-3.321968	-1.167496
C	4.301984	-0.632304	1.083638
F	4.591699	0.446619	0.257115
F	5.217553	-0.562583	2.085165
F	3.109657	-0.325355	1.639324
O	3.846379	-2.940482	1.219450
C	-2.318061	0.884157	-3.109756
H	-1.478430	1.576284	-3.276040
H	-1.998225	-0.122449	-3.424919
H	-3.140015	1.172429	-3.809738
O	-2.732005	0.903340	-1.767693
H	-2.344107	1.838147	-1.255990
C	-0.726805	3.247070	-0.672159
O	-0.243879	4.061154	0.194134
O	-1.982435	2.840201	-0.515151
O	-0.032040	2.797995	-1.664680
Cs	2.694562	3.405410	-0.342439

Vibrational frequencies

-109.4316	16.0965	20.6936
23.7492	29.4683	29.9016
36.9886	41.1671	46.1422
49.4413	54.6143	57.0754
60.7008	62.3677	71.3469
74.2540	85.8704	92.4444
99.0062	106.9577	113.5558
117.0608	121.1223	125.9740
145.6009	148.8055	157.7369
164.3859	170.0642	173.5068

M5

Zero-point correction= 0.565634
Thermal correction to Energy= 0.602210
Thermal correction to Enthalpy= 0.603155
Thermal correction to Gibbs Free Energy= 0.496366
Sum of electronic and zero-point Energies= -1889.064993
Sum of electronic and thermal Energies= -1889.028417
Sum of electronic and thermal Enthalpies= -1889.027472
Sum of electronic and thermal Free Energies= -1889.134261

Cartesian coordinates

C	-0.100580	1.646975	-0.925590
C	1.957507	2.607590	-0.241918
C	1.033138	3.776777	-0.362319
C	-0.353537	3.072896	-0.386220
H	-0.165923	1.581998	-2.014280
H	-0.753869	0.901705	-0.485637
H	1.146132	4.486084	0.459739
H	1.232539	4.310554	-1.298431
H	-0.750789	2.999048	0.629330
H	-1.083811	3.604813	-0.997130
N	1.307284	1.435929	-0.532060
N	3.209283	2.395995	0.055164
N	3.336815	1.013880	-0.058046
C	2.184700	0.418336	-0.419412
C	4.629590	0.434872	0.200345
C	5.516406	0.285304	-0.870020
C	4.960394	0.096091	1.519753
C	6.788087	-0.228471	-0.584478
C	6.239486	-0.409473	1.754019
C	7.166581	-0.576887	0.715071

H	7.493988	-0.359722	-1.400738
H	6.518837	-0.686107	2.768006
C	5.091853	0.632908	-2.271642
H	4.206888	0.038321	-2.537366
H	4.817513	1.691793	-2.350968
H	5.896259	0.434981	-2.985180
C	8.543517	-1.120469	1.009280
H	8.486236	-2.080520	1.534895
H	9.122241	-1.270609	0.093559
H	9.108254	-0.436676	1.654562
C	3.943309	0.223886	2.621191
H	3.510336	1.229372	2.657557
H	3.124063	-0.481706	2.444308
H	4.386401	0.005316	3.596057
C	1.983827	-1.060493	-0.888527
O	2.373549	-1.141968	-2.123487
C	0.512293	-1.436033	-0.604601
C	-0.385210	-1.521665	-1.670604
C	0.018439	-1.524333	0.702986
C	-1.756170	-1.630463	-1.438776
H	0.017396	-1.445800	-2.676300
C	-1.352377	-1.635706	0.934716
H	0.715401	-1.474890	1.534675
C	-2.265355	-1.661090	-0.130598
H	-2.460079	-1.626252	-2.263584
H	-1.728522	-1.657665	1.955464
C	-3.745091	-1.603900	0.098256
H	-4.000053	-1.952521	1.104473
H	-4.262342	-2.251645	-0.617065
C	-4.350721	-0.141527	-0.198671
C	-5.908904	-0.299502	-0.041619
C	-6.564387	-0.780637	1.102031
C	-6.680163	0.031774	-1.158878
C	-7.954575	-0.925164	1.121533
H	-5.992791	-1.034350	1.989053
C	-8.069005	-0.112159	-1.147425
H	-6.133228	0.400202	-2.022309
C	-8.713796	-0.593315	-0.004408
H	-8.445560	-1.298649	2.017376
H	-8.651009	0.150481	-2.028321
H	-9.794787	-0.708001	0.010625
C	-3.897555	0.809251	0.959747
F	-4.589547	1.980271	0.955630
F	-2.586011	1.160394	0.867529

F	-4.035838	0.301384	2.232512
O	-3.970196	0.363364	-1.356570
C	3.263482	-3.028548	-0.309103
H	2.441314	-3.760829	-0.374265
H	3.989534	-3.387000	0.428317
H	3.745755	-2.967492	-1.291808
O	2.819332	-1.763179	0.130586

Vibrational frequencies

18.2714	25.0636	34.1708
39.0929	42.2935	48.8877
52.9545	58.6160	65.3965
72.4966	79.4401	86.5530
91.2818	99.3228	114.7283
133.2108	137.1748	146.2977
149.6089	157.3675	177.4816
184.9263	191.1229	197.4085
210.8749	223.6642	232.7989
242.1406	243.1716	250.8203

M05

Zero-point correction= 0.607991
Thermal correction to Energy= 0.648826
Thermal correction to Enthalpy= 0.649771
Thermal correction to Gibbs Free Energy= 0.533117
Sum of electronic and zero-point Energies= -2154.111136
Sum of electronic and thermal Energies= -2154.070300
Sum of electronic and thermal Enthalpies= -2154.069356
Sum of electronic and thermal Free Energies= -2154.186009

Cartesian coordinates

C	0.326294	1.713171	0.036511
C	2.446281	2.376909	0.877083
C	1.556259	3.541184	1.176581
C	0.142626	2.918473	0.987278
H	0.182189	1.973991	-1.011108
H	-0.316582	0.872737	0.277142
H	1.721254	3.949501	2.175727
H	1.747962	4.339630	0.450725
H	-0.229352	2.559232	1.951403
H	-0.584330	3.621283	0.577966
N	1.746562	1.373881	0.257836
N	3.706418	2.065375	1.008536
N	3.786402	0.800035	0.432540

C	2.598197	0.374965	-0.038666
C	5.077519	0.167214	0.357190
C	5.896413	0.468340	-0.736916
C	5.481902	-0.672833	1.403841
C	7.166514	-0.120086	-0.772329
C	6.758043	-1.233224	1.324193
C	7.612150	-0.970515	0.243795
H	7.818712	0.094460	-1.615150
H	7.093636	-1.892769	2.121097
C	5.402245	1.364505	-1.839803
H	4.510216	0.909983	-2.289715
H	5.116696	2.349556	-1.452572
H	6.168813	1.507414	-2.606039
C	8.976683	-1.612519	0.179685
H	8.897308	-2.681191	-0.055465
H	9.603841	-1.150217	-0.588018
H	9.499216	-1.534015	1.139365
C	4.547529	-0.989655	2.539952
H	4.138567	-0.079435	2.991855
H	3.705692	-1.579087	2.161854
H	5.054989	-1.562507	3.320376
C	2.351459	-0.838618	-0.993546
O	2.776496	-0.511082	-2.173325
C	0.858257	-1.236840	-0.901315
C	0.003861	-0.907632	-1.954714
C	0.316704	-1.825599	0.247327
C	-1.370377	-1.128325	-1.853937
H	0.441720	-0.454353	-2.838457
C	-1.056189	-2.044735	0.349836
H	0.979393	-2.101604	1.061787
C	-1.924450	-1.685413	-0.692900
H	-2.030514	-0.846360	-2.668755
H	-1.468511	-2.479492	1.256787
C	-3.414553	-1.874261	-0.555486
H	-3.623491	-2.674089	0.160590
H	-3.843387	-2.177858	-1.515488
C	-4.227358	-0.588160	-0.163228
C	-5.710444	-1.012432	-0.010409
C	-6.151585	-1.907552	0.975971
C	-6.641393	-0.518013	-0.929264
C	-7.492575	-2.289430	1.043120
H	-5.450715	-2.301835	1.703642
C	-7.982842	-0.902168	-0.866976
H	-6.289089	0.168263	-1.690784

C	-8.415117	-1.789148	0.120542
H	-7.816254	-2.979528	1.817935
H	-8.690431	-0.506298	-1.591003
H	-9.458511	-2.088225	0.172113
C	-3.734186	-0.048360	1.208910
F	-4.609250	0.833623	1.747767
F	-2.553147	0.610691	1.107097
F	-3.541276	-1.024451	2.144973
O	-4.079235	0.400292	-1.102318
C	3.557317	-2.934129	-1.119823
H	2.726157	-3.575324	-1.457629
H	4.257753	-3.549024	-0.544962
H	4.066325	-2.538171	-2.005940
O	3.122153	-1.895606	-0.267441
C	-3.026990	3.153480	-0.784142
O	-2.576396	4.276002	-0.607446
O	-4.286399	2.831639	-0.484713
O	-2.283094	2.166507	-1.303960
H	-4.411947	1.823936	-0.678609
H	-2.817301	1.293998	-1.258132

Vibrational frequencies

14.3254	23.4724	29.1686
34.1634	41.1814	42.1655
51.2157	54.2275	58.1139
75.9839	78.7457	82.7158
86.4515	93.8397	100.1810
104.1138	107.6077	109.3872
129.6841	133.1212	142.4138
149.7419	153.3422	158.9965
163.6896	171.1263	186.6273
188.0780	195.4211	203.9154

TS6

Zero-point correction= 0.605218
Thermal correction to Energy= 0.645571
Thermal correction to Enthalpy= 0.646515
Thermal correction to Gibbs Free Energy= 0.531522
Sum of electronic and zero-point Energies= -2154.109591
Sum of electronic and thermal Energies= -2154.069238
Sum of electronic and thermal Enthalpies= -2154.068294
Sum of electronic and thermal Free Energies= -2154.183287

Cartesian coordinates

C	-0.277854	0.972039	-1.569407
C	-2.213943	2.198048	-0.947518
C	-1.253631	3.247415	-1.401549
C	-0.199173	2.399795	-2.165656
H	0.424152	0.820358	-0.754538
H	-0.162842	0.184616	-2.310865
H	-1.724677	4.018726	-2.013719
H	-0.778084	3.716875	-0.532414
H	-0.443957	2.366641	-3.231274
H	0.801451	2.815110	-2.044700
N	-1.644466	0.953028	-1.014677
N	-3.427724	2.133580	-0.469723
N	-3.599144	0.779791	-0.208716
C	-2.513909	0.052777	-0.521394
C	-4.885106	0.341956	0.267498
C	-5.154880	0.425015	1.639224
C	-5.835150	-0.067435	-0.673637
C	-6.439991	0.084125	2.063649
C	-7.107871	-0.405343	-0.198521
C	-7.427812	-0.333633	1.160839
H	-6.673853	0.135473	3.124297
H	-7.864316	-0.728106	-0.909610
C	-4.065562	0.803955	2.603986
H	-3.282146	0.039736	2.549278
H	-3.612680	1.767947	2.347619
H	-4.442712	0.860800	3.628413
C	-8.797581	-0.728719	1.656533
H	-8.788475	-1.750312	2.057274
H	-9.137121	-0.070011	2.462724
H	-9.540541	-0.698355	0.853874
C	-5.484968	-0.156826	-2.136229
H	-5.144613	0.811014	-2.522999
H	-4.669734	-0.874553	-2.283953
H	-6.348008	-0.474109	-2.727173
C	-2.327701	-1.475692	-0.154058
O	-3.035424	-1.790237	0.872243
C	-0.800376	-1.714942	0.001865
C	-0.218010	-1.384135	1.230347
C	0.026712	-2.179422	-1.024849
C	1.161393	-1.453448	1.408709
H	-0.864603	-1.055008	2.037606
C	1.409614	-2.260016	-0.842916
H	-0.420216	-2.443511	-1.977761
C	2.001970	-1.869353	0.365136

H	1.603837	-1.159529	2.355975
H	2.042571	-2.591740	-1.662239
C	3.500901	-1.842457	0.535783
H	3.976304	-2.555621	-0.142586
H	3.766763	-2.137413	1.555486
C	4.159077	-0.431277	0.351155
C	5.681526	-0.582095	0.579732
C	6.497050	-1.365859	-0.250495
C	6.260246	0.052644	1.683021
C	7.860082	-1.503230	0.016483
H	6.073792	-1.862148	-1.116878
C	7.623331	-0.086928	1.953564
H	5.622475	0.652806	2.321701
C	8.429714	-0.865154	1.121227
H	8.477125	-2.110288	-0.640676
H	8.054735	0.414724	2.815880
H	9.490561	-0.973743	1.329651
C	3.933527	0.074406	-1.100488
F	4.754595	1.102594	-1.411359
F	2.670119	0.520291	-1.296678
F	4.144334	-0.890618	-2.042083
O	3.595265	0.469639	1.233774
C	-3.174337	-3.424430	-1.318544
H	-2.345998	-4.095611	-1.038886
H	-3.571170	-3.750135	-2.286218
H	-3.955383	-3.513541	-0.554460
O	-2.749250	-2.083285	-1.473464
C	2.003270	2.920531	0.667567
O	1.392774	3.942689	0.362153
O	3.297157	2.775843	0.632758
O	1.286218	1.835413	1.097493
H	3.587665	1.653011	0.904607
H	1.910363	1.076313	1.203451

Vibrational frequencies

-820.8529	17.1724	29.6395
33.4653	37.2224	39.2838
44.4840	47.5988	51.1851
56.3519	60.6522	73.1388
85.9204	91.9136	95.6410
99.3659	103.0469	113.9395
124.8763	133.3630	142.2210
149.1288	153.9373	158.6479
171.8764	182.1422	189.1163

196.5402 203.5355 217.4594

M6

Zero-point correction= 0.579922
Thermal correction to Energy= 0.616829
Thermal correction to Enthalpy= 0.617774
Thermal correction to Gibbs Free Energy= 0.509149
Sum of electronic and zero-point Energies= -1889.577338
Sum of electronic and thermal Energies= -1889.540430
Sum of electronic and thermal Enthalpies= -1889.539486
Sum of electronic and thermal Free Energies= -1889.648110

Cartesian coordinates

C	-0.034255	1.745161	-0.851968
C	2.039842	2.650548	-0.140471
C	1.135311	3.838420	-0.220910
C	-0.263708	3.160589	-0.272713
H	-0.105855	1.710495	-1.941794
H	-0.695251	0.997214	-0.425217
H	1.257387	4.515003	0.626789
H	1.345705	4.402654	-1.136283
H	-0.666355	3.066815	0.739513
H	-0.978851	3.725383	-0.872164
N	1.369693	1.499780	-0.469240
N	3.286974	2.406440	0.149472
N	3.391756	1.027667	-0.010459
C	2.230976	0.464958	-0.392578
C	4.672859	0.414970	0.232265
C	5.566541	0.296953	-0.837675
C	4.983837	0.009079	1.536386
C	6.823313	-0.256205	-0.566026
C	6.250842	-0.534204	1.757151
C	7.183228	-0.672173	0.719984
H	7.534332	-0.364241	-1.381186
H	6.514312	-0.863637	2.759285
C	5.163705	0.720446	-2.224825
H	4.272716	0.155196	-2.528900
H	4.909457	1.786779	-2.254282
H	5.972099	0.542698	-2.938930
C	8.556067	-1.233547	0.997083
H	8.519014	-2.025856	1.751695
H	9.013610	-1.643380	0.091796
H	9.227169	-0.454374	1.380563
C	3.960833	0.105744	2.635469

H	3.548968	1.117460	2.717189
H	3.129381	-0.574598	2.420503
H	4.392166	-0.167940	3.601558
C	2.015304	-0.990537	-0.921975
O	2.424838	-1.033298	-2.151117
C	0.528185	-1.353576	-0.690851
C	-0.322952	-1.447509	-1.791035
C	-0.010453	-1.458868	0.597017
C	-1.699874	-1.578827	-1.610203
H	0.119307	-1.377057	-2.779619
C	-1.386289	-1.579269	0.778613
H	0.654961	-1.415253	1.453811
C	-2.253654	-1.605685	-0.323688
H	-2.353268	-1.640677	-2.477844
H	-1.800758	-1.612732	1.782783
C	-3.750785	-1.597471	-0.130054
H	-4.020530	-2.110902	0.794946
H	-4.239233	-2.142730	-0.945372
C	-4.405882	-0.181293	-0.129406
C	-5.937182	-0.308696	-0.057413
C	-6.556333	-1.082178	0.935694
C	-6.736514	0.354258	-0.994864
C	-7.945587	-1.201038	0.976175
H	-5.960355	-1.584888	1.689184
C	-8.126853	0.229565	-0.956942
H	-6.269058	0.974662	-1.750859
C	-8.736436	-0.550072	0.026673
H	-8.409152	-1.803738	1.751880
H	-8.731761	0.747437	-1.695843
H	-9.817838	-0.646766	0.056849
C	-3.930446	0.675484	1.066866
F	-4.670745	1.796019	1.197043
F	-2.645089	1.074180	0.955426
F	-4.032601	-0.015058	2.228113
O	-3.986863	0.575891	-1.254138
C	3.238663	-3.008337	-0.394227
H	2.406797	-3.722614	-0.510494
H	3.938841	-3.406516	0.347067
H	3.748093	-2.914380	-1.359935
O	2.801752	-1.752811	0.086507
H	-4.090723	0.018586	-2.039660

Vibrational frequencies

12.7713	18.3947	26.8470

30.1897	38.4811	45.2845
47.3819	58.5935	63.1897
66.7337	78.6177	89.1212
90.3043	91.7374	113.1853
129.0804	132.2809	146.0337
153.2170	173.3956	181.7006
185.8184	197.3187	203.1514
210.6558	226.9231	235.8162

TS7

Zero-point correction= 0.579182
Thermal correction to Energy= 0.615831
Thermal correction to Enthalpy= 0.616775
Thermal correction to Gibbs Free Energy= 0.508732
Sum of electronic and zero-point Energies= -1889.574999
Sum of electronic and thermal Energies= -1889.538350
Sum of electronic and thermal Enthalpies= -1889.537406
Sum of electronic and thermal Free Energies= -1889.645449

Cartesian coordinates

C	0.112679	1.632330	0.743744
C	-1.954533	2.672945	0.242705
C	-0.997112	3.814874	0.376032
C	0.373372	3.083512	0.275921
H	0.256008	1.503610	1.819674
H	0.706461	0.894582	0.212373
H	-1.137287	4.574866	-0.394929
H	-1.125543	4.297153	1.351609
H	0.707101	3.067601	-0.765261
H	1.148991	3.565681	0.872847
N	-1.315219	1.472394	0.432589
N	-3.223033	2.496148	0.003518
N	-3.350014	1.102845	0.052901
C	-2.199654	0.456919	0.311008
C	-4.649677	0.531383	-0.158474
C	-5.497511	0.383288	0.947191
C	-5.021421	0.156147	-1.455590
C	-6.769404	-0.152098	0.719713
C	-6.299713	-0.380892	-1.631874
C	-7.188459	-0.533550	-0.560602
H	-7.443421	-0.280547	1.562853
H	-6.608024	-0.687243	-2.628484
C	-5.016790	0.729905	2.331745
H	-4.176885	0.076247	2.595786

H	-4.664953	1.765914	2.387137
H	-5.813271	0.597414	3.068473
C	-8.577104	-1.078225	-0.788480
H	-9.271109	-0.274104	-1.064368
H	-8.590183	-1.811289	-1.601121
H	-8.973360	-1.556932	0.112021
C	-4.050071	0.273244	-2.599817
H	-3.591241	1.266615	-2.639501
H	-3.244312	-0.458384	-2.473595
H	-4.543337	0.083490	-3.556480
C	-2.027196	-1.400343	0.784472
O	-2.503283	-1.546572	1.932405
C	-0.520160	-1.545922	0.570500
C	0.311826	-1.548908	1.689808
C	0.056912	-1.614178	-0.704980
C	1.700464	-1.581989	1.541180
H	-0.147096	-1.511971	2.672362
C	1.440577	-1.641825	-0.854669
H	-0.586544	-1.631334	-1.577781
C	2.285907	-1.611905	0.266438
H	2.337680	-1.591919	2.422302
H	1.876853	-1.667564	-1.849335
C	3.789031	-1.571748	0.111890
H	4.097626	-2.086305	-0.800578
H	4.263084	-2.086378	0.952241
C	4.410014	-0.139780	0.107091
C	5.935518	-0.249155	0.123634
C	6.620087	-0.820387	-0.959106
C	6.662667	0.177913	1.239674
C	8.007795	-0.954801	-0.925664
H	6.074770	-1.152893	-1.835435
C	8.052112	0.038944	1.271315
H	6.140386	0.617222	2.080578
C	8.729786	-0.526560	0.190609
H	8.523217	-1.396065	-1.773813
H	8.603349	0.375148	2.144963
H	9.810374	-0.633169	0.216583
C	3.960514	0.670977	-1.137770
F	4.714591	1.770982	-1.323641
F	2.678133	1.098193	-1.013010
F	4.016194	-0.057179	-2.280351
O	3.998486	0.602883	1.239561
C	-3.855962	-2.744189	-0.002390
H	-3.613121	-3.595700	0.645059

H	-4.248120	-3.117146	-0.951979
H	-4.622843	-2.144287	0.493269
O	-2.694346	-1.988691	-0.332674
H	3.038529	0.493491	1.326614

Vibrational frequencies

-221.5976	13.5117	19.6135
29.7220	33.0053	40.0555
44.0998	46.5568	60.7329
65.1188	71.2877	75.9516
80.5879	93.5546	108.6162
110.2217	119.4862	128.3022
143.9032	155.8915	157.9787
166.0462	174.7654	183.3407
198.9873	207.3318	215.9996
229.0952	233.9593	243.4327

3a

Zero-point correction= 0.291053
Thermal correction to Energy= 0.311445
Thermal correction to Enthalpy= 0.312389
Thermal correction to Gibbs Free Energy= 0.240041
Sum of electronic and zero-point Energies= -1181.848099
Sum of electronic and thermal Energies= -1181.827708
Sum of electronic and thermal Enthalpies= -1181.826763
Sum of electronic and thermal Free Energies= -1181.899111

Cartesian coordinates

C	-4.913172	0.093496	-0.254632
O	-5.525362	1.084288	-0.614927
C	-3.442382	-0.086011	-0.399640
C	-2.776333	-1.238634	0.042982
C	-2.708492	0.940617	-1.009086
C	-1.400212	-1.356881	-0.126416
H	-3.336814	-2.037602	0.514603
C	-1.333096	0.815674	-1.173843
H	-3.229742	1.828749	-1.349794
C	-0.660506	-0.334004	-0.736435
H	-0.887275	-2.247451	0.221226
H	-0.770913	1.620061	-1.639214
C	0.833546	-0.471039	-0.922495
H	1.175868	0.175016	-1.734326
H	1.081599	-1.499499	-1.200873
C	1.706107	-0.165273	0.322289

C	3.186292	-0.365715	-0.038246
C	3.898282	0.566925	-0.806957
C	3.828006	-1.545717	0.356950
C	5.228750	0.329329	-1.151939
H	3.422805	1.482755	-1.136899
C	5.159467	-1.782324	0.008907
H	3.282286	-2.286570	0.930344
C	5.866272	-0.844354	-0.743649
H	5.766826	1.065491	-1.742123
H	5.640677	-2.702626	0.327152
H	6.902444	-1.026413	-1.013371
C	1.450006	1.271279	0.841312
F	2.369070	1.613650	1.776596
F	0.242702	1.388911	1.422107
F	1.505528	2.200431	-0.144487
O	1.287108	-1.048933	1.349768
H	1.847031	-0.895217	2.127918
O	-5.510236	-0.970268	0.321747
C	-6.937392	-0.869132	0.484430
H	-7.246550	-1.798996	0.962357
H	-7.196109	-0.015331	1.116437
H	-7.430789	-0.759405	-0.485270

Vibrational frequencies

19.6262	34.9008	37.0494
44.7304	64.0327	77.6312
90.1098	107.6915	147.2627
162.9795	179.6822	197.9369
204.8890	244.5789	279.7991
287.0115	301.6541	322.1329
334.9434	366.0438	369.4618
389.1903	411.2026	418.8549
432.5940	457.6734	490.6473
492.4002	522.6846	534.0534

M1b

Zero-point correction= 0.440503
Thermal correction to Energy= 0.465822
Thermal correction to Enthalpy= 0.466766
Thermal correction to Gibbs Free Energy= 0.384693
Sum of electronic and zero-point Energies= -1168.738176
Sum of electronic and thermal Energies= -1168.712857
Sum of electronic and thermal Enthalpies= -1168.711913
Sum of electronic and thermal Free Energies= -1168.793986

Cartesian coordinates

C	1.959618	-0.541769	0.034066
C	3.877229	0.536257	0.246247
C	4.273096	-1.798369	0.087176
H	4.239816	-2.295920	1.059451
H	4.006781	-2.513133	-0.685880
C	0.565307	1.564522	0.067420
C	0.102452	1.970358	-1.190050
C	-0.108196	1.858457	1.262690
C	-1.100151	2.684907	-1.232433
C	-1.304204	2.571629	1.166834
C	-1.816490	2.988024	-0.069597
H	-1.486645	3.002913	-2.196999
H	-1.855904	2.797318	2.075721
C	5.597852	-1.032971	-0.156437
H	5.807418	-1.010408	-1.229313
H	6.436914	-1.516237	0.345729
C	5.363630	0.419260	0.353335
H	5.886009	1.174337	-0.236604
H	5.666778	0.537614	1.399272
C	0.850667	1.607553	-2.445684
H	1.903198	1.903774	-2.384093
H	0.824790	0.523849	-2.609347
H	0.406532	2.092287	-3.318026
C	0.413988	1.356824	2.583327
H	0.385973	0.260984	2.610988
H	1.453618	1.660367	2.745697
H	-0.190229	1.733527	3.411624
C	-3.123735	3.737880	-0.131965
H	-3.028228	4.734280	0.315900
H	-3.466709	3.864290	-1.162444
H	-3.903591	3.208404	0.425872
N	2.979106	1.483719	0.271652
N	1.781021	0.799129	0.136001
N	3.299408	-0.692572	0.094951
C	-5.408706	-0.761360	0.144967
C	-5.113745	-2.017941	0.680344
C	-3.824567	-2.542937	0.576893
C	-2.799283	-1.830100	-0.069181
C	-3.112141	-0.564458	-0.598466
C	-4.400157	-0.037462	-0.495789
H	-6.410398	-0.349752	0.230426
H	-5.885855	-2.586422	1.191827

H	-3.599684	-3.508858	1.019575
H	-2.342231	0.009892	-1.103624
H	-4.613589	0.940619	-0.918787
C	-1.413906	-2.391918	-0.184215
C	-0.336590	-1.436869	-0.016992
H	-0.623694	-0.436187	0.263866
C	1.020696	-1.705484	-0.169230
O	1.605098	-2.794729	-0.452030
C	-1.247699	-3.716985	-0.445840
H	-0.254415	-4.138943	-0.528694
H	-2.103978	-4.364984	-0.608637

Vibrational frequencies

19.1187	34.6036	40.3489
52.8168	58.9714	64.7518
75.3705	94.1682	103.9367
118.9007	142.8778	150.6179
161.3769	168.7464	190.8300
197.2692	208.9276	226.4694
238.8253	241.1099	247.9879
274.7459	287.7233	293.7086
321.0614	338.1426	375.8592
399.0533	411.7728	414.2535

M1b+2b

Zero-point correction= 0.816274
Thermal correction to Energy= 0.864891
Thermal correction to Enthalpy= 0.865835
Thermal correction to Gibbs Free Energy= 0.735669
Sum of electronic and zero-point Energies= -3454.723526
Sum of electronic and thermal Energies= -3454.674909
Sum of electronic and thermal Enthalpies= -3454.673965
Sum of electronic and thermal Free Energies= -3454.804131

Cartesian coordinates

C	0.072979	2.242618	0.667071
C	0.092181	2.113792	-0.781067
C	0.499507	0.917067	-1.371646
C	0.902823	-0.203248	-0.537269
C	0.877455	-0.082637	0.852695
C	0.456315	1.164455	1.467104
C	-1.088014	3.037497	1.031649
C	-1.784647	3.403043	-0.190888
C	-1.055667	2.832623	-1.310664

C	-1.749800	2.324544	-2.409534
C	-0.225047	0.388539	-2.514654
C	0.425625	-1.424320	-1.164881
C	-0.045442	-2.475833	-0.380145
C	-0.065246	-2.350837	1.067977
C	0.388728	-1.177135	1.672712
C	-0.340594	-0.606661	2.793298
C	-0.297886	0.841427	2.666785
C	-1.411051	1.606653	3.016854
C	-1.814298	2.726661	2.182589
C	-3.179930	3.442892	-0.213656
C	-3.935531	3.119018	0.984372
C	-3.266666	2.767807	2.157853
C	-3.761054	1.673182	2.976424
C	-2.614365	0.955395	3.507244
C	-2.655827	-0.434302	3.628364
C	-1.496005	-1.231494	3.264848
C	-1.970060	-2.452570	2.634523
C	-1.269587	-2.999744	1.558210
C	-0.269548	-1.059829	-2.387907
C	-4.084463	-3.123943	-0.830834
C	-3.357706	-2.812033	-1.980759
C	-3.761466	-1.691759	-2.814491
C	-4.875854	-0.927410	-2.464954
C	-5.631980	-1.251560	-1.266699
C	-5.264148	-2.199983	0.980924
C	-4.117225	-2.918605	1.511014
C	-3.388515	-3.489676	0.391025
C	-1.993214	-3.529073	0.413608
C	-1.237291	-3.205514	-0.783819
C	-1.905611	-2.854461	-1.957293
C	-2.558841	-1.041366	-3.306026
C	-2.517279	0.347901	-3.428192
C	-3.676259	1.143758	-3.062643
C	-4.832331	0.519388	-2.591273
C	-5.561189	1.090211	-1.470928
C	-6.055244	-0.004384	-0.652349
C	-6.074432	0.117452	0.737561
C	-5.670955	-1.002731	1.570832
C	-3.422616	-2.410353	2.609426
C	-3.846400	-1.163347	3.223870
C	-4.947672	-0.473731	2.714995
C	-4.904341	0.973353	2.588972
C	-5.600757	1.338823	1.366676

C	-5.126658	2.389737	0.580717
C	-5.106421	2.262976	-0.866804
C	-3.902935	2.913813	-1.357607
C	-3.202051	2.365314	-2.432727
C	-1.410858	-1.760029	-2.776770
C	-1.325396	1.077296	-3.024017
C	-5.244229	-2.326957	-0.466561
C	4.288249	1.993227	-0.677829
C	4.488228	3.953364	0.321181
C	3.144055	4.169294	-1.623144
H	2.088481	3.962368	-1.434799
H	3.364646	3.950085	-2.663757
C	5.690848	0.769710	1.025688
C	6.855374	0.264901	0.428735
C	5.101917	0.187667	2.159272
C	7.403097	-0.900171	0.972318
C	5.689788	-0.975703	2.663106
C	6.824595	-1.544301	2.072198
H	8.295191	-1.320761	0.515912
H	5.241749	-1.454970	3.529581
C	3.584588	5.573927	-1.141620
H	4.404171	5.930132	-1.771489
H	2.766450	6.292500	-1.206436
C	4.095780	5.395258	0.317281
H	4.924637	6.058402	0.570329
H	3.296947	5.555218	1.049914
C	7.455061	0.916438	-0.789024
H	7.520542	2.003168	-0.673935
H	6.835077	0.714455	-1.670300
H	8.457486	0.528250	-0.984000
C	3.883133	0.790435	2.806422
H	3.122318	1.048334	2.066113
H	4.138918	1.714289	3.337178
H	3.438158	0.095871	3.522915
C	7.384787	-2.846951	2.585127
H	8.453998	-2.937633	2.372376
H	6.879970	-3.692142	2.100142
H	7.234830	-2.952635	3.663863
N	5.176823	3.143787	1.079238
N	5.051235	1.917987	0.442984
N	3.952036	3.298224	-0.750924
C	4.117154	-5.359595	-0.353384
C	4.382556	-5.187312	-1.714502
C	4.223973	-3.935165	-2.310065

C	3.792316	-2.826035	-1.562868
C	3.530186	-3.016113	-0.193690
C	3.688029	-4.266862	0.404121
H	4.244981	-6.333205	0.111209
H	4.725157	-6.027350	-2.312677
H	4.455389	-3.805503	-3.363205
H	3.181082	-2.180184	0.403295
H	3.468703	-4.386997	1.461639
C	3.613659	-1.482067	-2.197428
C	4.024524	-0.353369	-1.390757
H	4.520278	-0.585454	-0.461799
C	3.833160	0.988691	-1.706577
O	3.273886	1.505829	-2.719951
C	3.062799	-1.393010	-3.438933
H	2.724989	-2.281672	-3.963348
H	2.926893	-0.428990	-3.910765

Vibrational frequencies

9.1805	13.3303	15.8491
19.5040	21.7683	25.5770
33.9124	46.4735	48.6809
56.4115	60.8666	73.5906
86.8237	89.4373	106.2040
122.2274	131.2376	144.8408
154.8340	160.6680	174.9598
192.3334	196.7366	230.3726
231.5845	244.2699	250.0267
266.4393	266.8005	267.1781

TSb

Zero-point correction= 0.816269
Thermal correction to Energy= 0.863837
Thermal correction to Enthalpy= 0.864782
Thermal correction to Gibbs Free Energy= 0.739866
Sum of electronic and zero-point Energies= -3454.715642
Sum of electronic and thermal Energies= -3454.668074
Sum of electronic and thermal Enthalpies= -3454.667129
Sum of electronic and thermal Free Energies= -3454.792045

Cartesian coordinates

C	-0.279994	1.980228	-1.779643
C	-0.774017	1.025608	-2.771987
C	-0.405139	-0.311898	-2.702879
C	0.595897	-0.810865	-1.717390

C	0.957132	0.127956	-0.676526
C	0.525270	1.501820	-0.739632
C	-1.353684	2.904247	-1.486465
C	-2.502058	2.544045	-2.308035
C	-2.140138	1.384879	-3.102148
C	-3.090343	0.391645	-3.363455
C	-1.392618	-1.336272	-2.946151
C	0.016571	-2.099818	-1.232762
C	0.040700	-2.467140	0.106670
C	0.539554	-1.538097	1.122428
C	0.937486	-0.260557	0.712874
C	0.572582	0.896521	1.521395
C	0.318632	1.996098	0.615936
C	-0.700624	2.910724	0.888262
C	-1.558898	3.379956	-0.182607
C	-3.797179	2.667710	-1.800863
C	-4.005933	3.152496	-0.447347
C	-2.905680	3.491632	0.344344
C	-2.877472	3.106327	1.747344
C	-1.511218	2.746257	2.084710
C	-1.265045	1.685371	2.957622
C	-0.196058	0.740921	2.675957
C	-0.634393	-0.579688	3.084095
C	-0.282014	-1.689733	2.300666
C	-1.133744	-2.439630	-2.037337
C	-3.709201	-2.971207	1.727686
C	-3.513470	-3.433556	0.424668
C	-4.380827	-2.970450	-0.647024
C	-5.408967	-2.066180	-0.373471
C	-5.610602	-1.586104	0.982692
C	-4.295019	-1.092981	3.013753
C	-2.930765	-1.457005	3.354107
C	-2.564778	-2.611515	2.551431
C	-1.272057	-2.725511	2.035862
C	-1.069332	-3.203449	0.680916
C	-2.168247	-3.557342	-0.108559
C	-3.568197	-2.806307	-1.839887
C	-3.815257	-1.747434	-2.712009
C	-4.885181	-0.806715	-2.429534
C	-5.666665	-0.962039	-1.283381
C	-6.027935	0.199333	-0.488555
C	-5.997127	-0.187434	0.911707
C	-5.531113	0.712378	1.872807
C	-4.669272	0.250659	2.947496

C	-1.983263	-0.459334	3.602199
C	-2.372890	0.941748	3.531971
C	-3.684837	1.288100	3.208868
C	-3.942008	2.392356	2.298593
C	-5.083470	2.035861	1.473102
C	-5.111522	2.407044	0.127938
C	-5.595619	1.470079	-0.873874
C	-4.783369	1.631326	-2.065987
C	-4.436306	0.516803	-2.832426
C	-2.199650	-3.170174	-1.501633
C	-2.706461	-1.001442	-3.288633
C	-4.778353	-2.031235	2.012257
C	4.241365	1.977126	-0.749187
C	4.481771	3.941700	0.218219
C	3.036537	4.139228	-1.656816
H	1.996928	3.900990	-1.428114
H	3.222294	3.938771	-2.708352
C	5.697611	0.761182	0.916718
C	6.831458	0.228330	0.283581
C	5.154862	0.225911	2.094462
C	7.402269	-0.913667	0.848511
C	5.764141	-0.921010	2.614655
C	6.876402	-1.508841	2.002638
H	8.274555	-1.353020	0.371887
H	5.354507	-1.364648	3.517961
C	3.464363	5.550300	-1.182898
H	4.236736	5.937556	-1.852369
H	2.622879	6.243861	-1.194354
C	4.058186	5.373711	0.244150
H	4.880694	6.057205	0.459539
H	3.296165	5.502408	1.021038
C	7.377195	0.832461	-0.983624
H	7.476109	1.919724	-0.902142
H	6.709749	0.624842	-1.828249
H	8.357864	0.413799	-1.220597
C	3.974789	0.860076	2.782379
H	3.190023	1.137432	2.074898
H	4.275503	1.775743	3.303542
H	3.539923	0.177515	3.516129
C	7.483038	-2.776655	2.548284
H	8.576931	-2.732115	2.538246
H	7.189854	-3.636726	1.933770
H	7.154538	-2.972396	3.572638
N	5.206045	3.134768	0.948646

N	5.049135	1.906909	0.334426
N	3.899750	3.278029	-0.823447
C	4.043409	-5.469108	-0.499320
C	3.764434	-5.270777	-1.853351
C	3.512216	-3.987539	-2.338654
C	3.536072	-2.870506	-1.483578
C	3.819708	-3.088364	-0.121159
C	4.067924	-4.370581	0.364623
H	4.237292	-6.468534	-0.120944
H	3.748623	-6.115365	-2.536309
H	3.318339	-3.846433	-3.397470
H	3.813312	-2.253412	0.570848
H	4.269988	-4.511862	1.422646
C	3.262919	-1.506154	-2.012869
C	3.888501	-0.417507	-1.389049
H	4.557344	-0.630716	-0.570321
C	3.701477	0.950365	-1.723851
O	3.125208	1.446921	-2.715414
C	2.225881	-1.329007	-2.951571
H	1.786532	-2.200773	-3.424811
H	2.213084	-0.415297	-3.527886

Vibrational frequencies

-345.0682	12.6623	17.6578
22.3819	27.4267	37.2803
45.9207	50.7122	52.7562
56.4882	62.0463	69.9303
86.3048	99.7542	117.3271
129.9483	134.1647	141.1077
144.3778	155.1370	164.6716
199.2671	208.9521	228.4954
236.2389	245.7638	253.0549
258.7801	263.2385	264.6276

TSb'

Zero-point correction= 0.816584
Thermal correction to Energy= 0.863917
Thermal correction to Enthalpy= 0.864861
Thermal correction to Gibbs Free Energy= 0.740990
Sum of electronic and zero-point Energies= -3454.707732
Sum of electronic and thermal Energies= -3454.660399
Sum of electronic and thermal Enthalpies= -3454.659455
Sum of electronic and thermal Free Energies= -3454.783325

Cartesian coordinates

C	-0.147939	2.474955	-0.669000
C	-0.137151	1.656736	-1.879872
C	0.437452	0.391000	-1.883273
C	1.171290	-0.150794	-0.695115
C	0.973736	0.613227	0.532396
C	0.364484	1.907702	0.513321
C	-1.413188	3.174590	-0.628601
C	-2.166590	2.834588	-1.829146
C	-1.375211	1.898152	-2.600018
C	-1.999692	0.857829	-3.294819
C	-0.232339	-0.685963	-2.572106
C	0.689955	-1.573695	-0.606375
C	0.356465	-2.169468	0.603225
C	0.347685	-1.398499	1.847336
C	0.605170	-0.024483	1.764741
C	-0.184917	0.909476	2.560290
C	-0.338704	2.115907	1.778244
C	-1.541534	2.820253	1.805117
C	-2.095479	3.372841	0.580859
C	-3.556127	2.698337	-1.772939
C	-4.259075	2.895930	-0.519097
C	-3.534919	3.214647	0.634618
C	-3.874326	2.581164	1.900567
C	-2.639977	2.340236	2.627349
C	-2.490441	1.175035	3.381448
C	-1.235220	0.443555	3.351627
C	-1.534081	-0.975504	3.404919
C	-0.761347	-1.866952	2.644816
C	-0.072570	-1.899760	-1.786743
C	-3.551137	-3.436929	0.786126
C	-2.881810	-3.623616	-0.424673
C	-3.441612	-3.080827	-1.652308
C	-4.651367	-2.383780	-1.621912
C	-5.346148	-2.193499	-0.360418
C	-4.835670	-1.923788	2.040163
C	-3.602549	-2.171448	2.768570
C	-2.804692	-3.099718	1.988708
C	-1.416859	-2.951821	1.925249
C	-0.722227	-3.139366	0.667658
C	-1.438335	-3.473620	-0.486152
C	-2.343190	-2.600578	-2.470987
C	-2.494015	-1.437546	-3.222442
C	-3.749627	-0.709450	-3.192604

C	-4.808628	-1.171625	-2.407972
C	-5.601055	-0.232705	-1.632284
C	-5.937451	-0.867000	-0.368919
C	-5.959771	-0.108472	0.803987
C	-5.405593	-0.649510	2.033087
C	-2.974642	-1.124870	3.450902
C	-3.569201	0.204038	3.444646
C	-4.754541	0.436808	2.747478
C	-4.911629	1.650229	1.961771
C	-5.657663	1.312432	0.760478
C	-5.335417	1.921605	-0.453243
C	-5.308026	1.132088	-1.675216
C	-4.205908	1.611508	-2.489519
C	-3.443393	0.711359	-3.236062
C	-1.103689	-2.843886	-1.743540
C	-1.412185	-0.463617	-3.288100
C	-4.809913	-2.714761	0.819811
C	3.805630	2.126488	-0.596332
C	4.143317	4.076289	0.360294
C	2.796333	4.345662	-1.576909
H	1.733952	4.187895	-1.368373
H	3.000070	4.109103	-2.618275
C	5.152838	0.824473	1.092991
C	6.184374	0.171941	0.395887
C	4.665568	0.378833	2.331999
C	6.693772	-0.998909	0.960224
C	5.215972	-0.798288	2.849092
C	6.219051	-1.503663	2.176846
H	7.472614	-1.537470	0.427424
H	4.842645	-1.173928	3.797858
C	3.313193	5.730140	-1.112508
H	4.137889	6.042581	-1.757884
H	2.527757	6.484564	-1.168059
C	3.838293	5.538327	0.341014
H	4.710759	6.152224	0.570179
H	3.065306	5.754177	1.086379
C	6.706969	0.675120	-0.925407
H	6.814659	1.764077	-0.932568
H	6.036353	0.401837	-1.748267
H	7.683430	0.234707	-1.139958
C	3.603388	1.131883	3.090026
H	2.822386	1.510795	2.427356
H	4.036929	1.994344	3.608411
H	3.135144	0.487228	3.836942

C	6.791011	-2.776819	2.747123
H	7.773822	-2.595216	3.199307
H	6.925869	-3.530046	1.965168
H	6.141902	-3.196446	3.520693
N	4.774136	3.223904	1.129201
N	4.557081	2.005711	0.521032
N	3.565282	3.444849	-0.701891
C	5.408954	-4.817764	-0.515504
C	5.656426	-4.384339	-1.820666
C	4.990822	-3.269777	-2.330068
C	4.057553	-2.561672	-1.550741
C	3.832530	-3.000827	-0.234065
C	4.493203	-4.119283	0.274157
H	5.928990	-5.683774	-0.116352
H	6.378566	-4.907675	-2.441096
H	5.213941	-2.926194	-3.335463
H	3.127331	-2.477677	0.400767
H	4.294573	-4.438885	1.292991
C	3.365626	-1.361787	-2.113144
C	3.142431	-0.237244	-1.172656
H	3.516442	-0.427033	-0.175852
C	3.356358	1.117607	-1.617594
O	3.118710	1.579629	-2.743898
C	2.987587	-1.322886	-3.407932
H	3.140835	-2.176234	-4.060966
H	2.520697	-0.444328	-3.830651

Vibrational frequencies

-384.7368	10.9202	13.0857
22.3997	28.2684	40.3012
46.0989	58.6047	61.1901
73.8316	75.3278	88.6727
98.4765	105.7875	117.4989
122.5497	132.7262	140.9569
160.6411	178.6140	181.9372
206.7326	209.5572	221.8776
232.9801	235.5010	246.7997
261.8406	263.3242	268.3647

M2b

Zero-point correction= 0.819032

Thermal correction to Energy= 0.866419

Thermal correction to Enthalpy= 0.867363

Thermal correction to Gibbs Free Energy= 0.743365

Sum of electronic and zero-point Energies= -3454.727416
Sum of electronic and thermal Energies= -3454.680030
Sum of electronic and thermal Enthalpies= -3454.679085
Sum of electronic and thermal Free Energies= -3454.803083

Cartesian coordinates

C	-0.621661	1.843541	-2.290424
C	-1.057888	0.656346	-3.040706
C	-0.520282	-0.592207	-2.782188
C	0.710000	-0.818618	-1.877714
C	0.915113	0.386190	-0.971412
C	0.295420	1.645147	-1.241877
C	-1.782053	2.664650	-2.071244
C	-2.927896	2.029970	-2.716659
C	-2.475452	0.793257	-3.315727
C	-3.310077	-0.331602	-3.322254
C	-1.386747	-1.737283	-2.740340
C	0.212339	-2.023743	-1.046782
C	0.349719	-2.112017	0.327620
C	0.808853	-0.965024	1.124708
C	0.997144	0.254429	0.446351
C	0.540843	1.496350	1.075756
C	0.101312	2.368810	0.017169
C	-1.005414	3.199282	0.200560
C	-1.975194	3.364504	-0.863751
C	-4.197064	2.105154	-2.138170
C	-4.389541	2.814975	-0.886699
C	-3.289501	3.413414	-0.260510
C	-3.133303	3.304437	1.183512
C	-1.715448	3.172841	1.470152
C	-1.286100	2.329524	2.496770
C	-0.127725	1.472435	2.299826
C	-0.367943	0.211732	2.973113
C	0.075672	-0.978460	2.361190
C	-0.938431	-2.615084	-1.670585
C	-3.197620	-2.721844	2.314096
C	-3.025960	-3.401911	1.105656
C	-4.008030	-3.246452	0.043301
C	-5.121217	-2.425853	0.235585
C	-5.300748	-1.726046	1.495482
C	-3.933399	-0.715959	3.289113
C	-2.518346	-0.855711	3.580915
C	-2.059705	-2.087436	2.964636
C	-0.797945	-2.149152	2.368678

C	-0.621030	-2.847322	1.114044
C	-1.711943	-3.469418	0.493613
C	-3.295557	-3.218828	-1.222059
C	-3.724900	-2.378378	-2.246703
C	-4.884247	-1.526475	-2.049728
C	-5.568085	-1.547701	-0.832414
C	-6.023096	-0.306131	-0.231918
C	-5.863644	-0.418693	1.207096
C	-5.453055	0.693158	1.948995
C	-4.477712	0.540311	3.014331
C	-1.687114	0.271493	3.563065
C	-2.255683	1.582767	3.279319
C	-3.617646	1.713269	3.007898
C	-4.065251	2.591621	1.938068
C	-5.201634	1.960663	1.285757
C	-5.353187	2.068087	-0.098456
C	-5.776611	0.910794	-0.873376
C	-5.061999	0.933782	-2.134666
C	-4.626593	-0.259487	-2.716545
C	-1.873417	-3.356249	-0.934663
C	-2.752780	-1.630237	-3.034032
C	-4.356616	-1.874395	2.515345
C	4.237887	1.975448	-0.765883
C	4.382010	3.911103	0.262077
C	3.085675	4.148420	-1.715018
H	2.033383	3.899144	-1.566218
H	3.353629	3.976154	-2.753956
C	5.592010	0.721982	0.959462
C	6.756893	0.207502	0.366455
C	5.003384	0.165487	2.105426
C	7.300689	-0.949272	0.929097
C	5.589976	-0.993800	2.623600
C	6.724023	-1.571933	2.043606
H	8.193970	-1.377016	0.481997
H	5.143924	-1.454712	3.500420
C	3.469829	5.548542	-1.175695
H	4.291596	5.951377	-1.773046
H	2.628749	6.239573	-1.237259
C	3.949735	5.339551	0.289482
H	4.750356	6.018775	0.585547
H	3.128666	5.445621	1.007076
C	7.368777	0.839174	-0.857285
H	7.429296	1.927861	-0.762793
H	6.774781	0.617708	-1.752129

H	8.376439	0.452765	-1.025604
C	3.806785	0.792656	2.769753
H	3.043037	1.084944	2.046177
H	4.099223	1.697953	3.313068
H	3.353262	0.100671	3.482306
C	7.301969	-2.855687	2.582736
H	8.395842	-2.821206	2.608329
H	7.021063	-3.700224	1.941373
H	6.938039	-3.068666	3.591491
N	5.059450	3.087696	1.022729
N	4.960889	1.877890	0.371784
N	3.889863	3.272120	-0.837766
C	3.948467	-5.465419	-0.605878
C	3.505997	-5.237991	-1.910541
C	3.242162	-3.940212	-2.347918
C	3.432902	-2.839211	-1.492891
C	3.879602	-3.085229	-0.178518
C	4.129486	-4.382572	0.259978
H	4.142001	-6.477716	-0.263612
H	3.364395	-6.072039	-2.591476
H	2.912449	-3.782064	-3.369408
H	3.990607	-2.259667	0.516112
H	4.452781	-4.548029	1.283679
C	3.175692	-1.457549	-1.965680
C	3.942947	-0.441554	-1.478000
H	4.709562	-0.681531	-0.755069
C	3.800006	0.965684	-1.808807
O	3.383027	1.456463	-2.859717
C	1.963300	-1.193057	-2.798310
H	1.669846	-2.070128	-3.377320
H	2.122701	-0.358879	-3.477378

Vibrational frequencies

15.1259	18.0274	22.2699
25.8870	31.3157	45.6411
51.7436	56.3241	64.2912
72.0321	80.7168	81.5100
89.4837	127.2829	130.2742
140.9541	160.2049	167.5864
173.2143	188.9602	206.9593
213.6663	230.0965	243.9271
254.5706	257.8716	260.0607
261.6658	262.0202	269.1016

M1c

Zero-point correction= 0.540628
Thermal correction to Energy= 0.584666
Thermal correction to Enthalpy= 0.585610
Thermal correction to Gibbs Free Energy= 0.460141
Sum of electronic and zero-point Energies= -2739.802793
Sum of electronic and thermal Energies= -2739.758755
Sum of electronic and thermal Enthalpies= -2739.757811
Sum of electronic and thermal Free Energies= -2739.883280

Cartesian coordinates

C	-0.024761	-0.933967	2.055095
N	-1.422384	-1.181609	2.332738
C	-1.739893	-2.593073	2.515619
C	-0.367948	-3.299374	2.541123
C	0.663213	-2.160674	2.685804
H	0.271019	-0.002728	2.547998
H	-2.300024	-2.712635	3.452831
H	-2.382232	-2.972874	1.707896
H	-0.302002	-4.018909	3.361207
H	-0.201896	-3.833452	1.605334
H	0.851329	-1.943781	3.741903
H	1.617633	-2.400671	2.214627
C	-2.354522	-0.182470	2.457470
C	-3.700887	-0.335905	2.487666
H	-1.926081	0.817494	2.488942
H	-4.123983	-1.327764	2.366988
C	-4.594645	0.804904	2.534098
C	-5.918279	0.818141	2.275888
H	-4.120895	1.761016	2.762838
C	0.356916	-0.760086	0.510197
O	0.277091	-2.051922	-0.076039
Si	0.232519	-2.608370	-1.683001
C	-1.500145	-3.229941	-2.072347
H	-1.472004	-3.869063	-2.963400
H	-1.899435	-3.836970	-1.251805
H	-2.212790	-2.425224	-2.274583
C	1.417552	-4.070588	-1.721142
H	2.471154	-3.780423	-1.641955
H	1.203995	-4.769155	-0.904149
H	1.304681	-4.621396	-2.662674
C	0.759838	-1.286328	-2.911994
H	0.794035	-1.723465	-3.917744
H	0.060880	-0.445806	-2.943585

H	1.757571	-0.890370	-2.695890
C	-0.645951	0.165920	-0.205622
C	-1.938820	-0.340094	-0.410838
C	-2.919510	0.416720	-1.039747
C	-2.640225	1.703429	-1.500078
C	-1.353976	2.202274	-1.322876
C	-0.363778	1.444801	-0.686700
H	-2.179570	-1.335110	-0.069403
H	-3.405623	2.299486	-1.982333
H	0.623930	1.875006	-0.590182
C	1.801793	-0.241332	0.491859
C	2.151195	0.986690	1.072522
C	3.471469	1.437610	1.051884
C	4.482862	0.673297	0.471616
C	4.144636	-0.565289	-0.065598
C	2.827051	-1.021005	-0.042548
H	1.397191	1.614630	1.532856
H	5.504364	1.032317	0.446044
H	2.606404	-2.003269	-0.429985
C	-4.272286	-0.192383	-1.288145
C	-0.979709	3.544463	-1.889548
C	3.804298	2.747753	1.714161
C	5.176748	-1.407497	-0.763991
F	4.954233	-2.730215	-0.574545
F	6.430176	-1.139075	-0.342846
F	5.151820	-1.201215	-2.103485
F	4.921862	3.305070	1.201098
F	2.800634	3.644480	1.577021
F	4.011771	2.594825	3.043782
F	-0.095559	4.194698	-1.097744
F	-2.052149	4.349415	-2.048488
F	-0.392923	3.420565	-3.105151
F	-5.259878	0.727646	-1.264767
F	-4.317542	-0.787603	-2.511272
F	-4.581551	-1.148687	-0.385973
C	-6.767212	-0.351902	1.869218
H	-6.272213	-1.313454	2.028561
H	-7.714235	-0.368720	2.422982
H	-7.023736	-0.292701	0.802515
H	-6.430962	1.778102	2.318368

Vibrational frequencies

15.9147	19.0805	22.3118
24.7073	31.6679	33.1664

34.9764	37.3681	50.1030
58.4851	62.1171	70.9837
75.6921	80.3427	87.5626
97.7987	99.4631	102.2769
105.6761	114.0128	117.7374
128.5212	135.2149	150.9902
155.4189	162.7417	167.3794
177.0283	179.3643	189.4579

M1c+2c

Zero-point correction= 0.715002
Thermal correction to Energy= 0.773162
Thermal correction to Enthalpy= 0.774106
Thermal correction to Gibbs Free Energy= 0.616206
Sum of electronic and zero-point Energies= -3384.706730
Sum of electronic and thermal Energies= -3384.648570
Sum of electronic and thermal Enthalpies= -3384.647625
Sum of electronic and thermal Free Energies= -3384.805526

Cartesian coordinates

C	-0.431597	-1.231390	0.884355
N	0.986504	-0.917299	0.878864
C	1.520183	-0.655716	2.214478
C	0.454803	-1.232838	3.170163
C	-0.599084	-1.906936	2.261032
H	-0.643153	-1.908031	0.049648
H	2.493643	-1.148406	2.292774
H	1.672514	0.420590	2.374821
H	0.894227	-1.950715	3.866713
H	-0.004695	-0.431699	3.749134
H	-0.379464	-2.972137	2.144022
H	-1.604621	-1.802590	2.668984
C	1.729258	-0.790594	-0.248811
C	2.944298	-0.173637	-0.333180
H	1.279284	-1.213202	-1.140936
H	3.348726	0.312592	0.544241
C	3.699547	-0.136101	-1.555177
C	4.843137	0.553902	-1.777445
H	3.321148	-0.748277	-2.371456
C	-1.364876	0.053374	0.682940
O	-1.444060	0.693955	1.946637
Si	-2.598279	1.623971	2.760648
C	-1.686075	2.077958	4.336646
H	-2.295686	2.737259	4.965729

H	-1.446036	1.188394	4.929187
H	-0.746738	2.599549	4.121863
C	-4.137532	0.621331	3.160249
H	-4.728826	0.383852	2.271189
H	-3.891563	-0.319514	3.664711
H	-4.782283	1.195772	3.837360
C	-3.058999	3.174692	1.793359
H	-3.372805	3.961816	2.489932
H	-2.208900	3.566132	1.223677
H	-3.889954	3.009055	1.101612
C	-0.640514	0.963499	-0.313652
C	0.213380	1.958990	0.161373
C	1.116369	2.586975	-0.695913
C	1.169585	2.257800	-2.047254
C	0.286341	1.293751	-2.529198
C	-0.611115	0.651654	-1.675980
H	0.226745	2.183568	1.220113
H	1.905337	2.709379	-2.699712
H	-1.250437	-0.130152	-2.072217
C	-2.772880	-0.324790	0.195489
C	-3.359356	-1.565804	0.464062
C	-4.693874	-1.810135	0.133406
C	-5.478291	-0.826037	-0.462908
C	-4.891065	0.403761	-0.751263
C	-3.554799	0.647069	-0.440303
H	-2.797142	-2.359522	0.937590
H	-6.516179	-1.015147	-0.706309
H	-3.125561	1.610258	-0.688420
C	2.115800	3.529756	-0.086267
C	0.418136	0.788132	-3.937188
C	-5.293903	-3.137559	0.512833
C	-5.704000	1.529093	-1.330000
F	-5.986658	2.459089	-0.380361
F	-6.880287	1.108416	-1.836697
F	-5.037746	2.173313	-2.313327
F	-5.546135	-3.197648	1.842237
F	-6.458128	-3.374901	-0.126179
F	-4.455020	-4.161003	0.231041
F	1.013562	1.677422	-4.755535
F	-0.778818	0.466794	-4.476813
F	1.171974	-0.347782	-3.969577
F	3.022640	3.978883	-0.975912
F	1.520427	4.608567	0.472499
F	2.806245	2.915803	0.915911

N	5.371180	-2.093673	0.201717
N	4.247191	-2.323293	0.730313
C	6.151358	-1.151054	0.963039
C	3.431279	-3.264349	-0.006201
O	7.352897	-1.087073	0.816333
O	2.545120	-3.859003	0.571807
O	3.744444	-3.385890	-1.299218
O	5.428122	-0.363037	1.771905
C	6.168690	0.614809	2.544065
H	6.790793	1.207142	1.867313
H	6.833165	0.082902	3.232925
C	5.152077	1.465171	3.276914
H	4.520394	0.847147	3.922115
H	5.669900	2.198992	3.902838
H	4.508817	2.006258	2.576928
C	2.952473	-4.329561	-2.068678
H	3.568010	-4.532616	-2.947508
H	2.838984	-5.250012	-1.489098
C	1.599601	-3.757514	-2.457945
H	1.071161	-4.478713	-3.090617
H	0.991726	-3.575569	-1.568470
H	1.706313	-2.826037	-3.021813
C	5.514077	1.532193	-0.860595
H	5.621558	2.505491	-1.357294
H	4.960773	1.697083	0.064433
H	6.529525	1.200502	-0.605964
H	5.317824	0.429297	-2.749307

Vibrational frequencies

12.1472	15.7309	20.3680
21.9783	23.7778	26.5052
28.6623	33.5478	34.5498
37.4899	40.2395	44.3675
44.7595	48.0804	53.3849
61.8001	71.3838	74.3430
78.6389	82.1032	86.0492
95.7062	98.5355	102.6914
103.2985	107.1651	108.9206
117.5911	133.2068	136.2997

TSc

Zero-point correction= 0.716064

Thermal correction to Energy= 0.772724

Thermal correction to Enthalpy= 0.773669

Thermal correction to Gibbs Free Energy= 0.618768
Sum of electronic and zero-point Energies= -3384.680999
Sum of electronic and thermal Energies= -3384.624338
Sum of electronic and thermal Enthalpies= -3384.623394
Sum of electronic and thermal Free Energies= -3384.778295

Cartesian coordinates

C	0.384041	-1.392945	-0.363813
N	-0.943859	-0.853669	-0.700009
C	-1.363408	-1.271236	-2.049201
C	-0.755950	-2.672061	-2.157308
C	0.511626	-2.646042	-1.270104
H	0.396636	-1.632983	0.702690
H	-2.451242	-1.293035	-2.103098
H	-0.946667	-0.576253	-2.783611
H	-1.484213	-3.384178	-1.765339
H	-0.530267	-2.936925	-3.192662
H	0.581391	-3.551936	-0.662949
H	1.416062	-2.577352	-1.874605
C	-1.667088	-0.133231	0.140100
C	-2.865085	0.516319	-0.162581
H	-1.275735	-0.068729	1.151518
H	-3.185779	0.574227	-1.193410
C	-3.679480	1.015463	0.842002
C	-5.008138	1.405711	0.581339
H	-3.364504	0.898989	1.877175
C	1.503281	-0.309520	-0.636343
O	1.478400	-0.109839	-2.035198
Si	2.423020	0.515982	-3.293339
C	1.292314	0.284900	-4.771610
H	1.767709	0.656488	-5.686938
H	1.050893	-0.771704	-4.930804
H	0.350665	0.830697	-4.645871
C	4.014772	-0.459161	-3.521470
H	4.826492	-0.125006	-2.869951
H	3.859777	-1.529571	-3.347196
H	4.360043	-0.344927	-4.556558
C	2.786190	2.347347	-3.052343
H	3.300850	2.723848	-3.945671
H	1.872891	2.938558	-2.929748
H	3.438765	2.562186	-2.199851
C	1.113378	0.986928	0.092108
C	0.383275	1.965637	-0.580987
C	-0.075930	3.099210	0.088886

C	0.175422	3.275785	1.445626
C	0.901311	2.293973	2.122756
C	1.366986	1.159520	1.457364
H	0.150392	1.830954	-1.628177
H	-0.190138	4.151527	1.967555
H	1.921072	0.410317	2.011830
C	2.889254	-0.777790	-0.154373
C	3.159562	-2.054291	0.341783
C	4.456691	-2.409080	0.727031
C	5.510627	-1.509122	0.614291
C	5.239613	-0.227620	0.135366
C	3.947689	0.136701	-0.227939
H	2.378726	-2.793680	0.452902
H	6.514813	-1.789998	0.907192
H	3.764558	1.150973	-0.559863
C	-0.917889	4.078850	-0.682943
C	1.236479	2.485473	3.578665
C	4.704237	-3.814280	1.209379
C	6.360185	0.751935	-0.083609
F	6.815670	0.684351	-1.361260
F	7.412469	0.513516	0.724759
F	5.962952	2.027255	0.119375
F	4.794269	-4.681325	0.173829
F	5.848378	-3.915917	1.916005
F	3.694814	-4.251786	1.997672
F	0.301715	3.221872	4.216380
F	2.419845	3.122214	3.736019
F	1.337489	1.302615	4.227225
F	-1.096403	5.239436	-0.022882
F	-0.355513	4.368692	-1.881873
F	-2.145617	3.568681	-0.947002
N	-5.790594	-0.449799	0.503683
N	-5.213421	-1.194490	-0.439996
C	-7.147975	-0.168519	0.364200
C	-4.319124	-2.122464	0.062442
O	-7.725964	0.800720	0.838551
O	-3.669283	-2.872350	-0.666560
O	-4.255359	-2.213510	1.428316
O	-7.800403	-1.195464	-0.233564
C	-9.238897	-1.084485	-0.244388
H	-9.529464	-0.168516	-0.770518
H	-9.604020	-1.000558	0.785228
C	-9.772534	-2.324401	-0.933268
H	-9.471359	-3.228405	-0.395290

H	-10.866536	-2.290429	-0.968119
H	-9.395001	-2.393074	-1.958011
C	-3.493515	-3.312887	1.954481
H	-3.887665	-3.463942	2.963787
H	-3.687879	-4.211969	1.361822
C	-2.001582	-3.017682	1.993645
H	-1.465051	-3.843578	2.474092
H	-1.626644	-2.900458	0.975693
H	-1.802376	-2.104382	2.564464
C	-5.390229	1.961994	-0.771677
H	-4.781672	2.841488	-1.014534
H	-5.239746	1.218693	-1.562738
H	-6.441216	2.253929	-0.774141
H	-5.582148	1.774186	1.423092

Vibrational frequencies

-328.2717	11.8508	15.2488
17.0577	21.1249	25.1275
26.9316	28.1367	28.9294
30.6275	33.4917	36.8261
45.9276	48.8364	52.8800
56.8948	65.2336	74.7593
76.0280	81.9579	89.4842
95.1444	95.5298	99.3470
102.7169	107.5525	112.2458
121.4332	123.4024	127.9943

TSc'

Zero-point correction= 0.715339
Thermal correction to Energy= 0.772527
Thermal correction to Enthalpy= 0.773471
Thermal correction to Gibbs Free Energy= 0.616561
Sum of electronic and zero-point Energies= -3384.677529
Sum of electronic and thermal Energies= -3384.620341
Sum of electronic and thermal Enthalpies= -3384.619397
Sum of electronic and thermal Free Energies= -3384.776307

Cartesian coordinates

C	0.291060	-1.966404	-2.115622
C	0.167006	-1.094768	-0.855235
N	-1.226157	-0.647254	-0.921567
C	-1.748179	-0.620208	-2.303115
C	-0.661699	-1.319313	-3.141984
C	1.229975	0.089815	-0.798893

O	1.247410	0.678097	-2.085654
Si	1.914591	2.112979	-2.725472
C	2.607372	1.593137	-4.392633
C	-1.926320	-0.358616	0.154434
C	-3.270100	0.113585	0.162463
N	-4.272176	-1.472327	-0.224248
N	-4.781078	-2.059994	0.870167
C	-3.891998	-2.850408	1.538674
O	-4.194319	-3.567797	2.485246
C	2.568087	-0.595092	-0.477736
C	3.610260	-0.577356	-1.402341
C	4.828792	-1.195925	-1.126926
C	5.031263	-1.878415	0.069139
C	3.974378	-1.944822	0.975560
C	2.757546	-1.316944	0.708272
C	4.134392	-2.645522	2.298493
F	3.050702	-3.403094	2.589044
C	5.937172	-1.033945	-2.130954
F	6.934083	-1.921561	-1.948439
C	0.812718	1.153190	0.239282
C	-0.271119	1.977344	-0.100578
C	-0.753084	2.940670	0.777224
C	-0.160769	3.125259	2.025674
C	0.935957	2.335344	2.357101
C	1.423675	1.361972	1.477404
C	-1.885001	3.825950	0.330573
F	-1.415483	4.951009	-0.266367
C	1.584427	2.474152	3.709931
F	1.096519	1.562890	4.584349
F	-2.678992	3.210244	-0.575511
F	-2.663160	4.219263	1.359105
F	1.377776	3.693609	4.249129
F	2.920389	2.275865	3.644713
F	5.215895	-3.449293	2.325903
F	4.266362	-1.753968	3.309280
F	6.480359	0.206507	-2.054857
F	5.483501	-1.176638	-3.399154
C	-3.744057	0.635558	1.450066
C	-4.698796	1.565634	1.614196
C	3.253465	2.822651	-1.613037
C	0.553567	3.380493	-3.006405
C	-5.204908	-1.068104	-1.184794
O	-4.996158	-0.210793	-2.042232
O	-6.308667	-1.836475	-1.175979

C	-7.244428	-1.591032	-2.250554
C	-8.410576	-2.535417	-2.043019
O	-2.569272	-2.732871	1.116752
C	-1.613581	-3.515718	1.853698
C	-1.548614	-4.940225	1.328861
H	0.287166	-1.677412	0.058426
H	-2.710756	-1.129916	-2.314299
H	-1.919712	0.417535	-2.608391
H	-1.099577	-2.062868	-3.811182
H	-0.120700	-0.590233	-3.744450
H	-0.046000	-2.976337	-1.864484
H	1.317899	-2.030205	-2.477227
H	-1.409125	-0.499422	1.096629
H	-3.571210	0.648368	-0.729364
H	-3.286008	0.203782	2.338371
H	0.926250	4.158354	-3.684592
H	-0.325297	2.934398	-3.486093
H	0.222400	3.881832	-2.092755
H	3.428521	0.871682	-4.317346
H	1.827948	1.142450	-5.017456
H	2.992472	2.467696	-4.930333
H	3.565911	3.796623	-2.009645
H	2.897248	2.987720	-0.591330
H	4.145172	2.189940	-1.562764
H	-0.744317	1.868799	-1.064877
H	-0.538675	3.869965	2.715766
H	2.296742	0.797713	1.776451
H	1.962367	-1.402493	1.440630
H	5.977178	-2.359853	0.283413
H	3.473081	-0.097370	-2.358600
H	-7.555931	-0.541536	-2.223586
H	-6.743521	-1.762044	-3.209832
H	-0.654222	-3.003310	1.716360
H	-1.868002	-3.502891	2.917226
H	-9.152179	-2.389402	-2.835233
H	-8.078142	-3.577485	-2.068056
H	-8.892906	-2.352675	-1.078208
H	-0.774272	-5.506720	1.858082
H	-2.509960	-5.436114	1.482696
H	-1.315356	-4.949525	0.258971
C	-5.478157	2.265759	0.542932
H	-6.552564	2.185432	0.749495
H	-5.237778	3.336481	0.533116
H	-5.302899	1.860213	-0.455578

H	-4.941519	1.855703	2.635462

Vibrational frequencies

-417.7543	9.0052	12.7127
17.0149	19.8232	22.6121
24.9100	27.1977	31.0059
34.3054	34.8567	41.3616
46.4098	49.6283	53.9225
60.5461	67.0040	71.5518
75.1540	80.0517	82.7569
85.3512	93.3044	98.4647
98.6244	102.0012	108.6213
114.1757	121.5550	124.0423

M2c

Zero-point correction= 0.717857
Thermal correction to Energy= 0.774816
Thermal correction to Enthalpy= 0.775760
Thermal correction to Gibbs Free Energy= 0.620112
Sum of electronic and zero-point Energies= -3384.708760
Sum of electronic and thermal Energies= -3384.651801
Sum of electronic and thermal Enthalpies= -3384.650857
Sum of electronic and thermal Free Energies= -3384.806505

Cartesian coordinates

C	0.224130	-0.920424	-1.018923
N	-0.915892	-0.117134	-1.523376
C	-1.029920	-0.235943	-2.989046
C	-0.608961	-1.686221	-3.220520
C	0.471439	-1.951985	-2.151523
H	-0.085448	-1.400548	-0.087914
H	-2.055855	-0.048614	-3.301337
H	-0.349643	0.484806	-3.451776
H	-1.486387	-2.315265	-3.051731
H	-0.240579	-1.849972	-4.235930
H	0.400714	-2.973127	-1.770184
H	1.470982	-1.816842	-2.564096
C	-1.796151	0.460921	-0.734326
C	-2.926653	1.194998	-1.128621
H	-1.650727	0.296155	0.326626
H	-3.104179	1.396828	-2.176295
C	-3.904573	1.432235	-0.196804
C	-5.339566	1.540247	-0.579680
H	-3.706480	1.234588	0.854554

C	1.457288	0.017828	-0.713334
O	1.850613	0.569101	-1.951937
Si	3.270758	0.739481	-2.865420
C	2.582647	1.218966	-4.542153
H	3.389811	1.408291	-5.259175
H	1.950516	0.425708	-4.956128
H	1.979026	2.131162	-4.477800
C	4.245023	-0.863971	-2.971448
H	4.659551	-1.170407	-2.006993
H	3.645969	-1.693282	-3.362203
H	5.088345	-0.722321	-3.659157
C	4.351171	2.116691	-2.175403
H	4.988706	2.514704	-2.974565
H	3.752179	2.952067	-1.795312
H	5.015050	1.778157	-1.374766
C	0.963009	1.141524	0.210153
C	0.810193	2.443639	-0.258468
C	0.206598	3.414959	0.545273
C	-0.298143	3.092768	1.801064
C	-0.140777	1.786176	2.266384
C	0.518887	0.829348	1.499611
H	1.132191	2.690268	-1.262081
H	-0.811666	3.834607	2.399737
H	0.633993	-0.176980	1.889410
C	2.618222	-0.716644	-0.022276
C	2.733478	-2.104759	0.065735
C	3.869640	-2.686837	0.635043
C	4.914659	-1.903865	1.115787
C	4.790011	-0.516598	1.049825
C	3.651726	0.069149	0.504249
H	1.953878	-2.758941	-0.298391
H	5.795226	-2.361785	1.548629
H	3.570987	1.149739	0.489720
C	0.105925	4.816591	0.004753
C	-0.835759	1.332756	3.519407
C	3.975615	-4.189110	0.653575
C	5.905652	0.381561	1.512648
F	6.603866	0.871724	0.455792
F	6.785119	-0.259399	2.307097
F	5.434284	1.449562	2.192721
F	4.329902	-4.670323	-0.561151
F	4.894120	-4.623498	1.540112
F	2.792969	-4.764684	0.970620
F	-1.996109	0.693290	3.195270

F	-1.157604	2.352003	4.336200
F	-0.094772	0.450972	4.223307
F	-0.657295	5.614312	0.778049
F	1.328485	5.391089	-0.089476
F	-0.422472	4.824960	-1.240896
N	-5.649908	0.075258	-0.628549
N	-5.223149	-0.643554	-1.746520
C	-6.207678	-0.482531	0.505890
C	-4.266578	-1.563091	-1.501397
O	-6.386299	0.123471	1.557097
O	-3.770381	-2.303486	-2.358565
O	-3.822395	-1.654808	-0.173345
O	-6.580959	-1.760130	0.299996
C	-7.056768	-2.453214	1.469694
H	-7.959679	-1.959558	1.845297
H	-6.296872	-2.393361	2.257048
C	-7.327061	-3.885407	1.056114
H	-6.414760	-4.360001	0.682174
H	-7.691486	-4.458950	1.914765
H	-8.082617	-3.926032	0.265960
C	-2.931056	-2.727648	0.111439
H	-3.394416	-3.686408	-0.150980
H	-2.025370	-2.642872	-0.502735
C	-2.606913	-2.661452	1.594126
H	-1.882536	-3.437358	1.865558
H	-2.194150	-1.685189	1.871778
H	-3.509989	-2.811327	2.193691
C	-5.681795	2.235177	-1.889642
H	-5.233968	1.723752	-2.743098
H	-6.765763	2.232980	-2.034101
H	-5.335698	3.273468	-1.862161
H	-5.927665	1.948883	0.240942

Vibrational frequencies

8.6553	13.3267	18.1572
19.7848	24.2599	25.2872
28.1757	33.3366	34.0620
37.4422	38.7322	42.7459
46.4202	51.8270	54.8172
69.9179	74.1888	77.7098
78.3536	86.9615	91.0886
98.9408	100.5927	105.5424
105.8499	109.3072	113.9353
125.8492	129.6005	139.3082

1d

Zero-point correction= 0.205697
Thermal correction to Energy= 0.217936
Thermal correction to Enthalpy= 0.218880
Thermal correction to Gibbs Free Energy= 0.165870
Sum of electronic and zero-point Energies= -576.695413
Sum of electronic and thermal Energies= -576.683174
Sum of electronic and thermal Enthalpies= -576.682230
Sum of electronic and thermal Free Energies= -576.735240

Cartesian coordinates

C	3.593044	1.536202	-0.065354
C	2.252786	1.163006	-0.092814
C	1.885530	-0.196213	-0.015397
C	2.905854	-1.161463	0.085079
C	4.248079	-0.785381	0.115330
C	4.595987	0.565013	0.040456
H	3.859950	2.587173	-0.128509
H	1.488290	1.928603	-0.180885
H	2.636468	-2.212869	0.141873
H	5.020389	-1.544805	0.195304
H	5.640613	0.861594	0.061143
C	0.495152	-0.650832	-0.035208
H	0.351852	-1.730453	-0.048349
C	-0.615919	0.109886	-0.029821
H	-0.587906	1.194123	-0.001056
C	-1.948700	-0.521322	-0.053288
O	-2.922535	0.412641	0.006426
C	-4.285877	-0.081240	-0.009396
H	-4.413400	-0.796373	0.809554
H	-4.457086	-0.615119	-0.950258
C	-5.202144	1.115093	0.137137
H	-6.244792	0.782070	0.126065
H	-5.017388	1.636327	1.081631
H	-5.058214	1.822667	-0.685291
O	-2.172656	-1.721319	-0.116622

Vibrational frequencies

39.0739	63.2203	70.9224
92.6813	112.7625	184.0026
192.6875	238.8041	280.2768
291.6044	324.5719	390.8834
414.0853	500.5441	521.9026

585.4505	631.4924	697.1435
724.0013	751.4064	784.3324
830.0877	853.6677	859.5590
889.2190	904.7981	942.7975
985.6804	1005.4512	1010.8347

1d+B•

Zero-point correction= 0.356652
Thermal correction to Energy= 0.379127
Thermal correction to Enthalpy= 0.380071
Thermal correction to Gibbs Free Energy= 0.303205
Sum of electronic and zero-point Energies= -907.469593
Sum of electronic and thermal Energies= -907.447118
Sum of electronic and thermal Enthalpies= -907.446173
Sum of electronic and thermal Free Energies= -907.523040

Cartesian coordinates

C	0.500717	-1.349936	0.677133
C	-0.592408	-1.385157	-0.108092
H	-0.541726	-1.372983	-1.190479
C	-1.935618	-1.363227	0.492811
O	-2.886810	-1.232457	-0.458343
C	-4.258748	-1.188298	0.007801
H	-4.362146	-0.376886	0.734274
H	-4.486504	-2.128355	0.521134
C	-5.141444	-0.977469	-1.203895
H	-6.190228	-0.945756	-0.892278
H	-4.902167	-0.033382	-1.703635
H	-5.020803	-1.792422	-1.924353
O	-2.190429	-1.432333	1.687585
C	-1.077934	1.743626	-1.279657
C	0.233102	1.796727	-1.642610
H	-1.967199	1.592638	-1.870758
H	0.699055	1.709757	-2.611390
C	0.140401	2.057149	0.612373
N	-1.133080	1.904285	0.090743
N	0.972915	1.987844	-0.492373
C	-2.349050	1.934344	0.885563
H	-2.458816	2.905389	1.377538
H	-3.201354	1.767073	0.227108
H	-2.322465	1.151673	1.647273
C	2.416117	2.142819	-0.435874
H	2.851333	1.394038	0.228976
H	2.822840	2.012368	-1.438531

H	2.676209	3.139793	-0.066984
B	0.530945	2.228796	2.054828
H	1.687803	2.339339	2.349562
H	-0.319271	2.258071	2.899430
C	1.897283	-1.301115	0.245937
C	2.284627	-1.303402	-1.109242
C	2.900884	-1.216937	1.229720
C	3.628680	-1.221942	-1.461056
H	1.532871	-1.361642	-1.889805
C	4.247276	-1.135264	0.875490
H	2.614474	-1.207522	2.277860
C	4.615441	-1.135869	-0.471776
H	3.910519	-1.221622	-2.509998
H	5.006410	-1.068459	1.649284
H	5.662723	-1.069383	-0.751680
H	0.336838	-1.338578	1.753026

Vibrational frequencies

29.4572	36.8420	45.8119
50.7171	66.0596	68.8259
74.0834	81.6162	96.7408
114.0095	121.9827	156.5851
180.1057	184.2815	190.4089
195.9125	239.4845	242.9874
249.3019	277.2436	292.7843
308.4002	315.2780	326.9121
390.5870	410.8654	413.0537
472.4029	500.0719	523.6573

TSd

Zero-point correction= 0.356625
Thermal correction to Energy= 0.378031
Thermal correction to Enthalpy= 0.378975
Thermal correction to Gibbs Free Energy= 0.304737
Sum of electronic and zero-point Energies= -907.464927
Sum of electronic and thermal Energies= -907.443521
Sum of electronic and thermal Enthalpies= -907.442576
Sum of electronic and thermal Free Energies= -907.516815

Cartesian coordinates

C	0.375256	-1.886721	0.130180
H	0.234628	-2.740492	0.789970
C	-0.733319	-1.141570	-0.176812
H	-0.695706	-0.342674	-0.906356

C	-2.073232	-1.582233	0.226967
O	-3.035445	-0.901035	-0.452278
C	-4.402072	-1.183645	-0.080482
H	-4.523623	-1.008086	0.993919
H	-4.616233	-2.240514	-0.272674
C	-5.290895	-0.272313	-0.901711
H	-6.341235	-0.464420	-0.660195
H	-5.074796	0.779482	-0.688826
H	-5.146574	-0.447804	-1.972453
O	-2.335116	-2.461383	1.037804
C	0.516590	3.112142	-0.791777
C	1.611089	2.811940	-0.037334
H	0.410867	3.738311	-1.663605
H	2.639013	3.124258	-0.130426
C	-0.154798	1.721890	0.860434
N	-0.556078	2.447274	-0.236017
N	1.192507	1.972082	0.973482
C	-1.922465	2.477493	-0.742871
H	-1.934254	3.036409	-1.678685
H	-2.279630	1.460376	-0.916095
H	-2.583528	2.966164	-0.021722
C	2.065417	1.376760	1.975488
H	2.159227	0.301313	1.808219
H	3.049760	1.838349	1.895927
H	1.661327	1.553191	2.974478
B	-1.003566	0.768297	1.688763
H	-0.494239	0.174990	2.593130
H	-2.192084	0.809719	1.586521
C	1.736526	-1.588850	-0.264107
C	2.079921	-0.481332	-1.078470
C	2.791693	-2.404094	0.209566
C	3.406849	-0.207110	-1.391375
H	1.303610	0.178238	-1.451573
C	4.118639	-2.127883	-0.110234
H	2.554192	-3.257704	0.839750
C	4.437237	-1.026615	-0.912426
H	3.641983	0.654527	-2.010433
H	4.908079	-2.770488	0.270140
H	5.471913	-0.807913	-1.159495

Vibrational frequencies

-189.5632	34.5807	38.3452
41.1036	51.9542	69.0249
80.6784	91.2059	96.9870

111.5068	131.7215	146.5288
156.3917	168.0825	190.6096
210.8395	241.1348	264.3754
271.4245	300.9216	312.2563
316.7052	327.7116	330.1265
392.1442	419.9448	473.8774
506.2911	517.0920	532.3356

TSd'

Zero-point correction= 0.356822
Thermal correction to Energy= 0.378029
Thermal correction to Enthalpy= 0.378973
Thermal correction to Gibbs Free Energy= 0.305755
Sum of electronic and zero-point Energies= -907.464421
Sum of electronic and thermal Energies= -907.443214
Sum of electronic and thermal Enthalpies= -907.442270
Sum of electronic and thermal Free Energies= -907.515488

Cartesian coordinates

C	0.110238	-1.437820	0.460752
C	-1.009480	-1.147446	-0.289848
H	-0.937985	-0.755493	-1.298186
C	-2.332828	-1.249964	0.281098
O	-3.288287	-0.804040	-0.595321
C	-4.644616	-0.812995	-0.106484
H	-4.701383	-0.224003	0.815632
H	-4.934475	-1.840371	0.141623
C	-5.525416	-0.232611	-1.194400
H	-6.569289	-0.230692	-0.864340
H	-5.236160	0.797852	-1.424719
H	-5.455911	-0.824843	-2.112295
O	-2.622022	-1.655660	1.406184
C	0.109672	2.931630	-0.824189
C	1.463481	2.819236	-0.733244
H	-0.509439	3.485845	-1.511883
H	2.250273	3.255721	-1.327998
C	0.564953	1.569778	0.920780
N	-0.431823	2.166147	0.188722
N	1.732002	1.983821	0.329009
C	-1.867203	2.076923	0.440073
H	-2.279058	3.085189	0.533365
H	-2.364125	1.552716	-0.377913
H	-2.037112	1.532109	1.365652
C	3.070343	1.646236	0.801299

H	3.183172	0.565456	0.870982
H	3.795727	2.038209	0.088722
H	3.246558	2.095179	1.782327
B	0.431636	0.541900	2.044461
H	1.426313	0.162189	2.585888
H	-0.630268	0.358268	2.556854
C	1.482138	-1.466036	-0.054508
C	1.859539	-0.828823	-1.255340
C	2.480306	-2.154592	0.667135
C	3.176855	-0.876729	-1.707533
H	1.123523	-0.272449	-1.826509
C	3.795520	-2.204370	0.211985
H	2.211024	-2.648828	1.597134
C	4.154053	-1.561707	-0.978706
H	3.444311	-0.368745	-2.630219
H	4.544054	-2.742837	0.786871
H	5.180649	-1.593238	-1.331727
H	-0.052689	-1.933179	1.414188

Vibrational frequencies

-173.1770	33.8046	39.2842
58.7406	70.5413	76.6511
77.1079	87.1870	94.2331
108.0986	137.4330	151.8464
179.3629	182.5791	199.7378
226.1099	238.4489	267.2753
272.0364	287.7644	308.6571
322.5908	339.7493	349.4323
390.6166	416.9490	470.5229
509.9912	524.7872	531.8788

M1d

Zero-point correction= 0.358608
Thermal correction to Energy= 0.379880
Thermal correction to Enthalpy= 0.380825
Thermal correction to Gibbs Free Energy= 0.306504
Sum of electronic and zero-point Energies= -907.488797
Sum of electronic and thermal Energies= -907.467524
Sum of electronic and thermal Enthalpies= -907.466580
Sum of electronic and thermal Free Energies= -907.540901

Cartesian coordinates

C	-0.100509	-1.512033	0.384703
H	-0.320082	-2.196772	1.200273

C	-1.129237	-0.487489	0.100223
H	-1.096455	-0.128698	-0.932149
C	-2.516348	-0.964068	0.401042
O	-3.431325	-0.354984	-0.389842
C	-4.820457	-0.647070	-0.106174
H	-5.024265	-0.429506	0.947520
H	-5.002647	-1.714968	-0.267869
C	-5.659758	0.211739	-1.029457
H	-6.722111	0.017697	-0.849868
H	-5.468294	1.274870	-0.853007
H	-5.440999	-0.011619	-2.078456
O	-2.828421	-1.760075	1.272920
C	1.963876	2.826026	-0.447854
C	2.639454	2.184581	0.541473
H	2.300415	3.507513	-1.212894
H	3.683971	2.188567	0.809441
C	0.471535	1.594682	0.708779
N	0.637697	2.453896	-0.328968
N	1.708411	1.438227	1.241822
C	-0.436155	2.923364	-1.201806
H	0.005129	3.518814	-2.000917
H	-0.966219	2.074062	-1.634421
H	-1.140625	3.536816	-0.636874
C	2.069607	0.562008	2.352962
H	2.639692	-0.290459	1.977410
H	2.674194	1.122492	3.068964
H	1.163258	0.205804	2.836680
B	-0.904934	0.874497	1.111149
H	-0.878933	0.517291	2.271946
H	-1.823528	1.651774	0.925516
C	1.176195	-1.599006	-0.217897
C	1.599450	-0.751999	-1.287994
C	2.126875	-2.553266	0.261790
C	2.879898	-0.846486	-1.816305
H	0.914136	-0.013759	-1.690125
C	3.402116	-2.639606	-0.276850
H	1.835357	-3.214650	1.074169
C	3.796187	-1.785689	-1.319957
H	3.172999	-0.181078	-2.624301
H	4.101900	-3.373113	0.115420
H	4.796613	-1.852076	-1.736874

Vibrational frequencies

25.4168	33.5546	56.4272

57.2234	66.1103	80.3034
89.5593	90.4845	100.3606
108.4489	127.5996	165.5360
167.7017	190.8468	200.7408
253.3586	281.9737	288.7860
303.8208	312.7105	332.3541
342.4416	386.0271	393.3881
422.0880	472.3189	492.9040
521.4870	575.2969	577.9973

1e

Zero-point correction= 0.151544
Thermal correction to Energy= 0.161025
Thermal correction to Enthalpy= 0.161969
Thermal correction to Gibbs Free Energy= 0.116232
Sum of electronic and zero-point Energies= -384.991909
Sum of electronic and thermal Energies= -384.982429
Sum of electronic and thermal Enthalpies= -384.981485
Sum of electronic and thermal Free Energies= -385.027221

Cartesian coordinates

C	2.440314	0.147931	0.000019
H	2.484992	1.236762	0.000033
C	1.230119	-0.427650	-0.000067
H	1.110411	-1.507436	-0.000079
C	-0.002016	0.387474	-0.000148
O	-1.098876	-0.400791	-0.000052
C	-2.377937	0.281996	0.000022
H	-2.436508	0.924675	-0.884585
H	-2.436394	0.924701	0.884617
C	-3.458774	-0.778615	0.000108
H	-4.442639	-0.298897	0.000169
H	-3.385373	-1.413121	-0.888550
H	-3.385252	-1.413098	0.888772
O	-0.054473	1.607989	-0.000052
C	3.741126	-0.583536	0.000089
H	4.337818	-0.303987	0.878111
H	3.604828	-1.668797	0.000083
H	4.337909	-0.303990	-0.877873

Vibrational frequencies

32.8389	76.9536	121.9086
148.3164	210.2774	227.0384
252.7991	270.8929	352.8230

401.6108	463.7234	700.9228
755.8641	813.7472	853.2263
887.3205	929.9184	1006.6686
1011.4471	1060.3663	1081.7022
1130.9734	1138.1420	1177.3389
1219.6174	1303.8936	1325.1210
1347.0199	1397.9733	1407.6380

1e+B•

Zero-point correction= 0.302634
Thermal correction to Energy= 0.322332
Thermal correction to Enthalpy= 0.323276
Thermal correction to Gibbs Free Energy= 0.252703
Sum of electronic and zero-point Energies= -715.762236
Sum of electronic and thermal Energies= -715.742538
Sum of electronic and thermal Enthalpies= -715.741594
Sum of electronic and thermal Free Energies= -715.812167

Cartesian coordinates

C	0.706806	2.399206	0.072927
H	0.530097	2.680020	1.110314
C	-0.240973	1.686952	-0.552348
H	-0.126431	1.357828	-1.580474
C	-1.463718	1.267806	0.157596
O	-2.236714	0.487237	-0.628511
C	-3.456008	-0.024351	-0.034458
H	-4.140123	0.812824	0.141659
H	-3.219742	-0.474818	0.933733
C	-4.037631	-1.035244	-0.999776
H	-4.970579	-1.437971	-0.592815
H	-4.254636	-0.574580	-1.968449
H	-3.343791	-1.867028	-1.157699
O	-1.759847	1.558991	1.308147
C	1.230022	-1.542715	-1.414119
C	0.136721	-1.805245	-0.647775
H	1.399951	-1.684674	-2.469796
H	-0.827451	-2.207963	-0.912768
C	1.732451	-0.937077	0.718056
N	2.198352	-1.012044	-0.583773
N	0.441803	-1.435217	0.646959
C	3.533928	-0.618312	-0.996784
H	3.618698	-0.741554	-2.077071
H	3.719080	0.427155	-0.739200
H	4.286535	-1.240487	-0.502812

C	-0.449866	-1.558933	1.787909
H	0.015987	-2.169358	2.566557
H	-0.684903	-0.573495	2.197492
H	-1.372076	-2.039077	1.459807
B	2.453995	-0.411516	1.928619
H	1.899845	-0.397769	2.991503
H	3.580137	-0.012791	1.823403
C	1.992888	2.843242	-0.540160
H	2.838676	2.509326	0.072495
H	2.119359	2.461217	-1.557034
H	2.045073	3.939800	-0.567744

Vibrational frequencies

23.0402	30.5468	46.5588
58.6136	72.3752	81.1000
105.2274	123.9276	130.2878
133.5954	160.8109	162.5154
183.2176	205.5416	231.0076
238.9211	243.6676	255.6999
290.3121	304.6114	309.1514
355.4088	404.6290	413.7281
467.1672	470.5680	576.5395
593.8574	631.7595	700.4564

TSe

Zero-point correction= 0.302419
Thermal correction to Energy= 0.321050
Thermal correction to Enthalpy= 0.321994
Thermal correction to Gibbs Free Energy= 0.254359
Sum of electronic and zero-point Energies= -715.748756
Sum of electronic and thermal Energies= -715.730125
Sum of electronic and thermal Enthalpies= -715.729181
Sum of electronic and thermal Free Energies= -715.796815

Cartesian coordinates

C	0.083452	2.640988	-0.536184
H	0.586519	3.404501	0.053687
C	0.567552	1.344235	-0.465345
H	0.212104	0.604801	-1.176920
C	1.908055	1.101904	0.091384
O	2.422760	-0.082236	-0.343415
C	3.686465	-0.478841	0.231313
H	3.601513	-0.474132	1.323437
H	4.454584	0.251538	-0.045211

C	4.010623	-1.860682	-0.299673
H	4.978866	-2.190734	0.090568
H	3.250607	-2.586038	0.007854
H	4.063981	-1.855709	-1.393003
O	2.530919	1.850667	0.832723
C	-2.418398	-2.150836	-0.737780
C	-3.363927	-1.225399	-0.421230
H	-2.474345	-3.037774	-1.348946
H	-4.402359	-1.150501	-0.702789
C	-1.445007	-0.619518	0.612404
N	-1.251299	-1.773026	-0.104126
N	-2.762393	-0.296243	0.407761
C	0.013876	-2.494995	-0.173605
H	-0.090529	-3.310752	-0.889417
H	0.809353	-1.821362	-0.494162
H	0.269871	-2.904882	0.807498
C	-3.434844	0.872438	0.958223
H	-3.175805	1.770616	0.391462
H	-4.512186	0.711783	0.904636
H	-3.142615	1.010660	1.999921
B	-0.373247	0.178532	1.370911
H	-0.726503	1.121952	2.017426
H	0.599748	-0.424447	1.721015
C	-1.176029	3.022933	-1.240264
H	-1.590889	2.189123	-1.816907
H	-1.951428	3.356891	-0.532153
H	-1.018762	3.865889	-1.927925

Vibrational frequencies

-370.1683	31.3458	53.6074
57.6085	73.5323	79.9985
88.3192	103.7868	112.9733
130.0485	141.6215	154.2627
176.6233	188.7984	235.3535
260.1690	266.2348	278.4359
301.3287	325.8358	336.1921
356.0815	395.6467	467.9745
476.6908	579.7161	604.6116
646.3595	671.2254	692.2930

TSe'

Zero-point correction= 0.302827

Thermal correction to Energy= 0.321315

Thermal correction to Enthalpy= 0.322259

Thermal correction to Gibbs Free Energy= 0.255035
Sum of electronic and zero-point Energies= -715.753082
Sum of electronic and thermal Energies= -715.734594
Sum of electronic and thermal Enthalpies= -715.733650
Sum of electronic and thermal Free Energies= -715.800875

Cartesian coordinates

C	0.253240	2.107560	-0.212780
H	0.007244	2.728180	0.644865
C	-0.724373	1.265558	-0.682634
H	-0.575963	0.700536	-1.598815
C	-1.934590	1.002965	0.067173
O	-2.715468	0.068868	-0.560412
C	-3.930253	-0.300813	0.122714
H	-4.555136	0.588674	0.260852
H	-3.682482	-0.686596	1.118001
C	-4.627602	-1.346685	-0.723441
H	-5.560131	-1.653661	-0.238989
H	-4.868370	-0.950044	-1.714911
H	-3.996907	-2.232782	-0.848483
O	-2.261411	1.507553	1.140365
C	2.832228	-1.735203	-0.804567
C	1.614510	-2.265199	-0.511779
H	3.613599	-2.081836	-1.462398
H	1.129109	-3.161317	-0.865344
C	1.833506	-0.359847	0.689916
N	2.958623	-0.573074	-0.070330
N	1.009672	-1.420069	0.399037
C	4.143882	0.275724	-0.057000
H	4.896651	-0.171298	-0.706706
H	3.902765	1.275843	-0.419708
H	4.540865	0.349578	0.958348
C	-0.297640	-1.689653	0.987678
H	-0.260070	-2.622370	1.557823
H	-0.570382	-0.872347	1.650508
H	-1.047834	-1.773008	0.199308
B	1.524468	0.867479	1.545827
H	0.604439	0.832956	2.308357
H	2.389421	1.679143	1.704210
C	1.399360	2.550479	-1.083540
H	2.217424	2.975251	-0.497990
H	1.793565	1.722339	-1.681884
H	1.063209	3.326681	-1.787199

Vibrational frequencies

-266.9174	25.2354	44.3301
56.2158	67.8867	92.9561
103.6632	116.5285	121.3636
135.5086	165.1250	168.2640
194.5914	213.0245	248.3452
256.6718	262.5938	282.7781
302.0443	330.7210	336.3510
357.5869	397.8903	464.7236
468.2274	557.0786	578.3342
611.9941	658.0506	683.2756

M1e

Zero-point correction= 0.305157
Thermal correction to Energy= 0.323274
Thermal correction to Enthalpy= 0.324219
Thermal correction to Gibbs Free Energy= 0.257018
Sum of electronic and zero-point Energies= -715.772759
Sum of electronic and thermal Energies= -715.754642
Sum of electronic and thermal Enthalpies= -715.753698
Sum of electronic and thermal Free Energies= -715.820899

Cartesian coordinates

C	-0.293484	-1.967026	0.038776
H	0.163192	-2.765406	0.637658
C	0.761166	-1.129143	-0.536605
H	0.538199	-0.500666	-1.395607
C	2.044292	-0.948360	0.089768
O	2.773799	0.035450	-0.526254
C	4.067933	0.314920	0.045643
H	4.699966	-0.577129	-0.034694
H	3.951434	0.541540	1.111200
C	4.655900	1.486639	-0.714190
H	5.645848	1.728926	-0.314514
H	4.762297	1.250151	-1.777653
H	4.019629	2.372244	-0.617323
O	2.473695	-1.570786	1.062148
C	-3.209155	1.681291	-0.542152
C	-2.063943	2.362592	-0.283545
H	-4.125374	1.985005	-1.023385
H	-1.778896	3.381284	-0.493819
C	-1.806240	0.270481	0.523730
N	-3.035204	0.403217	-0.039703
N	-1.217083	1.486319	0.372192

C	-4.057617	-0.635304	-0.150263
H	-5.026397	-0.207825	0.115290
H	-4.096462	-1.014696	-1.173818
H	-3.818226	-1.449105	0.530027
C	0.135677	1.850242	0.791218
H	0.435595	1.222671	1.628223
H	0.841477	1.711355	-0.030101
H	0.134357	2.896754	1.100148
B	-1.152120	-1.047377	1.182130
H	-0.402907	-0.705164	2.078856
H	-2.037360	-1.758295	1.629283
C	-1.225387	-2.564566	-1.026675
H	-2.023173	-3.153799	-0.562638
H	-1.703592	-1.776764	-1.621371
H	-0.687798	-3.218851	-1.725213

Vibrational frequencies

16.0096	32.4173	48.8865
72.5360	83.0731	100.3352
116.5999	126.3179	132.5920
164.4792	192.5588	217.7958
256.2365	266.3785	268.9021
276.5234	291.1461	325.9989
343.6076	378.2441	397.9507
452.0819	465.8042	471.4723
572.5692	623.5892	626.4997
643.6699	704.8725	725.7229

II+III

Zero-point correction= 0.827001
Thermal correction to Energy= 0.889028
Thermal correction to Enthalpy= 0.889972
Thermal correction to Gibbs Free Energy= 0.722356
Sum of electronic and zero-point Energies= -3483.567918
Sum of electronic and thermal Energies= -3483.505891
Sum of electronic and thermal Enthalpies= -3483.504947
Sum of electronic and thermal Free Energies= -3483.672563

Cartesian coordinates

C	-1.275883	-1.526113	2.985706
C	-0.046803	-1.391403	3.865220
C	1.061481	-0.945337	2.937341
C	0.351099	-0.043639	1.908761
N	-1.057024	-0.473365	2.003437

H	-2.193159	-1.353766	3.555771
H	1.456767	-1.843926	2.457411
H	0.414800	1.010475	2.204515
H	-1.314939	-2.529179	2.539691
H	1.863294	-0.443645	3.478094
F	0.247530	-2.550583	4.532273
F	-0.270660	-0.433483	4.834044
C	1.025882	-0.080594	0.475668
C	2.444233	0.489865	0.698342
C	2.651085	1.855225	0.507789
C	3.522052	-0.280015	1.157685
C	3.909192	2.426796	0.699416
H	1.828453	2.479873	0.195346
C	4.773214	0.301098	1.363253
H	3.407119	-1.340618	1.343325
C	4.987290	1.659410	1.125295
H	5.965729	2.101901	1.266022
C	1.018583	-1.463806	-0.204816
C	2.101499	-1.924867	-0.959406
C	-0.150536	-2.236421	-0.218999
C	2.020470	-3.114111	-1.687797
H	3.021526	-1.358008	-1.011101
C	-0.217545	-3.430874	-0.930252
H	-1.038363	-1.897807	0.287773
C	0.863654	-3.886446	-1.681476
H	0.801882	-4.806516	-2.249467
C	4.055877	3.893192	0.409149
C	5.891532	-0.548833	1.899710
C	-1.533384	-4.155028	-0.958107
C	3.207378	-3.499117	-2.524265
F	-1.408907	-5.441520	-1.348893
F	-2.405368	-3.561895	-1.812217
F	-2.132332	-4.157562	0.258678
F	3.070205	-4.712620	-3.097971
F	3.412021	-2.603533	-3.524633
F	4.349195	-3.522808	-1.795027
F	5.870044	-0.604100	3.255360
F	5.813458	-1.826429	1.459864
F	7.107814	-0.075222	1.547962
F	5.332745	4.318645	0.497852
F	3.618098	4.191584	-0.843867
F	3.318272	4.650292	1.256797
O	0.269680	0.831164	-0.319318
Si	0.160313	1.109187	-2.003621

C	-0.910850	-0.247239	-2.752454
H	-1.798541	-0.439080	-2.141088
H	-1.247949	0.024361	-3.757768
H	-0.349958	-1.183423	-2.833742
C	1.875227	1.066996	-2.782678
H	2.330249	0.076076	-2.689243
H	1.805757	1.277549	-3.855497
H	2.559308	1.795989	-2.338100
C	-0.702900	2.836322	-2.086144
C	-0.565528	3.576358	-3.467654
C	-2.213406	2.629738	-1.804187
C	-0.166914	3.754336	-0.963103
H	-1.300724	4.395720	-3.414096
H	-2.383238	2.209523	-0.810143
H	-2.737485	3.594480	-1.833047
H	-2.704731	1.971918	-2.526850
H	-0.655590	4.737700	-1.012966
H	-0.380021	3.335073	0.025021
H	0.910819	3.929458	-1.024191
C	-0.954131	2.722435	-4.687129
H	-1.025128	3.352291	-5.581488
H	-0.206452	1.950683	-4.902498
H	-1.922226	2.229037	-4.561720
C	0.796118	4.246394	-3.722669
H	1.036436	5.000598	-2.968387
H	1.618112	3.526465	-3.748868
H	0.780713	4.757555	-4.692517
C	-2.070367	0.043592	1.249435
C	-3.341701	-0.493845	1.145232
H	-1.790078	0.907772	0.665494
H	-3.574828	-1.395423	1.705814
C	-4.326961	0.067426	0.316698
C	-5.672677	-0.408945	0.150710
C	-6.258614	-1.408738	0.971749
C	-6.488560	0.153728	-0.866852
C	-7.572199	-1.821397	0.773754
H	-5.682223	-1.850915	1.778826
C	-7.800725	-0.263179	-1.057292
H	-6.069737	0.929834	-1.502342
C	-8.356143	-1.257236	-0.240851
H	-7.994188	-2.587234	1.420198
H	-8.397510	0.187436	-1.846616
H	-9.381554	-1.583457	-0.390012
H	-4.043055	0.914228	-0.300073

C	-5.804061	3.054909	0.830042
C	-5.433375	3.892971	-0.201420
H	-6.815200	2.648835	0.787597
H	-4.460106	4.370978	-0.250116
H	-6.127864	4.115620	-1.005910
C	-5.029233	2.639511	1.924242
C	-3.615565	3.083758	2.145157
H	-2.980088	2.229881	2.416461
H	-3.170586	3.569026	1.273165
H	-3.553662	3.790162	2.987167
C	-5.627303	1.795251	3.010922
H	-6.623159	1.424944	2.749619
H	-4.987925	0.930418	3.236600
H	-5.715403	2.363083	3.950735

Vibrational frequencies

8.5035	11.9578	17.6442
18.4733	20.6081	23.8334
25.5990	26.1505	27.1456
28.6085	30.4390	32.3186
35.2215	37.7875	46.8127
54.7903	58.1338	59.8385
65.3138	72.7168	78.9218
91.3725	94.5169	95.0128
96.5131	101.7741	104.3995
107.1976	112.2061	116.1819

III

Zero-point correction= 0.122595
Thermal correction to Energy= 0.129260
Thermal correction to Enthalpy= 0.130204
Thermal correction to Gibbs Free Energy= 0.092226
Sum of electronic and zero-point Energies= -195.801658
Sum of electronic and thermal Energies= -195.794993
Sum of electronic and thermal Enthalpies= -195.794049
Sum of electronic and thermal Free Energies= -195.832027

Cartesian coordinates

C	0.399034	-0.034686	-0.014722
C	-0.845961	-0.672232	-0.010377
H	-0.820333	-1.763414	-0.017095
C	0.562764	1.457754	-0.003580
H	0.906963	1.806947	0.981725
H	1.330600	1.770503	-0.723695

H	-0.357693	1.997026	-0.241094
C	1.669670	-0.833292	0.007880
H	2.295801	-0.609790	-0.868732
H	2.282000	-0.580050	0.886664
H	1.484788	-1.911949	0.025815
C	-2.099288	-0.084664	0.008183
H	-2.995309	-0.697998	0.005480
H	-2.244135	0.991446	0.026626

Vibrational frequencies

74.3318	158.7504	240.4619
300.2551	358.9743	400.5999
541.6306	571.8418	765.4124
770.0082	949.7839	979.3967
1004.5113	1019.0241	1072.0649
1079.9385	1237.8292	1256.3838
1367.5199	1413.6649	1424.8247
1458.9989	1471.9229	1477.8820
1484.2131	1516.8292	1533.2732
3000.5919	3010.3603	3041.1618

***(S)*-^{os}TSf**

Zero-point correction= 0.826842
Thermal correction to Energy= 0.887996
Thermal correction to Enthalpy= 0.888940
Thermal correction to Gibbs Free Energy= 0.724773
Sum of electronic and zero-point Energies= -3483.529288
Sum of electronic and thermal Energies= -3483.468134
Sum of electronic and thermal Enthalpies= -3483.467190
Sum of electronic and thermal Free Energies= -3483.631356

Cartesian coordinates

C	-1.458649	1.455386	-2.900411
C	-0.561248	0.609134	-3.787850
C	0.588279	0.179399	-2.903035
C	-0.102842	-0.047571	-1.549400
N	-1.312089	0.806795	-1.592150
H	-2.491403	1.431603	-3.251010
H	1.307467	1.001057	-2.859932
H	-0.444029	-1.083726	-1.486561
H	-1.100654	2.490860	-2.893783
H	1.082752	-0.712434	-3.286524
F	-0.166100	1.262607	-4.921370
F	-1.265582	-0.510009	-4.209681

C	0.824562	0.137298	-0.291391
C	1.728057	-1.107427	-0.325255
C	1.293298	-2.251119	0.344103
C	2.881090	-1.196632	-1.110891
C	2.016517	-3.438830	0.277593
H	0.377007	-2.216723	0.914962
C	3.601740	-2.392050	-1.171751
H	3.226533	-0.342607	-1.682053
C	3.184962	-3.525019	-0.474520
H	3.749628	-4.447367	-0.523852
C	1.580434	1.469867	-0.243697
C	2.889023	1.574927	0.231266
C	0.885069	2.652136	-0.521769
C	3.483378	2.826173	0.413252
H	3.456547	0.690053	0.489669
C	1.489889	3.893244	-0.354425
H	-0.148633	2.603263	-0.833248
C	2.796679	3.999807	0.120223
H	3.258771	4.967649	0.268352
C	1.458622	-4.626903	1.004589
C	4.872193	-2.417732	-1.973596
C	0.654585	5.117405	-0.591734
C	4.881425	2.857662	0.960747
F	1.397765	6.234858	-0.735334
F	-0.199071	5.336556	0.440808
F	-0.112293	4.994397	-1.702751
F	5.324830	4.110553	1.190924
F	4.962967	2.177973	2.132426
F	5.762688	2.267189	0.116920
F	4.725397	-1.785271	-3.162225
F	5.883274	-1.786961	-1.326221
F	5.293534	-3.673790	-2.234112
F	2.333250	-5.648444	1.089431
F	1.084551	-4.303331	2.269480
F	0.342820	-5.105427	0.391792
O	-0.048506	0.078239	0.831441
Si	0.176758	0.423831	2.489089
C	0.282523	2.291179	2.716255
H	-0.480903	2.813873	2.131782
H	0.149222	2.564658	3.766878
H	1.260132	2.665717	2.397269
C	1.768540	-0.369355	3.106907
H	2.634555	0.010675	2.555019
H	1.922077	-0.114297	4.161332

H	1.759120	-1.459482	3.017876
C	-1.431525	-0.315084	3.244615
C	-1.417789	-0.503863	4.803503
C	-2.587447	0.649601	2.875223
C	-1.741283	-1.675188	2.574751
H	-2.471270	-0.690777	5.067986
H	-2.634124	0.837417	1.798613
H	-3.551689	0.213861	3.171031
H	-2.500278	1.620639	3.371052
H	-2.638893	-2.121605	3.024587
H	-1.939104	-1.555110	1.508406
H	-0.930942	-2.403476	2.678778
C	-0.973952	0.737570	5.596095
H	-1.176365	0.592824	6.662996
H	0.103246	0.914770	5.497407
H	-1.495421	1.646483	5.284403
C	-0.624665	-1.724171	5.303246
H	-1.004232	-2.664740	4.896512
H	0.437526	-1.654521	5.052620
H	-0.697569	-1.789642	6.394682
C	-2.407611	0.357794	-0.889318
C	-3.701232	0.812913	-0.966197
H	-2.177878	-0.447657	-0.206221
H	-3.945384	1.644060	-1.622023
C	-4.725653	0.148261	-0.260705
C	-6.125290	0.491726	-0.249818
C	-6.690133	1.503533	-1.067970
C	-7.006035	-0.214153	0.609718
C	-8.050891	1.789128	-1.019122
H	-6.056412	2.064751	-1.747378
C	-8.364724	0.075804	0.653094
H	-6.599559	-0.997596	1.244688
C	-8.901562	1.081502	-0.160903
H	-8.454945	2.570423	-1.657356
H	-9.011700	-0.482832	1.324014
H	-9.962775	1.308378	-0.128264
H	-4.417790	-0.616920	0.446551
C	-3.615718	-2.403704	-2.195995
C	-4.911403	-2.187416	-1.737180
H	-3.346993	-1.942941	-3.147205
H	-5.296236	-2.656216	-0.838477
H	-5.623754	-1.636815	-2.339579
C	-2.607492	-3.130119	-1.566726
C	-2.804879	-3.799024	-0.233944

H	-1.863529	-3.852224	0.322327
H	-3.541771	-3.285968	0.390195
H	-3.148457	-4.837426	-0.359963
C	-1.322429	-3.443496	-2.283982
H	-1.162898	-2.791558	-3.147475
H	-0.454097	-3.364796	-1.619714
H	-1.327594	-4.484316	-2.645438

Vibrational frequencies

-68.8968	12.7709	14.1236
18.0586	19.2975	20.5503
22.7839	23.5858	26.6978
27.6355	33.6085	35.9292
39.8761	42.1762	48.7908
51.3354	57.1734	58.9844
64.6952	73.3829	75.7572
82.9341	86.7102	94.7555
95.6995	99.5419	105.8031
109.0676	110.6276	113.9385

***(S)*-^{os}TSf'**

Zero-point correction= 0.826736
Thermal correction to Energy= 0.887800
Thermal correction to Enthalpy= 0.888744
Thermal correction to Gibbs Free Energy= 0.724501
Sum of electronic and zero-point Energies= -3483.523566
Sum of electronic and thermal Energies= -3483.462503
Sum of electronic and thermal Enthalpies= -3483.461559
Sum of electronic and thermal Free Energies= -3483.625802

Cartesian coordinates

C	-1.595172	1.465468	-2.493074
C	-0.635339	1.055895	-3.596242
C	0.617287	0.588235	-2.885508
C	0.067591	-0.086445	-1.614208
N	-1.272522	0.495860	-1.448613
H	-2.634152	1.371956	-2.816241
H	1.208222	1.474612	-2.641390
H	-0.043547	-1.165633	-1.773823
H	-1.402823	2.501956	-2.191202
H	1.211483	-0.080817	-3.506715
F	-0.405903	2.055527	-4.500825
F	-1.189180	0.004513	-4.308017
C	1.012021	0.031183	-0.354248

C	2.226574	-0.852557	-0.691678
C	2.230314	-2.171768	-0.241795
C	3.290293	-0.428374	-1.497683
C	3.304869	-3.018890	-0.502514
H	1.395592	-2.539100	0.335332
C	4.353620	-1.290257	-1.774300
H	3.313714	0.576357	-1.902513
C	4.384194	-2.589752	-1.268171
H	5.225604	-3.242514	-1.463011
C	1.368381	1.475778	0.032265
C	2.651757	1.870041	0.418265
C	0.332581	2.408725	0.165675
C	2.890289	3.161995	0.894364
H	3.480818	1.175255	0.381452
C	0.582867	3.700648	0.616061
H	-0.685058	2.109739	-0.038473
C	1.864957	4.097735	0.990058
H	2.054616	5.097137	1.360177
C	3.252531	-4.398506	0.087891
C	5.461930	-0.799138	-2.662466
C	-0.594854	4.618158	0.770300
C	4.293571	3.505222	1.305419
F	-0.236238	5.886046	1.059008
F	-1.420096	4.198002	1.762777
F	-1.347889	4.657517	-0.358128
F	4.383414	4.717386	1.891033
F	4.785356	2.594505	2.182299
F	5.139360	3.508191	0.245912
F	5.111238	-0.846643	-3.971859
F	5.783003	0.489719	-2.398290
F	6.589749	-1.530540	-2.530414
F	4.419480	-5.062897	-0.030783
F	2.945246	-4.352993	1.413635
F	2.293424	-5.159385	-0.492433
O	0.270917	-0.544445	0.717219
Si	0.525995	-0.552553	2.408313
C	0.063523	1.129001	3.120170
H	-0.867485	1.513188	2.693225
H	-0.063676	1.064624	4.205028
H	0.851213	1.862208	2.920256
C	2.338653	-0.883353	2.798557
H	2.976235	-0.126346	2.329576
H	2.496384	-0.812151	3.880479
H	2.680677	-1.867481	2.469207

C	-0.699965	-1.929254	2.966298
C	-0.441777	-2.508659	4.402776
C	-2.119701	-1.306908	2.929586
C	-0.690948	-3.095362	1.949465
H	-1.348484	-3.091592	4.632934
H	-2.346530	-0.866488	1.954261
H	-2.876054	-2.080320	3.122009
H	-2.256937	-0.521007	3.677590
H	-1.369292	-3.890826	2.287778
H	-1.035249	-2.769028	0.964631
H	0.296551	-3.548638	1.821534
C	-0.305423	-1.446117	5.506923
H	-0.315858	-1.925885	6.491748
H	0.641888	-0.900659	5.428178
H	-1.117940	-0.714859	5.490616
C	0.740178	-3.489924	4.503829
H	0.625213	-4.354539	3.845523
H	1.693683	-3.011807	4.263501
H	0.816393	-3.870170	5.528754
C	-2.244587	-0.182050	-0.758427
C	-3.526341	0.257295	-0.542619
H	-1.930199	-1.147973	-0.380407
H	-3.797829	1.263726	-0.849325
C	-4.517853	-0.593287	-0.003083
C	-5.848631	-0.218270	0.374655
C	-6.453796	1.008646	-0.005955
C	-6.641877	-1.123229	1.130465
C	-7.753987	1.321631	0.388073
H	-5.894004	1.724934	-0.596935
C	-7.940436	-0.809097	1.508875
H	-6.208970	-2.076236	1.423343
C	-8.507142	0.422346	1.147189
H	-8.185215	2.273776	0.090720
H	-8.516347	-1.520486	2.094525
H	-9.520191	0.670654	1.448878
H	-4.195808	-1.585712	0.305898
C	-5.761046	-0.611068	-2.945431
C	-7.052089	-0.157084	-2.849343
H	-5.044940	0.035125	-3.455589
H	-7.835288	-0.730175	-2.363739
H	-7.339070	0.799448	-3.273772
C	-5.230991	-1.804155	-2.411589
C	-6.105992	-2.847118	-1.779361
H	-5.522073	-3.511806	-1.133592

H	-6.907415	-2.412132	-1.175543
H	-6.581578	-3.479825	-2.544862
C	-3.832324	-2.218000	-2.758353
H	-3.252883	-1.409928	-3.214483
H	-3.281726	-2.566353	-1.874426
H	-3.840215	-3.060739	-3.466840

Vibrational frequencies

-133.4428	8.1018	14.6291
17.5026	19.2491	20.4190
20.9421	23.5133	27.2193
28.2074	29.6745	34.6235
40.1637	46.9468	47.9835
49.6597	56.0471	60.7979
65.8499	70.7757	76.0463
88.9691	95.2541	95.5528
98.8887	99.4952	109.6878
110.9196	115.2569	118.5949

IV

Zero-point correction= 0.833056
Thermal correction to Energy= 0.893324
Thermal correction to Enthalpy= 0.894269
Thermal correction to Gibbs Free Energy= 0.732361
Sum of electronic and zero-point Energies= -3483.622114
Sum of electronic and thermal Energies= -3483.561845
Sum of electronic and thermal Enthalpies= -3483.560901
Sum of electronic and thermal Free Energies= -3483.722809

Cartesian coordinates

C	-1.217069	1.640774	-2.988637
C	-0.222040	0.891875	-3.856555
C	0.867528	0.435361	-2.912355
C	0.066210	0.068321	-1.651504
N	-1.148686	0.924201	-1.708746
H	-2.215046	1.600163	-3.428932
H	1.543283	1.276151	-2.736848
H	-0.250107	-0.977565	-1.729314
H	-0.911657	2.689051	-2.892263
H	1.433445	-0.400699	-3.322942
F	0.237524	1.635972	-4.909761
F	-0.846722	-0.217402	-4.404331
C	0.884666	0.137464	-0.304466
C	1.794110	-1.103988	-0.367065

C	1.326117	-2.301376	0.181177
C	2.998075	-1.125042	-1.076332
C	2.064606	-3.476217	0.064640
H	0.379248	-2.312586	0.700372
C	3.734711	-2.307078	-1.187184
H	3.378518	-0.225489	-1.545389
C	3.281257	-3.493688	-0.616826
H	3.859561	-4.406276	-0.699736
C	1.629597	1.463899	-0.096567
C	2.909673	1.535809	0.460867
C	0.949434	2.662714	-0.337674
C	3.492922	2.771306	0.749762
H	3.463922	0.637038	0.697125
C	1.543194	3.890989	-0.059856
H	-0.064484	2.629601	-0.712922
C	2.821222	3.963344	0.489346
H	3.276704	4.919058	0.718400
C	1.508492	-4.751270	0.633192
C	5.005031	-2.287944	-1.990768
C	0.726361	5.131294	-0.281741
C	4.886108	2.801390	1.313464
F	1.469369	6.258085	-0.245616
F	-0.240852	5.261954	0.661465
F	0.090874	5.104576	-1.479356
F	5.125934	3.925742	2.024340
F	5.120820	1.748406	2.132211
F	5.825762	2.747643	0.336565
F	4.753950	-2.381406	-3.321116
F	5.696880	-1.137946	-1.810408
F	5.830457	-3.309252	-1.673753
F	2.480282	-5.576009	1.082775
F	0.664372	-4.521809	1.668916
F	0.803636	-5.450023	-0.293622
O	-0.075479	-0.013955	0.737349
Si	0.005848	0.242707	2.423762
C	0.092843	2.091759	2.774700
H	-0.619690	2.659463	2.168558
H	-0.124071	2.300279	3.826717
H	1.094074	2.481026	2.564667
C	1.546503	-0.585671	3.120560
H	2.449306	-0.183873	2.647941
H	1.629339	-0.379986	4.193654
H	1.550205	-1.670470	2.979332
C	-1.659111	-0.525563	3.011517

C	-1.763325	-0.801094	4.556130
C	-2.784634	0.464142	2.613464
C	-1.927324	-1.847190	2.251567
H	-2.834072	-0.999532	4.727935
H	-2.768278	0.693845	1.543262
H	-3.767545	0.026407	2.838332
H	-2.724560	1.415543	3.150146
H	-2.849800	-2.310223	2.627355
H	-2.064908	-1.676659	1.181918
H	-1.125569	-2.582596	2.367355
C	-1.388311	0.392755	5.450826
H	-1.671930	0.187272	6.489563
H	-0.308036	0.579652	5.448957
H	-1.891950	1.316833	5.153789
C	-1.012263	-2.051069	5.047986
H	-1.357747	-2.967061	4.561353
H	0.067464	-1.975261	4.889441
H	-1.173600	-2.180265	6.124767
C	-2.304085	0.342329	-1.181898
C	-3.593741	0.609774	-1.441788
H	-2.072110	-0.428331	-0.460161
H	-3.891337	1.384195	-2.143996
C	-4.684670	-0.255938	-0.836514
C	-5.983192	0.506475	-0.640491
C	-6.657990	1.084099	-1.727944
C	-6.546449	0.638662	0.635919
C	-7.855810	1.776038	-1.542999
H	-6.242122	0.992596	-2.728159
C	-7.745287	1.330932	0.826077
H	-6.038402	0.196420	1.489930
C	-8.404776	1.902990	-0.263607
H	-8.361505	2.217205	-2.398248
H	-8.162260	1.423346	1.825767
H	-9.336790	2.442826	-0.118972
H	-4.347593	-0.593825	0.150213
C	-3.680707	-2.422742	-1.729400
C	-4.917360	-1.562683	-1.673629
H	-2.946783	-2.130750	-2.479298
H	-5.762144	-2.103947	-1.234353
H	-5.219047	-1.279894	-2.690043
C	-3.358702	-3.437618	-0.909414
C	-4.247124	-3.962361	0.190837
H	-3.710040	-3.962996	1.147332
H	-5.167198	-3.388791	0.322726

H	-4.525528	-5.007338	-0.004971
C	-2.029138	-4.144696	-1.015148
H	-1.388243	-3.716098	-1.791965
H	-1.491145	-4.093791	-0.060926
H	-2.160895	-5.213736	-1.232500

Vibrational frequencies

10.8074	13.2243	18.1368
20.5386	24.6510	28.4353
29.6988	32.5348	33.3528
33.9239	37.4776	39.5574
40.9426	45.9276	46.8261
55.8752	58.7877	64.3836
68.3930	72.9427	75.6223
95.1713	96.2231	97.3002
98.7634	102.8682	108.6410
112.0894	115.3615	116.4490

M3(B3LYP)

Zero-point correction= 0.404892
Thermal correction to Energy= 0.428548
Thermal correction to Enthalpy= 0.429492
Thermal correction to Gibbs Free Energy= 0.351727
Sum of electronic and zero-point Energies= -1091.276904
Sum of electronic and thermal Energies= -1091.253248
Sum of electronic and thermal Enthalpies= -1091.252304
Sum of electronic and thermal Free Energies= -1091.330070

Cartesian coordinates

C	-2.086234	2.742876	-0.438982
C	0.124672	2.931077	0.417911
C	-0.439905	4.307514	0.575804
C	-1.962481	4.052621	0.379568
H	-2.127813	2.914924	-1.517614
H	-2.926972	2.118573	-0.139627
H	-0.202971	4.754221	1.543040
H	-0.031579	4.959793	-0.204009
H	-2.437676	3.914426	1.354108
H	-2.457297	4.882782	-0.125643
N	-0.806774	2.082310	-0.120647
N	1.269597	2.327506	0.592545
N	1.036316	1.044038	0.126483
C	-0.224862	0.883843	-0.316257
C	2.090888	0.061691	0.185157

C	3.020194	0.022557	-0.865689
C	2.165007	-0.781710	1.303158
C	4.052071	-0.914745	-0.774088
C	3.217600	-1.702189	1.342422
C	4.163203	-1.788511	0.314617
H	4.784322	-0.965047	-1.575805
H	3.298077	-2.365526	2.199544
C	2.900428	0.946793	-2.048335
H	1.947176	0.773037	-2.558846
H	2.930981	1.998523	-1.741975
H	3.714439	0.776145	-2.756864
C	5.269615	-2.812763	0.366642
H	4.970778	-3.736845	-0.144282
H	6.174827	-2.447967	-0.128166
H	5.522760	-3.077766	1.397419
C	1.162251	-0.704008	2.427108
H	1.056573	0.319299	2.803591
H	0.170107	-1.037928	2.102781
H	1.470615	-1.340778	3.259532
C	-0.764061	-0.314491	-1.069523
O	-0.078449	-0.628730	-2.076051
C	-1.955934	-0.917803	-0.608650
C	-2.537291	-1.991952	-1.373279
C	-2.638436	-0.560530	0.607614
C	-3.679854	-2.620552	-0.987544
H	-2.030104	-2.286119	-2.287728
C	-3.782675	-1.184682	1.006174
H	-2.224626	0.216698	1.246268
C	-4.394646	-2.259461	0.233027
H	-4.089780	-3.422635	-1.597968
H	-4.262287	-0.889425	1.936798
C	-5.544875	-2.882679	0.621534
H	-6.061056	-2.601678	1.535172
H	-5.982924	-3.681215	0.029687

Vibrational frequencies

23.3191	44.0853	51.7882
58.6735	66.9459	74.1543
98.0356	101.5420	125.8781
137.0584	154.0880	163.0012
168.5152	181.3084	192.6218
224.3402	234.1611	238.7402
243.8829	265.0666	278.6422
286.6631	322.1157	332.3447

363.1689	380.8986	413.8594
431.0141	456.7295	482.9717

ε-TS4(B3LYP)

Zero-point correction= 0.521553
Thermal correction to Energy= 0.555606
Thermal correction to Enthalpy= 0.556551
Thermal correction to Gibbs Free Energy= 0.453449
Sum of electronic and zero-point Energies= -1773.777472
Sum of electronic and thermal Energies= -1773.743419
Sum of electronic and thermal Enthalpies= -1773.742475
Sum of electronic and thermal Free Energies= -1773.845576

Cartesian coordinates

C	1.094090	3.006294	-0.447716
C	3.303050	2.814460	0.415013
C	2.973678	4.262452	0.585842
C	1.429296	4.260608	0.395946
H	1.098039	3.200490	-1.523148
H	0.157684	2.523926	-0.170802
H	3.287605	4.652705	1.555495
H	3.480555	4.844372	-0.191759
H	0.940860	4.180925	1.370486
H	1.072936	5.168891	-0.091035
N	2.246637	2.134505	-0.131892
N	4.328488	2.024627	0.599856
N	3.890406	0.800191	0.131371
C	2.625133	0.858609	-0.316272
C	4.766706	-0.346819	0.203986
C	5.677764	-0.554157	-0.841612
C	4.703146	-1.170426	1.340483
C	6.542398	-1.647967	-0.728389
C	5.587951	-2.249533	1.397407
C	6.513367	-2.504012	0.376902
H	7.254298	-1.833222	-1.528126
H	5.556636	-2.902928	2.265613
C	5.711360	0.341094	-2.052809
H	4.780646	0.239916	-2.621119
H	5.820487	1.395039	-1.775604
H	6.545202	0.074443	-2.706262
C	7.460658	-3.673572	0.479710
H	8.064232	-3.779869	-0.425504
H	8.144387	-3.554401	1.328368
H	6.916294	-4.611395	0.636787

C	3.723228	-0.913603	2.457500
H	3.779552	0.120123	2.815079
H	2.691382	-1.094481	2.135510
H	3.925979	-1.574726	3.303159
C	1.869690	-0.247264	-1.034706
O	2.447823	-0.719252	-2.024387
C	0.563317	-0.591425	-0.548813
C	-0.265961	-1.441216	-1.333018
C	0.044569	-0.120317	0.691618
C	-1.537235	-1.764090	-0.927567
H	0.124346	-1.815244	-2.274557
C	-1.225708	-0.446494	1.100105
H	0.662780	0.492935	1.342003
C	-2.084056	-1.267470	0.300979
H	-2.161978	-2.395078	-1.551346
H	-1.597410	-0.073252	2.050156
C	-3.436973	-1.499265	0.637594
H	-3.756516	-1.267481	1.649826
H	-3.914411	-2.371862	0.203057
C	-4.603460	-0.220401	-0.647266
C	-5.960944	-0.642086	-0.105625
C	-6.504624	-0.221442	1.119450
C	-6.716948	-1.506486	-0.911695
C	-7.768375	-0.657134	1.520614
H	-5.950476	0.449435	1.765202
C	-7.975136	-1.948707	-0.505987
H	-6.294842	-1.812262	-1.863231
C	-8.508207	-1.524905	0.713980
H	-8.174847	-0.316724	2.469343
H	-8.544061	-2.618677	-1.145411
H	-9.490296	-1.864068	1.031646
C	-4.091466	1.159039	-0.154918
F	-4.968905	2.133900	-0.529416
F	-2.907159	1.472806	-0.712814
F	-3.936267	1.302365	1.190602
O	-4.301405	-0.482875	-1.834227

Vibrational frequencies

-216.1054	15.0321	20.0476
25.0559	28.1649	44.2864
51.2676	54.0927	58.7415
71.2558	76.8386	77.1794
83.1766	101.6159	113.6161
117.7038	130.2072	143.5123

150.1756	158.9930	164.3652
178.2403	186.8465	195.9782
218.3219	236.1107	244.0785
249.2935	260.4995	271.3593

M3(M06-2X)

Zero-point correction= 0.408747
Thermal correction to Energy= 0.432202
Thermal correction to Enthalpy= 0.433146
Thermal correction to Gibbs Free Energy= 0.355696
Sum of electronic and zero-point Energies= -1090.802522
Sum of electronic and thermal Energies= -1090.779068
Sum of electronic and thermal Enthalpies= -1090.778124
Sum of electronic and thermal Free Energies= -1090.855573

Cartesian coordinates

C	2.136648	2.661466	0.457257
C	-0.056591	2.923811	-0.411462
C	0.564707	4.273165	-0.579645
C	2.069186	3.948745	-0.393653
H	2.170761	2.858854	1.530789
H	2.951773	1.994755	0.177870
H	0.340766	4.720870	-1.547886
H	0.190535	4.939030	0.203717
H	2.521880	3.756248	-1.368717
H	2.609962	4.765571	0.082901
N	0.837541	2.050948	0.141553
N	-1.216160	2.357445	-0.587630
N	-1.030364	1.088180	-0.108085
C	0.209838	0.887072	0.341168
C	-2.084784	0.112749	-0.187645
C	-3.031791	0.077064	0.839081
C	-2.105764	-0.743010	-1.288030
C	-4.049766	-0.865497	0.728870
C	-3.147849	-1.669387	-1.353163
C	-4.121218	-1.744258	-0.357392
H	-4.802128	-0.923182	1.512166
H	-3.192312	-2.349195	-2.200057
C	-2.917672	1.008451	2.011655
H	-1.972584	0.817238	2.530489
H	-2.923657	2.054867	1.689501
H	-3.743207	0.856470	2.709172
C	-5.232870	-2.756259	-0.434443
H	-5.149303	-3.486352	0.377068

H	-6.209410	-2.272875	-0.336058
H	-5.211049	-3.299326	-1.381596
C	-1.037932	-0.679713	-2.345511
H	-0.896233	0.342810	-2.710441
H	-0.078389	-1.028950	-1.946923
H	-1.301491	-1.314049	-3.193718
C	0.685640	-0.349306	1.079969
O	-0.034129	-0.669578	2.045926
C	1.871769	-0.946429	0.622385
C	2.440141	-2.035972	1.373183
C	2.558758	-0.569884	-0.585547
C	3.580630	-2.656436	0.990806
H	1.920900	-2.342092	2.277463
C	3.698956	-1.185635	-0.985662
H	2.142004	0.215618	-1.215645
C	4.306364	-2.273064	-0.220144
H	3.987686	-3.468805	1.588518
H	4.184920	-0.883189	-1.910067
C	5.452931	-2.883886	-0.606119
H	5.974215	-2.585524	-1.510575
H	5.884280	-3.690897	-0.021992

Vibrational frequencies

23.8239	44.6911	45.3187
57.7212	64.3029	72.6978
98.5184	101.4988	129.5219
134.1138	160.2846	165.7912
173.7998	190.7006	211.5089
226.1882	233.3596	241.5036
248.5836	260.6837	278.9301
296.2540	329.8472	341.1920
357.6012	385.8718	417.8081
435.4145	457.5762	482.6005

ε-TS4(M06-2X)

Zero-point correction= 0.528201
Thermal correction to Energy= 0.561690
Thermal correction to Enthalpy= 0.562634
Thermal correction to Gibbs Free Energy= 0.461890
Sum of electronic and zero-point Energies= -1773.060319
Sum of electronic and thermal Energies= -1773.026830
Sum of electronic and thermal Enthalpies= -1773.025886
Sum of electronic and thermal Free Energies= -1773.126630

Cartesian coordinates

C	0.888446	2.895648	-0.431040
C	3.121672	2.828326	0.368966
C	2.719425	4.259516	0.520971
C	1.177337	4.157751	0.408147
H	0.868449	3.091661	-1.505167
H	-0.014530	2.361548	-0.136629
H	3.055768	4.690066	1.463894
H	3.150244	4.841483	-0.299374
H	0.747616	4.029693	1.404062
H	0.737791	5.044015	-0.047961
N	2.087859	2.091864	-0.136607
N	4.182847	2.089740	0.537567
N	3.790331	0.852987	0.108197
C	2.523510	0.840889	-0.304942
C	4.690342	-0.268430	0.183708
C	5.608104	-0.443586	-0.854813
C	4.605502	-1.111158	1.291860
C	6.485727	-1.518977	-0.749096
C	5.503832	-2.177079	1.347514
C	6.449901	-2.390152	0.344070
H	7.210076	-1.685340	-1.542754
H	5.461176	-2.854051	2.196828
C	5.602740	0.474314	-2.044780
H	4.641173	0.396804	-2.563650
H	5.742302	1.517924	-1.744994
H	6.398195	0.205766	-2.741818
C	7.428995	-3.529918	0.438616
H	7.568927	-4.009823	-0.533615
H	8.408680	-3.170118	0.770738
H	7.090011	-4.284474	1.151900
C	3.572429	-0.890912	2.363327
H	3.591284	0.140448	2.730350
H	2.565449	-1.091395	1.979190
H	3.749566	-1.559119	3.207734
C	1.812260	-0.337294	-0.944747
O	2.408822	-0.859975	-1.885997
C	0.523738	-0.665287	-0.423922
C	-0.297487	-1.573296	-1.145769
C	0.020838	-0.140505	0.801740
C	-1.549822	-1.899290	-0.707610
H	0.090759	-1.988122	-2.071617
C	-1.227900	-0.467979	1.250269
H	0.643728	0.511708	1.412385

C	-2.090192	-1.341278	0.502254
H	-2.174222	-2.573951	-1.284611
H	-1.591915	-0.062574	2.189989
C	-3.419288	-1.559652	0.854032
H	-3.786304	-1.219165	1.817996
H	-3.945002	-2.398652	0.410277
C	-4.441273	-0.270037	-0.695906
C	-5.816247	-0.599271	-0.174850
C	-6.429207	0.058364	0.897268
C	-6.509895	-1.616014	-0.838412
C	-7.712510	-0.305373	1.297315
H	-5.914740	0.854514	1.424150
C	-7.786637	-1.983643	-0.430407
H	-6.024872	-2.105905	-1.676543
C	-8.393427	-1.328507	0.640468
H	-8.182223	0.213226	2.127605
H	-8.312383	-2.778699	-0.950591
H	-9.391898	-1.611578	0.959105
C	-3.840692	1.076532	-0.242007
F	-4.636303	2.079774	-0.677373
F	-2.635543	1.271505	-0.781452
F	-3.716813	1.254085	1.086028
O	-4.063042	-0.669839	-1.800146

Vibrational frequencies

-190.1537	18.1532	23.7019
28.4297	36.3808	44.4523
52.9695	56.0722	60.1826
71.7012	79.1086	102.3313
107.7235	117.2646	125.5047
130.4544	138.3444	149.0729
151.6674	166.4861	171.2125
184.2187	187.5034	199.6805
218.6289	239.3033	240.3844
257.0002	268.4137	276.8438

M3(ωB97X-D)

Zero-point correction= 0.410337
Thermal correction to Energy= 0.433579
Thermal correction to Enthalpy= 0.434523
Thermal correction to Gibbs Free Energy= 0.357574
Sum of electronic and zero-point Energies= -1090.925823
Sum of electronic and thermal Energies= -1090.902581
Sum of electronic and thermal Enthalpies= -1090.901637

Sum of electronic and thermal Free Energies= -1090.978586

Cartesian coordinates

C	2.121859	2.715256	0.476320
C	-0.040180	2.923508	-0.477596
C	0.576512	4.265299	-0.693118
C	2.075538	3.970702	-0.422738
H	2.137821	2.950071	1.542419
H	2.941184	2.038092	0.238600
H	0.393557	4.655451	-1.694459
H	0.162171	4.973241	0.031015
H	2.580175	3.755519	-1.367233
H	2.578998	4.813571	0.049712
N	0.835395	2.091228	0.156238
N	-1.184883	2.336332	-0.678956
N	-1.004304	1.087903	-0.133812
C	0.216359	0.928380	0.379744
C	-2.050557	0.106376	-0.200911
C	-3.012780	0.098101	0.811015
C	-2.059345	-0.781681	-1.278328
C	-4.030671	-0.847493	0.713493
C	-3.099217	-1.707923	-1.329576
C	-4.088127	-1.755498	-0.345813
H	-4.794178	-0.878217	1.486256
H	-3.133026	-2.413569	-2.155384
C	-2.921475	1.057473	1.963523
H	-1.985626	0.882857	2.505016
H	-2.925990	2.096935	1.619034
H	-3.757406	0.920816	2.652501
C	-5.182129	-2.787895	-0.411312
H	-4.877872	-3.704129	0.107105
H	-6.097410	-2.428092	0.066266
H	-5.413336	-3.056047	-1.445707
C	-0.980450	-0.753785	-2.325873
H	-0.829368	0.254909	-2.723394
H	-0.027084	-1.094660	-1.907170
H	-1.235505	-1.413443	-3.157760
C	0.709345	-0.268427	1.169783
O	0.044673	-0.511382	2.197264
C	1.849221	-0.921990	0.677904
C	2.424717	-2.006484	1.430825
C	2.492504	-0.597308	-0.569247
C	3.525732	-2.671541	1.011619
H	1.944751	-2.277169	2.367200

C	3.594247	-1.255158	-1.004526
H	2.077898	0.188624	-1.198561
C	4.205537	-2.342055	-0.241258
H	3.933823	-3.480950	1.612640
H	4.046314	-0.984846	-1.955725
C	5.314480	-2.996874	-0.663248
H	5.802734	-2.738574	-1.598955
H	5.749832	-3.803456	-0.079926

Vibrational frequencies

19.0345	44.9866	47.5597
59.6144	69.1500	76.2633
93.8800	114.2605	138.8782
149.0524	164.4210	168.2379
183.7860	193.6735	208.6151
226.8284	241.4199	246.0626
253.7990	263.5512	286.6489
295.2940	332.4495	342.4282
365.2003	390.1403	420.7070
433.3462	452.6360	489.3525

ε-TS4(ωB97X-D)

Zero-point correction= 0.528878
Thermal correction to Energy= 0.562240
Thermal correction to Enthalpy= 0.563184
Thermal correction to Gibbs Free Energy= 0.462997
Sum of electronic and zero-point Energies= -1773.230567
Sum of electronic and thermal Energies= -1773.197205
Sum of electronic and thermal Enthalpies= -1773.196261
Sum of electronic and thermal Free Energies= -1773.296448

Cartesian coordinates

C	0.869456	2.863828	-0.438947
C	3.087587	2.809344	0.396643
C	2.674381	4.232215	0.564919
C	1.135833	4.128486	0.405006
H	0.845102	3.061169	-1.512411
H	-0.028261	2.320691	-0.147807
H	2.980388	4.647365	1.525081
H	3.127073	4.833459	-0.229357
H	0.673891	4.006787	1.387477
H	0.710721	5.013762	-0.066689
N	2.072648	2.074713	-0.142765
N	4.150683	2.078248	0.579805

N	3.775894	0.841708	0.121413
C	2.519599	0.829279	-0.321489
C	4.691027	-0.263810	0.191207
C	5.619446	-0.412026	-0.840171
C	4.618229	-1.119912	1.292984
C	6.520154	-1.470316	-0.737082
C	5.538302	-2.163664	1.346359
C	6.497594	-2.347862	0.347754
H	7.254558	-1.612419	-1.525450
H	5.507295	-2.849275	2.189132
C	5.615191	0.516168	-2.022405
H	4.655411	0.445802	-2.544844
H	5.756392	1.557406	-1.714844
H	6.410688	0.254946	-2.722780
C	7.502421	-3.463418	0.459556
H	7.031315	-4.387029	0.807633
H	7.986759	-3.662300	-0.499581
H	8.284371	-3.203621	1.181615
C	3.575196	-0.934829	2.361337
H	3.576190	0.088273	2.751109
H	2.573769	-1.141125	1.967987
H	3.753640	-1.616870	3.194824
C	1.815582	-0.324605	-1.011425
O	2.393258	-0.770719	-2.004593
C	0.550020	-0.709362	-0.480165
C	-0.279797	-1.588783	-1.227380
C	0.057391	-0.235604	0.769852
C	-1.528718	-1.927640	-0.791874
H	0.095595	-1.971777	-2.171659
C	-1.186505	-0.577850	1.215792
H	0.682302	0.395460	1.398469
C	-2.062274	-1.409242	0.437470
H	-2.156269	-2.578947	-1.391090
H	-1.540465	-0.203377	2.171610
C	-3.394448	-1.620162	0.785508
H	-3.742765	-1.329659	1.772538
H	-3.930919	-2.438560	0.316511
C	-4.458194	-0.221763	-0.679958
C	-5.826268	-0.591992	-0.158913
C	-6.380230	-0.096624	1.026449
C	-6.577827	-1.473361	-0.940634
C	-7.660397	-0.478009	1.415290
H	-5.817816	0.584182	1.654113
C	-7.853652	-1.860209	-0.546464

H	-6.140901	-1.843476	-1.862055
C	-8.401173	-1.361621	0.633725
H	-8.080641	-0.081902	2.334887
H	-8.425662	-2.545438	-1.164940
H	-9.399488	-1.657606	0.941536
C	-3.860893	1.115708	-0.172915
F	-4.673872	2.128813	-0.559929
F	-2.664920	1.346815	-0.722164
F	-3.715533	1.247423	1.160876
O	-4.099521	-0.555560	-1.812836

Vibrational frequencies

-259.2965	18.2919	27.3252
33.7693	36.0628	49.8671
50.9878	58.4193	62.2073
73.9993	76.1543	83.2800
99.5571	114.9957	125.8479
138.9500	148.2431	152.1237
170.5186	172.9287	181.1820
187.7141	190.8452	203.6155
215.7740	242.1188	243.5058
245.6184	260.6412	274.5577

ε-TS4$_{\Phi = -60°}$

Zero-point correction= 0.522397
Thermal correction to Energy= 0.556182
Thermal correction to Enthalpy= 0.557126
Thermal correction to Gibbs Free Energy= 0.455034
Sum of electronic and zero-point Energies= -1773.856514
Sum of electronic and thermal Energies= -1773.822730
Sum of electronic and thermal Enthalpies= -1773.821785
Sum of electronic and thermal Free Energies= -1773.923878

Cartesian coordinates

C	0.648336	2.647858	-0.498167
C	2.874563	2.806412	0.330617
C	2.340000	4.197287	0.451738
C	0.808545	3.959089	0.308057
H	0.618122	2.810121	-1.578344
H	-0.206242	2.043290	-0.198477
H	2.615691	4.675174	1.393125
H	2.735115	4.808380	-0.367212
H	0.365757	3.826477	1.298679
H	0.305189	4.791183	-0.184793

N	1.917925	1.965244	-0.174354
N	4.003982	2.173981	0.524585
N	3.732413	0.885930	0.105676
C	2.470009	0.750865	-0.322244
C	4.735513	-0.143086	0.202871
C	5.642820	-0.277709	-0.855003
C	4.760993	-0.944676	1.352160
C	6.618300	-1.270862	-0.734384
C	5.754021	-1.925028	1.420182
C	6.685243	-2.103742	0.388946
H	7.335589	-1.400907	-1.540333
H	5.801046	-2.562643	2.299038
C	5.539346	0.598920	-2.074087
H	4.586183	0.414773	-2.582342
H	5.573988	1.661050	-1.808028
H	6.351976	0.393302	-2.774241
C	7.719214	-3.197850	0.476729
H	8.083833	-3.322074	1.501210
H	7.290609	-4.158822	0.166045
H	8.575770	-2.995023	-0.172431
C	3.758855	-0.756397	2.462104
H	3.739062	0.281920	2.810925
H	2.745231	-1.006288	2.128287
H	3.997360	-1.397530	3.313548
C	1.854845	-0.476155	-0.962494
O	2.484573	-0.963257	-1.910497
C	0.571156	-0.878810	-0.458882
C	-0.251703	-1.731924	-1.241926
C	0.062579	-0.415839	0.787672
C	-1.530636	-2.038590	-0.843890
H	0.138334	-2.100295	-2.185999
C	-1.207295	-0.739849	1.196030
H	0.684634	0.194737	1.436546
C	-2.075161	-1.526225	0.376875
H	-2.167056	-2.647445	-1.476998
H	-1.581509	-0.366950	2.144455
C	-3.453285	-1.667453	0.669594
H	-3.790162	-1.407430	1.669492
H	-3.976384	-2.508353	0.224030
C	-4.406418	-0.318540	-0.640686
C	-5.814792	-0.568050	-0.122134
C	-6.322383	-0.063073	1.085766
C	-6.647095	-1.367631	-0.918211
C	-7.629867	-0.350598	1.479439

H	-5.701542	0.554652	1.723492
C	-7.950291	-1.662658	-0.520042
H	-6.246345	-1.743504	-1.853685
C	-8.449406	-1.153638	0.681811
H	-8.008382	0.052533	2.415072
H	-8.579747	-2.285224	-1.150596
H	-9.465641	-1.378819	0.993210
C	-3.770303	1.017409	-0.164749
F	-4.553691	2.066172	-0.545983
F	-2.561097	1.215679	-0.729971
F	-3.595852	1.157901	1.179557
O	-4.111972	-0.631353	-1.820704

Vibrational frequencies

-179.4986	14.4626	23.5150
24.5982	30.4806	40.9920
43.6609	55.3277	61.5258
70.3618	80.1812	87.8031
92.3138	107.2997	125.0842
130.7828	141.2616	147.8949
154.5491	168.0339	174.8062
179.7113	191.5662	198.1758
219.1446	237.7376	238.7983
253.2946	266.2868	275.2007

ε-TS4$_{\Phi = 171°}$

Zero-point correction= 0.522369
Thermal correction to Energy= 0.556136
Thermal correction to Enthalpy= 0.557080
Thermal correction to Gibbs Free Energy= 0.455696
Sum of electronic and zero-point Energies= -1773.858465
Sum of electronic and thermal Energies= -1773.824698
Sum of electronic and thermal Enthalpies= -1773.823754
Sum of electronic and thermal Free Energies= -1773.925138

Cartesian coordinates

C	0.347814	2.788429	0.183866
C	2.598173	2.755842	0.955987
C	2.087079	4.091844	1.386985
C	0.548573	3.899432	1.243278
H	0.282993	3.173019	-0.836900
H	-0.499290	2.133639	0.380775
H	2.396886	4.351048	2.400672
H	2.467901	4.861720	0.706927

H	0.133627	3.562127	2.196603
H	0.041092	4.820041	0.953890
N	1.616598	2.046524	0.315350
N	3.720292	2.083246	0.988297
N	3.417915	0.911820	0.320904
C	2.143262	0.881857	-0.089943
C	4.403156	-0.131597	0.194826
C	5.268165	-0.099577	-0.906301
C	4.460215	-1.110403	1.196018
C	6.229354	-1.110222	-0.988584
C	5.441335	-2.096738	1.066238
C	6.330717	-2.112123	-0.015319
H	6.915794	-1.112833	-1.831036
H	5.512532	-2.868361	1.828272
C	5.139438	0.965312	-1.962479
H	4.182545	0.854613	-2.483817
H	5.166323	1.969586	-1.525840
H	5.945475	0.889231	-2.695852
C	7.360106	-3.206666	-0.144112
H	7.688273	-3.565249	0.836144
H	6.944292	-4.066920	-0.683503
H	8.239419	-2.867071	-0.699276
C	3.493761	-1.099718	2.352490
H	3.506400	-0.136649	2.874662
H	2.466904	-1.271204	2.008416
H	3.741250	-1.882223	3.072870
C	1.492431	-0.198345	-0.929260
O	2.063750	-0.469477	-1.993216
C	0.261091	-0.750982	-0.436167
C	-0.539080	-1.540757	-1.306019
C	-0.206342	-0.530699	0.887823
C	-1.752435	-2.031389	-0.891924
H	-0.181924	-1.721425	-2.315041
C	-1.407880	-1.050740	1.313486
H	0.395342	0.042562	1.588220
C	-2.247487	-1.794097	0.429205
H	-2.370430	-2.597189	-1.582989
H	-1.757035	-0.862557	2.322367
C	-3.576535	-2.118782	0.794877
H	-3.800873	-2.237156	1.850303
H	-4.131389	-2.779635	0.134204
C	-4.496443	-0.226944	0.736959
C	-4.128265	0.247076	-0.658224
C	-4.568925	-0.332544	-1.858120

C	-3.220854	1.314235	-0.726417
C	-4.116057	0.150364	-3.087207
H	-5.259019	-1.166662	-1.840369
C	-2.759823	1.789938	-1.953377
H	-2.891595	1.751674	0.209422
C	-3.207225	1.210151	-3.142613
H	-4.470954	-0.309376	-4.005792
H	-2.054445	2.616664	-1.982557
H	-2.851498	1.576891	-4.101470
C	-5.936489	-0.766506	0.912151
F	-6.826440	0.254645	0.772844
F	-6.120307	-1.280254	2.146468
F	-6.336115	-1.729701	0.035175
O	-4.081431	0.423782	1.731930

Vibrational frequencies

-199.6094	20.8895	22.2046
26.9884	34.8465	47.4643
52.5459	59.3487	63.7129
68.0601	72.0532	88.8829
95.9522	101.5843	115.5955
130.8107	138.5410	140.9273
154.0328	165.7684	170.2123
177.3400	196.1382	201.8186
232.9715	234.9741	241.6708
245.7840	259.5437	276.7013

ε-TS4$_{\Phi = -161°}$

Zero-point correction= 0.522944
Thermal correction to Energy= 0.556420
Thermal correction to Enthalpy= 0.557364
Thermal correction to Gibbs Free Energy= 0.456418
Sum of electronic and zero-point Energies= -1773.857488
Sum of electronic and thermal Energies= -1773.824013
Sum of electronic and thermal Enthalpies= -1773.823069
Sum of electronic and thermal Free Energies= -1773.924014

Cartesian coordinates

C	-0.089267	1.814086	-1.249159
C	2.170899	2.552471	-1.100399
C	1.437352	3.735812	-1.641560
C	-0.038908	3.358913	-1.327070
H	-0.286855	1.343616	-2.215654
H	-0.796041	1.438434	-0.507885

H	1.752743	4.673474	-1.181102
H	1.621142	3.807584	-2.719393
H	-0.322111	3.772486	-0.355662
H	-0.733211	3.739634	-2.076544
N	1.312878	1.508784	-0.877083
N	3.407196	2.217046	-0.827611
N	3.308262	0.896767	-0.438610
C	2.042938	0.458645	-0.465572
C	4.476216	0.175839	-0.001387
C	5.263259	-0.458551	-0.970920
C	4.773334	0.162732	1.367385
C	6.406643	-1.124645	-0.524444
C	5.927605	-0.520332	1.760901
C	6.753000	-1.166009	0.832325
H	7.038536	-1.625778	-1.252924
H	6.186001	-0.546758	2.816150
C	4.863269	-0.443716	-2.421975
H	3.908898	-0.967046	-2.547277
H	4.733901	0.578481	-2.793800
H	5.614595	-0.940793	-3.039582
C	7.976077	-1.923114	1.285682
H	8.758798	-1.912328	0.521250
H	8.389406	-1.505440	2.208474
H	7.728573	-2.973499	1.484267
C	3.870995	0.837365	2.368790
H	3.659598	1.874152	2.085672
H	2.909314	0.315300	2.441090
H	4.324946	0.840451	3.362108
C	1.561238	-0.957516	-0.223879
O	2.163662	-1.855231	-0.818933
C	0.366194	-1.070270	0.573353
C	-0.494526	-2.183937	0.395596
C	-0.046656	-0.025355	1.437877
C	-1.754314	-2.184082	0.951143
H	-0.168387	-2.996869	-0.245786
C	-1.292275	-0.044163	2.020529
H	0.619276	0.811109	1.632527
C	-2.219529	-1.087227	1.736442
H	-2.436224	-3.003755	0.743363
H	-1.606333	0.775888	2.656707
C	-3.596976	-0.884271	2.016786
H	-3.833034	-0.222107	2.846632
H	-4.268648	-1.732620	1.918135
C	-4.068208	0.389723	0.460554

C	-4.259368	-0.632187	-0.651491
C	-5.316295	-1.555013	-0.728683
C	-3.272965	-0.668881	-1.646780
C	-5.381089	-2.476414	-1.774214
H	-6.092448	-1.559400	0.026391
C	-3.331803	-1.595338	-2.688249
H	-2.465111	0.050480	-1.583460
C	-4.388108	-2.505326	-2.757878
H	-6.209981	-3.178111	-1.818003
H	-2.552189	-1.606774	-3.445869
H	-4.438953	-3.229065	-3.566692
C	-5.373486	0.930854	1.091896
F	-6.093205	1.623377	0.166192
F	-5.108229	1.788921	2.100948
F	-6.226590	-0.001642	1.604551
O	-3.185387	1.288308	0.320330

Vibrational frequencies

-232.9772	14.1141	19.7342
24.8664	36.7493	44.1601
49.5716	60.1634	63.6183
72.8482	80.3318	95.0336
96.3667	109.9364	122.8223
136.5296	145.9174	158.4598
169.4576	176.4202	187.0741
188.8480	190.8765	206.4174
234.1932	239.0156	243.8507
250.5566	266.6202	275.5504

ε-TS4$_{\Phi = 78°}$

Zero-point correction= 0.523106
Thermal correction to Energy= 0.556573
Thermal correction to Enthalpy= 0.557517
Thermal correction to Gibbs Free Energy= 0.457047
Sum of electronic and zero-point Energies= -1773.857297
Sum of electronic and thermal Energies= -1773.823830
Sum of electronic and thermal Enthalpies= -1773.822886
Sum of electronic and thermal Free Energies= -1773.923357

Cartesian coordinates

C	0.329513	2.617118	-0.949559
C	2.556926	2.873968	-0.152232
C	2.015927	4.267356	-0.183233
C	0.484265	4.005957	-0.285020

H	0.290356	2.663881	-2.040739
H	-0.515852	2.042320	-0.577112
H	2.298510	4.845978	0.697720
H	2.397764	4.786857	-1.068849
H	0.051558	3.970445	0.718403
H	-0.030390	4.779871	-0.855041
N	1.601381	1.980404	-0.559341
N	3.678785	2.265151	0.135856
N	3.404029	0.935713	-0.123228
C	2.144606	0.755278	-0.543380
C	4.388496	-0.083411	0.137712
C	5.301437	-0.401713	-0.875617
C	4.376972	-0.705665	1.392994
C	6.242676	-1.394642	-0.593342
C	5.338421	-1.693429	1.622559
C	6.275884	-2.048387	0.645007
H	6.960394	-1.669234	-1.361690
H	5.352089	-2.198774	2.584527
C	5.232305	0.273675	-2.219083
H	4.302844	-0.008953	-2.725874
H	5.238668	1.364523	-2.120242
H	6.075204	-0.018759	-2.849463
C	7.319226	-3.099556	0.928994
H	8.224570	-2.644334	1.349945
H	6.957727	-3.836358	1.652469
H	7.614182	-3.627182	0.017092
C	3.354211	-0.335995	2.435933
H	3.329477	0.746111	2.604871
H	2.348256	-0.641704	2.124893
H	3.573739	-0.825412	3.387323
C	1.528761	-0.548146	-1.008528
O	2.144232	-1.145124	-1.900955
C	0.280496	-0.929446	-0.405272
C	-0.459094	-2.009613	-0.959705
C	-0.251999	-0.275037	0.738202
C	-1.671637	-2.380520	-0.431451
H	-0.048138	-2.527277	-1.820858
C	-1.459903	-0.657184	1.273592
H	0.303195	0.525898	1.217929
C	-2.230818	-1.716408	0.705315
H	-2.233368	-3.190986	-0.885386
H	-1.849629	-0.140412	2.145174
C	-3.528944	-2.022916	1.205227
H	-3.729874	-1.724971	2.229843

H	-3.943119	-2.993255	0.942188
C	-5.093575	-0.875649	0.536921
C	-4.464586	0.509289	0.523184
C	-4.612364	1.269545	1.693358
C	-3.765403	1.073634	-0.554452
C	-4.070569	2.549540	1.794928
H	-5.171891	0.831965	2.513549
C	-3.248395	2.369299	-0.463953
H	-3.627095	0.518202	-1.473204
C	-3.388628	3.110846	0.710681
H	-4.193740	3.116547	2.714021
H	-2.737199	2.799525	-1.321274
H	-2.982369	4.116464	0.777308
C	-5.297434	-1.532488	-0.849812
F	-6.207562	-0.820073	-1.570936
F	-5.785110	-2.784469	-0.732285
F	-4.190435	-1.627165	-1.638206
O	-6.038972	-1.109411	1.338767

Vibrational frequencies

-240.3751	18.3848	21.9100
25.3522	36.4228	45.0557
52.4849	59.4576	67.6433
73.9533	83.5275	91.3633
98.5074	110.8472	127.8595
137.3693	144.2453	151.1977
167.6057	176.5521	182.6805
190.4146	200.1282	230.7477
235.9226	239.0718	245.9702
249.0235	260.5872	267.2507