Supporting Information for

Electron–Electrophile Coupled Dinitrogen Reduction in a Cerium–Meta-Tetraphenolate System: A Computational Study

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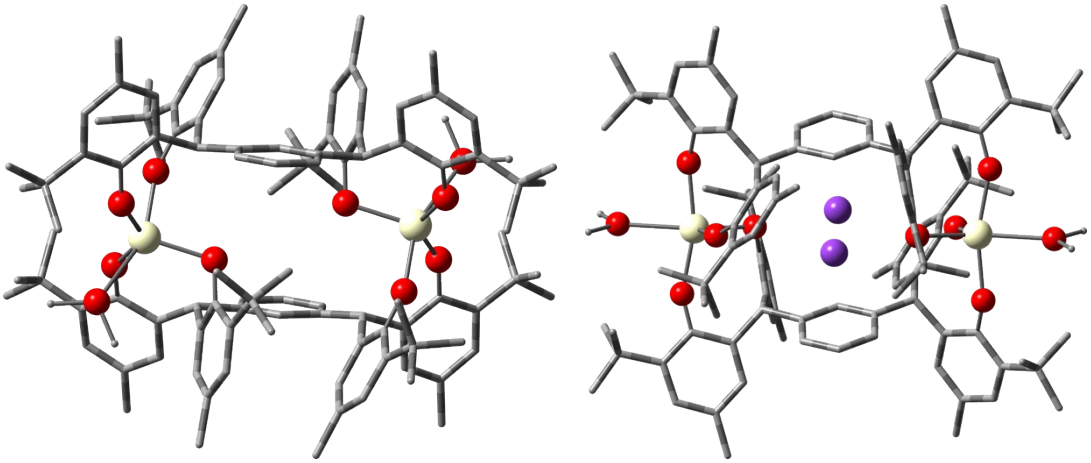
Contents

Section S1. Structural Effects of K^+ Incorporation on N_2 Reduction

Optimised Geometries of K^+-Free vs K^+-Bound Starting Complexes

Both starting complexes contained two Ce centres and were optimised in the triplet spin state, as this configuration corresponds to the expected ground state for a pair of Ce(III) ions, each bearing one unpaired 4f electron. Upon incorporation of two K^+ cations, a marked expansion of the Ce···Ce separation was observed, increasing from 8.33 Å in the K^+-free species to 9.75 Å in the K^+-bound analogue. In the latter, the two K^+ centres were positioned in close proximity to each other (K···K = 4.54 Å) and engaged in electrostatic interactions with the ligand framework, as indicated by short K···O distances of 2.88 Å to the nearest aryloxide oxygen atoms. These structural changes reflect a redistribution of the coordination environment upon K^+ incorporation, with the cations occupying the central cavity and influencing the overall geometry of the bimetallic core (**Figure S1.1**).



K^+-Free Starting Complex
Ce···Ce distance = 8.33 Å
Triplet State, Overall Charge –2

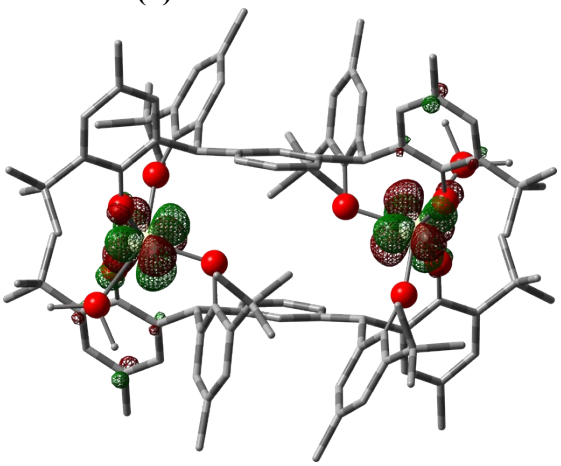
K^+-Bound Starting Complex
Ce···Ce distance = 9.75 Å
K···K = 4.54 Å
Triplet State, Overall Charge 0

Figure S1.1. Optimised geometries of the K^+-free starting complex (left) and K^+-bound starting complex (right), both in the triplet spin state. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, potassium = purple. All hydrogen atoms are omitted for clarity.

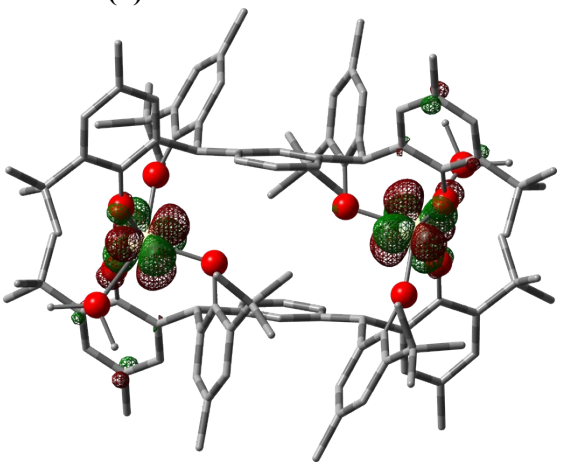
α-Spin HOMO–1 and HOMO Analysis for K^+-Free and K^+-Bound Starting Complexes

The α-spin HOMO–1 and HOMO of the K^+-free and K^+-bound starting complexes are both dominated by Ce 4f character, with minimal contributions from the ligand framework. In both cases, each Ce atom contributes almost equally to the orbital, though the K^+-bound complex shows a slightly more asymmetric distribution between the two Ce centres, particularly in the HOMO–1 (46.33 % vs 49.73 %). The atomic orbital (AO) composition remains overwhelmingly f-character (>93 % in all cases), but the K^+-bound complex exhibits slightly higher f-character in the HOMO (96.08 %) compared to the K^+-free system (93.00 %). Minor variations in the s and p components are also observed, with the K^+-bound complex displaying a marginally higher s-character (**Figures S1.2–1.3**).

HOMO–1 (α):



HOMO (α):



Atomic contributions – HOMO–1(α):

Atom		Contribution (%)
1	Ce	46.72
2	Ce	46.83
AO composition (%) – HOMO–1(α):		

s	p	d	f
0.51	5.53	0.76	93.20

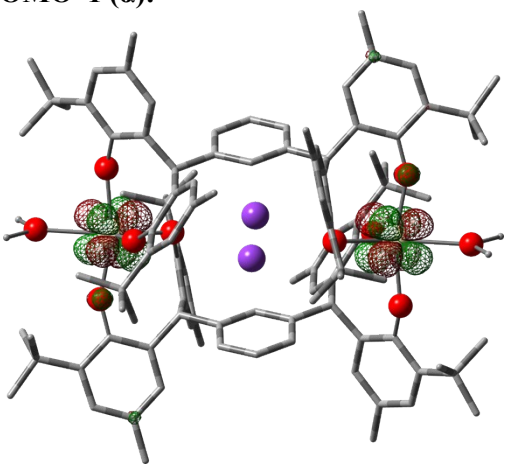
Atomic contributions – HOMO–1(α):

Atom		Contribution (%)
1	Ce	46.75
2	Ce	46.63
AO composition (%) – HOMO (α):		

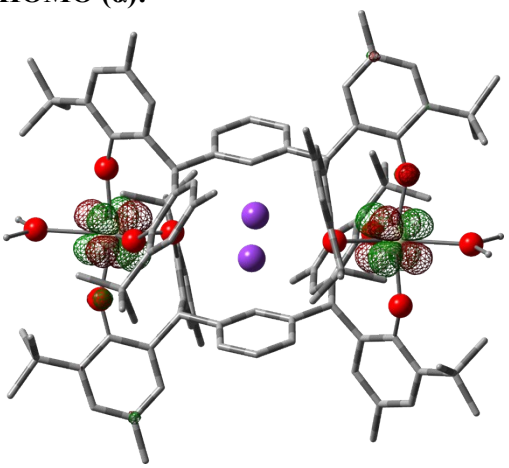
s	p	d	f
0.59	5.68	0.74	93.00

Figure S1.2. Selected α-spin molecular orbitals HOMO–1 and HOMO of the K^+-Free starting complex in the triplet spin state (atom colour coding: Ce = yellow, O = red, C = grey), calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Isosurfaces are plotted at an isovalue of 0.03. Orbital phases are represented by red (positive) and green (negative) regions. Atomic and AO composition analyses were performed using Multiwfn (Version 3.8)[S1].

HOMO–1 (α):



HOMO (α):



Atomic contributions – HOMO–1(α):

Atom		Contribution (%)
1	Ce	46.33
2	Ce	49.73
AO composition (%) – HOMO–1(α):		
s	p	d	f
0.48	3.29	0.29	95.94

Atomic contributions – HOMO (α):

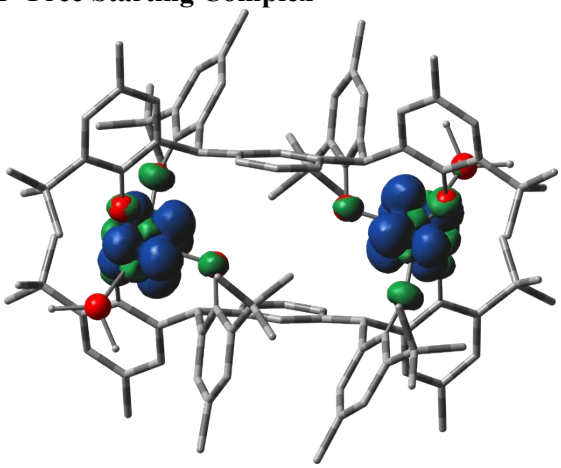
Atom		Contribution (%)
1	Ce	49.80
2	Ce	46.39
AO composition (%) – HOMO (α):		
s	p	d	f
0.62	3.02	0.28	96.08

Figure S1.3. Selected α-spin molecular orbitals HOMO–1 and HOMO of the K^+-Bound starting complex in the triplet spin state (atom colour coding: Ce = yellow, O = red, C = grey), calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Isosurfaces are plotted at an isovalue of 0.03. Orbital phases are represented by red (positive) and green (negative) regions. Atomic and AO composition analyses were performed using Multiwfn (Version 3.8)[S1].

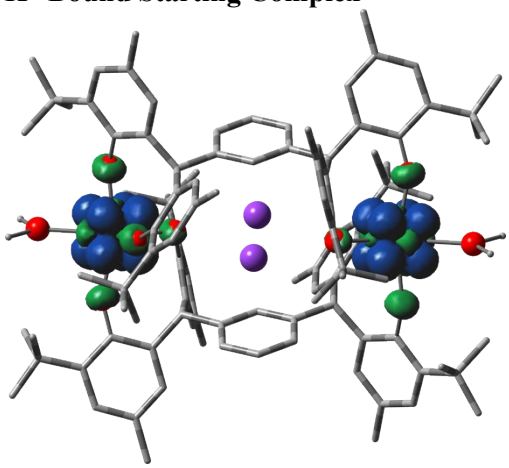
Spin Density and CM5 Charge Distributions in K^+-Free vs K^+-Bound Starting Complexes

The CM5 charge and spin population analyses reveal that both the K^+-Free and K^+-Bound starting complexes exhibit nearly identical spin distributions, with each Ce centre having a spin population of ~1.03–1.04, consistent with two Ce(III) centres in the triplet state. However, K^+ coordination induces a slight increase in the CM5 charges on Ce from 1.34 to 1.37, indicating marginally greater electron withdrawal from the metal centres. The spin density plots for both systems show localised α spin density primarily on the Ce atoms, with minor delocalisation onto the ligand framework, and the spatial distribution remains qualitatively similar regardless of K^+ binding (**Figure S1.4**).

K^+-Free Starting Complex



K^+-Bound Starting Complex



CM5 Charges and Spin Population (K^+-Free Starting Complex):

Atom		Charges	Spin Population
1	Ce	1.34	1.03
2	Ce	1.34	1.03

CM5 Charges and Spin Population (K^+-Bound Starting Complex):

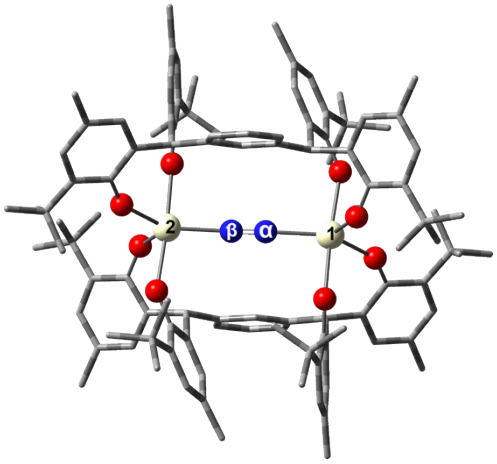
Atom		Charges	Spin Population
1	Ce	1.37	1.04
2	Ce	1.37	1.04

Figure S1.4. Spin density distribution and CM5 charges of the K^+-Free and K^+-Bound starting complexes in the triplet spin state (atom colour coding: Ce = yellow, K = purple, O = red, C = grey), calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Isosurfaces are plotted at an isovalue of 0.0009, with blue representing excess α spin density and green representing excess β spin density. Hydrogen atoms are omitted for clarity.

Section S2. Comparison of Electronic Structure and N_2 Activation Pathways in Ce–mTP Complexes Following Two-Electron Reduction via Different K^+ Incorporation Strategies

K^+-Free vs K^+-Bound Geometries following $2e^-$ Electrochemical Reduction

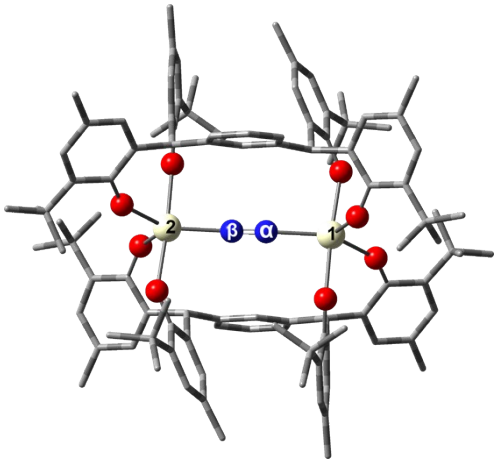
Comparison of the optimised geometries for the K^+-free and K^+-bound complexes following two-electron reduction reveals that in both cases, the quintet spin state is more stable than the triplet, by 5.3 and 6.2 kcal mol^{-1}, respectively. Upon moving from triplet to quintet, both systems show elongation of the Ce–N bonds (K^+-free: 2.30 → 2.36 Å; K^+-bound: 2.31 → 2.42 Å) and slight contraction of the N–N bond (K^+-free: 1.22 → 1.21 Å; K^+-bound: 1.25 → 1.24 Å). The presence of K^+ cations leads to overall longer Ce–N bonds in both spin states and slightly longer N–N distances compared to the K^+-free analogue, consistent with enhanced activation of the N_2 ligand via cation coordination (**Figures S2.1–2.2**).



K^+-Free Complex Following Two-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.30
Ce2–Nβ = 2.30
Nα–Nβ = 1.22

Triplet Spin State, Overall Charge –4

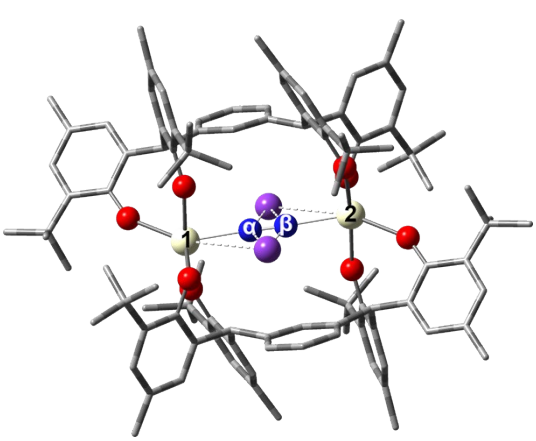


K^+-Free Complex Following Two-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.36
Ce2–Nβ = 2.36
Nα–Nβ = 1.21

Quintet Spin State, Overall Charge –4

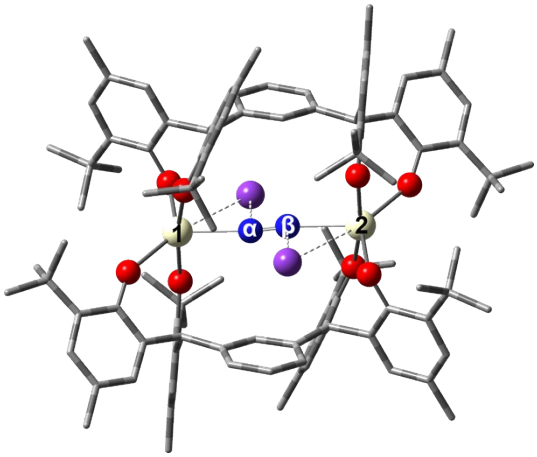
Figure S2.1. Optimised geometries of the K^+-free complex following two-electron reduction in the triplet (left) and quintet (right) spin states. The quintet state is lower in energy by 5.3 kcal mol^{-1}. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase, with relative free energies calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, nitrogen = blue. All hydrogen atoms are omitted for clarity.



K^+-Bound Complex Following Two-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.31
Ce2–Nβ = 2.31
Nα–Nβ = 1.25

Triplet Spin State, Overall Charge –2



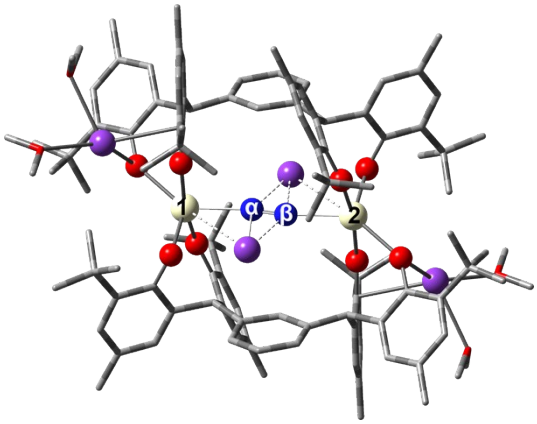
K^+-Bound Complex Following Two-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.42
Ce2–Nβ = 2.42
Nα–Nβ = 1.24

Quintet Spin State, Overall Charge –2

Figure S2.2. Optimised geometries of the K^+-bound complex following two-electron reduction in the triplet (left) and quintet (right) spin states. The quintet state is lower in energy by 6.2 kcal mol^{-1}. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase, with relative free energies calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, nitrogen = blue. All hydrogen atoms are omitted for clarity.

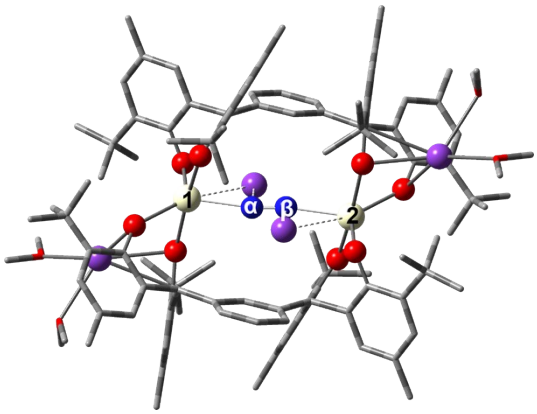
Across all three systems examined following two-electron reduction—K^+-free, K^+-bound, and K^0 as reductant—the quintet spin state was consistently more stable than the triplet, with energy differences of 5.3, 6.2, and 9.1 kcal mol^{-1}, respectively. In each case, the quintet geometry showed slightly elongated Ce–N bonds and a marginally longer N–N bond. The larger stabilisation of the quintet in the K^0 system suggests that additional K^+ coordination further favours high-spin configurations by stabilising electron density delocalisation across the $\{Ce_2(\mu\text{-}\eta^1\text{:}\eta^1\text{-}N_2)\}$ core. Given this consistent trend and the substantial 9.1 kcal mol^{-1} preference in the chemically relevant K^0 case, the quintet spin state was used for electronic structure analysis in the main text.



K^+-Bound Complex Following Two-Electron Reduction (K^0 as Redundant)

Bond Lengths (Å):
Ce1–Nα = 2.39
Ce2–Nβ = 2.39
Nα–Nβ = 1.22

Triplet Spin State, Overall Charge 0



K^+-Bound Complex Following Two-Electron Reduction (K^0 as Redundant)

Bond Lengths (Å):
Ce1–Nα = 2.38
Ce2–Nβ = 2.38
Nα–Nβ = 1.24

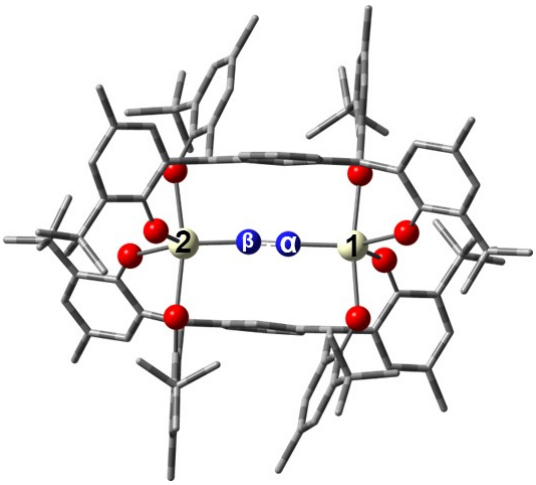
Quintet Spin State, Overall Charge 0

Figure S2.3. Optimised geometries of the K^+-bound complex (K^0 as reductant) following two-electron reduction in the triplet (left) and quintet (right) spin states. The quintet state is lower in energy by 9.1 kcal mol^{-1}. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase, with relative free energies calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, nitrogen = blue, potassium = purple. All hydrogen atoms are omitted for clarity.

Section S3. Computational Analysis of the Four-Electron-Reduced Species

K^+-Free Geometries following $4e^-$ Electrochemical Reduction

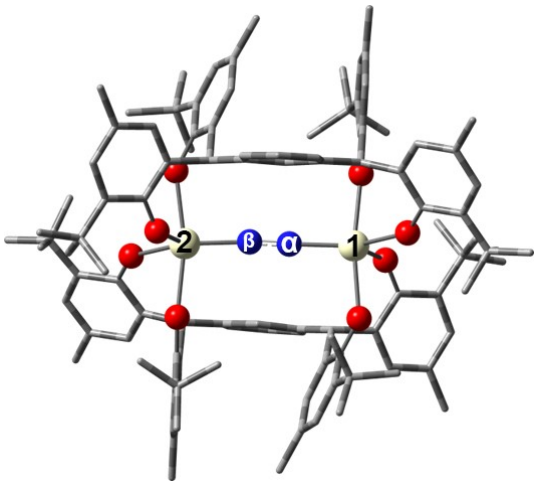
Following four-electron reduction of the K^+-free complex, both the triplet and quintet spin states were examined. The quintet state is more stable by 1.9 kcal mol^{-1}, indicating a preference for high-spin electronic configurations in this system. Structurally, the quintet state exhibits elongated Ce–N bonds (2.27 Å vs. 2.15 Å in the triplet) and a shorter N–N distance (1.23 Å vs 1.27 Å). This combination of energetic and structural changes supports the assignment of the quintet state as the ground state under these reduction conditions, justifying its inclusion as the reference state in the main text discussion of four-electron-reduced species. (**Figure S3.1**).



K^+-Free Complex Following Four-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.15
Ce2–Nβ = 2.15
Nα–Nβ = 1.27

Triplet Spin State, Overall Charge –6



K^+- Free Complex Following Four-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.27
Ce2–Nβ = 2.27
Nα–Nβ = 1.23

Quintet Spin State, Overall Charge –6

Figure S3.1. Optimised geometries of the K^+-free complex following four-electron reduction in the triplet (left) and quintet (right) spin states. The quintet state is lower in energy by 1.9 kcal mol^{-1}. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase, with relative free energies calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, nitrogen = blue, potassium = purple. All hydrogen atoms are omitted for clarity.

Spin Density Distribution of K^+-Free Complex following $4e^-$ Electrochemical Reduction

In the K^+-free four-electron-reduced complex, spin density was predominantly localised on the cerium centres and the ligand framework, with minimal delocalisation onto the N_2 unit. Significant α spin density was observed at the Ce sites, while the nitrogen atoms of the N_2 moiety exhibited only minor β spin density contributions, confirming that full reduction to an N_2^{4-} species was not achieved. The distribution of spin density supports a mixed-valent electronic structure, with excess electron density delocalised across the metal–ligand scaffold rather than concentrated on the N_2 ligand (**Figure S3.2**).

CM5 Charges and Spin Population:

Atom		Spin Population	Charges
1	Ce	1.02	1.27
2	Ce	1.02	1.27
7	C	-0.06	-0.04
12	C	0.06	-0.13
17	C	0.29	-0.08
21	C	0.10	-0.05
24	C	0.27	-0.18
26	C	0.08	0.02
28	C	0.07	0.01
33	C	-0.08	-0.10
125	C	-0.06	-0.04
130	C	0.06	-0.13
135	C	0.29	-0.08
139	C	0.10	-0.05
142	C	0.27	-0.18
144	C	0.08	0.02
146	C	0.07	0.01
151	C	-0.08	-0.10
239	N	0.03	-0.51
240	N	0.03	-0.51

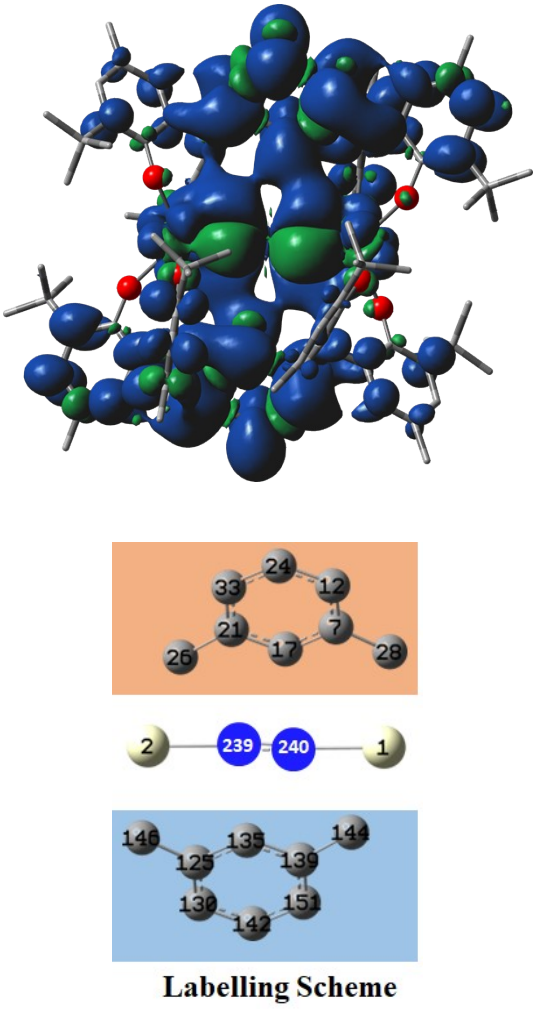
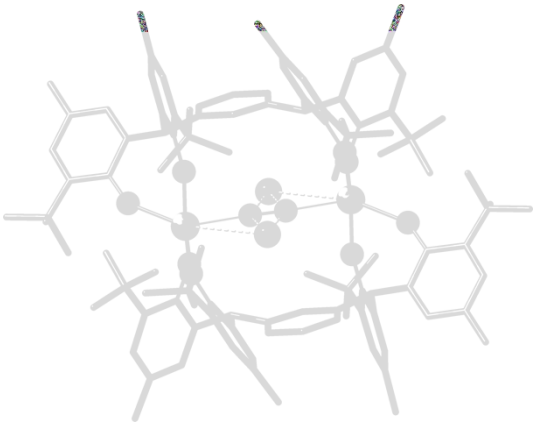


Figure S3.2. Spin density distribution of the four-electron-reduced K^+-free complex in the quintet spin state (atom colour coding: Ce = yellow, N = blue, O = red, C = grey), with CM5 charges listed for selected atoms. Calculations were performed at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Isosurfaces are plotted at an isovalue of 0.0009, with blue representing excess α spin density and green representing excess β spin density. Hydrogen atoms are omitted for clarity.

K^+-Bound Geometries following $4e^-$ Electrochemical Reduction

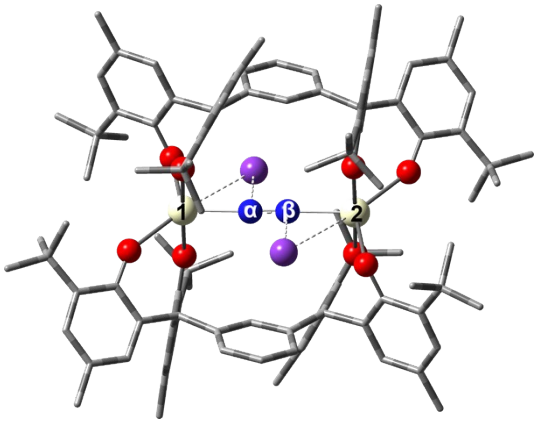
In the K^+-bound four-electron-reduced complex, elongation of the Ce–N bonds and slight contraction of the N–N bond was observed in the quintet spin state relative to the triplet, consistent with enhanced electron density delocalisation across the metal–ligand framework. The quintet geometry exhibited Ce–N distances of 2.28 Å and an N–N bond length of 1.26 Å, compared to 2.17 Å and 1.28 Å, respectively, in the triplet state (**Figure S3.3**). These energetic and structural features confirm the quintet state as the ground state for the K^+-bound four-electron-reduced species, providing the basis for its use as the representative configuration in the discussion of spin density distribution in the main text.



K^+-Bound Complex Following Four-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.17
Ce2–Nβ = 2.17
Nα–Nβ = 1.28

Triplet Spin State, Overall Charge –4



K^+- Bound Complex Following Four-Electron Reduction (Electrochemical Reduction)

Bond Lengths (Å):
Ce1–Nα = 2.28
Ce2–Nβ = 2.28
Nα–Nβ = 1.26

Quintet Spin State, Overall Charge –4

Figure S3.3. Optimised geometries of the K^+-bound complex following four-electron reduction in the triplet (left) and quintet (right) spin states. The quintet state is lower in energy by 1.3 kcal mol^{-1}. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase, with relative free energies calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, nitrogen = blue, potassium = purple. All hydrogen atoms are omitted for clarity.

Spin Density Distribution of K^+-Bound Complex following $4e^-$ Electrochemical Reduction

In the K^+-bound four-electron-reduced complex, the additional electrons were predominantly localised on the K^+ cations and the cerium centres, rather than on the N_2 unit. The spin density plot shows substantial α spin density on the Ce atoms, while the nitrogen atoms of the N_2 moiety display only minimal contributions. This distribution indicates that, although K^+ coordination influences electron delocalisation, full reduction to an N_2^{4-} species is not achieved, as also evidenced by the CM5 charges.

CM5 Charges and Spin Population:

Atom		Spin Population	Charges
1	Ce	1.13	1.17
2	Ce	1.13	1.17
α	N	0.33	-0.70
β	N	0.33	-0.70
κ_1	K^0	0.40	0.50
κ_2	K^0	0.40	0.50

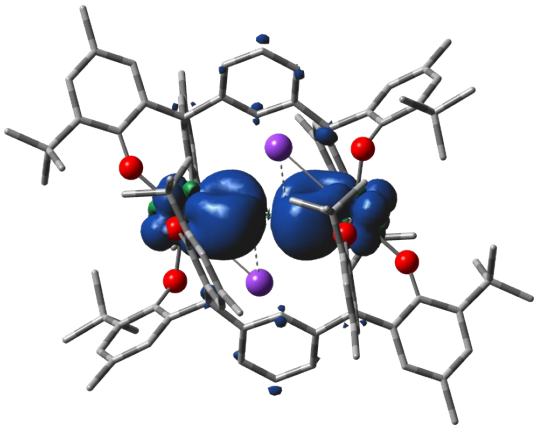
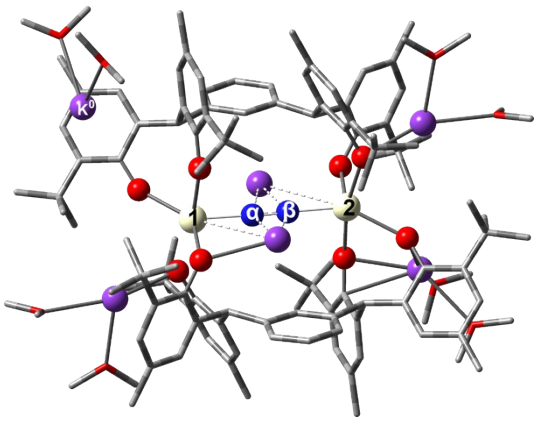


Figure S3.4. Spin density distribution of the four-electron-reduced K^+-bound complex in the quintet spin state (atom colour coding: Ce = yellow, N = blue, O = red, C = grey), with CM5 charges listed for selected atoms. Calculations were performed at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Isosurfaces are plotted at an isovalue of 0.0009, with blue representing excess α spin density and green representing excess β spin density. Hydrogen atoms are omitted for clarity.

K^+-Bound Complex Reduced with K^0 following $4e^-$ Reduction

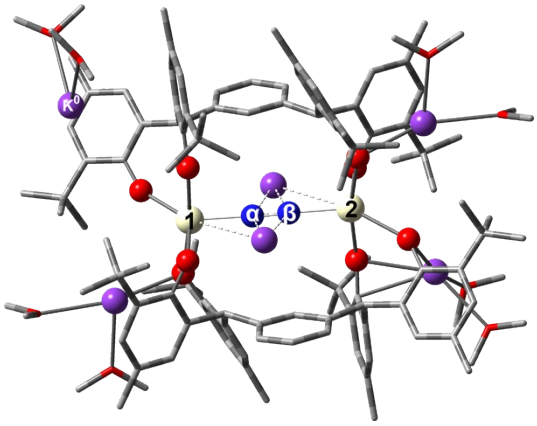
Following four-electron reduction of the K^+-bound complex using K^0 as the reductant, both the triplet and quintet spin states were optimised and compared. The two spin states exhibited very similar structural metrics, with Ce–N bond lengths of 2.18–2.22 Å in the triplet and 2.18–2.23 Å in the quintet, and identical N–N distances of 1.29 Å. Despite these small structural differences, the quintet spin state was calculated to be marginally lower in energy by 0.2 kcal mol^{-1}. The quintet spin state was discussed in the main text because it is slightly more stable than the triplet state by 0.2 kcal mol^{-1}, making it the thermodynamically preferred configuration under these conditions.



K^+-Bound Complex Following Four-Electron Reduction (Reduced using K^0)

Bond Lengths (Å):
Ce1–Nα = 2.18
Ce2–Nβ = 2.22
Nα–Nβ = 1.29

Triplet Spin State, Overall Charge 0



K^+- Bound Complex Following Four-Electron Reduction (Reduced using K^0)

Bond Lengths (Å):
Ce1–Nα = 2.23
Ce2–Nβ = 2.18
Nα–Nβ = 1.29

Quintet Spin State, Overall Charge 0

Figure S3.5. Optimised geometries of the K^+-bound complex following four-electron reduction in the triplet (left) and quintet (right) spin states using K^0 as reductant. The quintet state is lower in energy by 0.2 kcal mol^{-1}. Geometries were fully optimised at the PBE0-D3BJ/BS1 level of theory in the gas phase, with relative free energies calculated at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Atom colour coding: oxygen = red, cerium = yellow, carbon = grey, nitrogen = blue, potassium = purple. All hydrogen atoms are omitted for clarity.

Spin Density Distribution of K^+-Bound Complex Reduced with K^0 following $4e^-$ Reduction

Spin-density analysis revealed that, as in the quintet, in the triplet spin state, one unpaired electron was localised on an outer K^0 atom, with the remaining unpaired electrons distributed across the {$Ce_2(\mu\text{-}\eta^1{:}\eta^1\text{-}N_2)$} core. CM5 charge and spin population values confirmed that the N_2 unit in the triplet state carries a similar charge and spin distribution to that in the quintet, indicating that the extra electron remains localised on potassium rather than the N_2 π^* manifold. This behaviour further supports the conclusion that additional reduction beyond **Intermediate 3** results in electron localisation on external potassium species, without achieving greater population of the N_2 π^* orbitals or further weakening of the N–N bond.

CM5 Charges and Spin Population:

Atom		Spin Population	Charges
1	Ce	-1.01	1.23
2	Ce	1.19	1.20
α	N	0.27	-0.85
β	N	0.43	-0.83
K^0	K	1.21	0.07

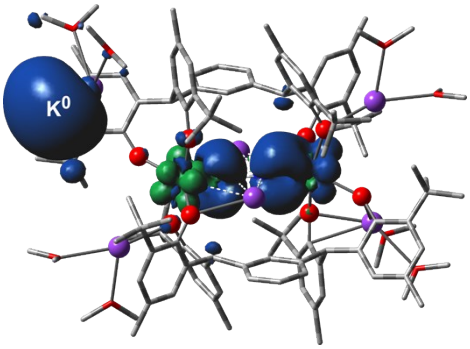
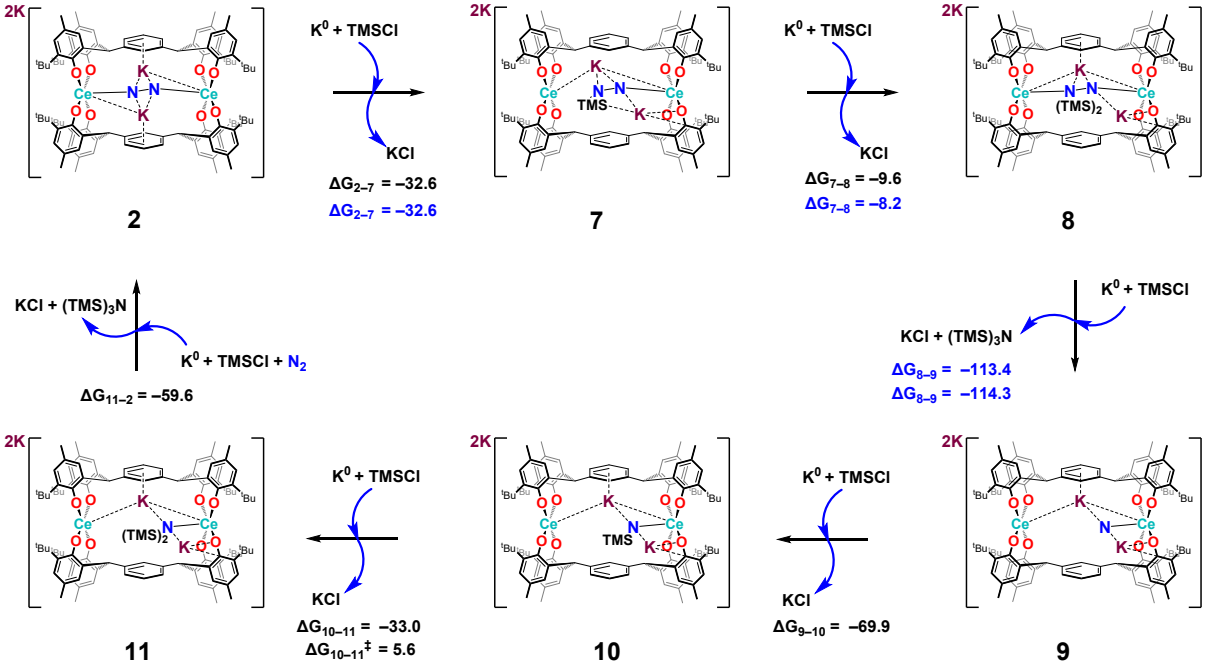


Figure S3.6. Spin density distribution of the four-electron-reduced K^+-bound complex in the quintet spin state (atom colour coding: Ce = yellow, N = blue, O = red, C = grey) using K^0 as reductant, with CM5 charges listed for selected atoms. Calculations were performed at the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 level of theory. Isosurfaces are plotted at an isovalue of 0.0009, with blue representing excess α spin density and green representing excess β spin density. Hydrogen atoms are omitted for clarity.

Section S4. Comparison of BS1 and BS1′ Optimisation Protocols

For all steps in the catalytic sequence illustrated in Scheme S__, free energy changes (ΔG, kcal mol^{-1}) were computed at both the PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1 and PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1′ levels to assess the reliability of the mixed-basis optimisation protocol. Values obtained from PBE0-D3BJ/BS1′ optimisations are shown in **black**, whereas the corresponding PBE0-D3BJ/BS1 values are given in **blue**. In all cases, PBE0-D3BJ/BS1′ results were found to be in excellent agreement with PBE0-D3BJ/BS1, with deviations typically within 1–2 kcal mol^{-1}. This consistency confirms that the BS1′ protocol, which applies a reduced 3-21G(d) basis to peripheral atoms, preserves the structural and energetic accuracy of the full BS1 model while offering substantial computational savings.



Scheme S4.1. DFT-computed catalytic cycle for N_2 reductive silylation mediated by Ce–mTP: benchmarking PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1′ against PBE0-D3BJ/BS2/SMD // PBE0-D3BJ/BS1.

Section S5. XYZ Coordinates and SCF Energies (a.u.) for Optimised Ce–mTP Species — PBE0-D3BJ/BS1 (default); PBE0-D3BJ/BS1′ where indicated

K^+-Free Starting Complex – Quintet
SCF Energy (a.u.): -5895.146252

Ce	4.128287	0.082000	-0.372753
Ce	-4.128361	-0.082078	0.372918
O	-4.851199	1.838997	1.347582
O	1.986100	0.484442	-0.939869
O	5.043058	1.898471	0.689323
O	-3.835722	1.130726	-1.437457
C	1.171730	3.474245	0.884491
C	-2.540399	3.116851	-1.400041
C	1.916204	1.551085	-1.724369
C	4.937312	3.199667	0.886223
C	3.698268	3.853903	0.647072
C	1.130708	4.037586	2.164149
H	2.057340	4.217285	2.700818
C	3.606231	5.237484	0.764029
H	2.642963	5.710908	0.583012
C	-3.790597	3.846030	0.626624
C	-0.035893	3.227767	0.229811
H	-0.025008	2.767227	-0.751198
C	-4.873205	3.154745	1.227887
C	-3.256944	2.117447	-2.104755
C	-1.271593	3.540742	0.802179
C	5.881697	5.356016	1.463095
H	6.716466	5.958052	1.812130
C	-0.090314	4.365594	2.742108
H	-0.112902	4.807329	3.735825
C	-2.563565	3.104551	0.119550
H	-2.665537	2.058648	0.425005
C	2.497385	3.013867	0.271198
H	2.654609	2.028260	0.728513
C	4.695687	6.017217	1.144051
C	-1.899426	4.129738	-2.105053
H	-1.323471	4.869989	-1.553701
C	-1.285664	4.125463	2.069730
H	-2.234926	4.373092	2.534033
C	-3.836224	5.230127	0.491903
H	-2.992807	5.729743	0.018874
C	2.435774	3.902100	-2.094073
H	2.808395	4.846052	-1.701922
C	2.341562	2.813582	-1.229680
C	-1.948489	4.198768	-3.493832
C	-2.675480	3.220566	-4.171920
H	-2.717106	3.282447	-5.255835
C	2.065818	3.803956	-3.430542
C	0.790308	0.161884	-3.557459
C	-4.910598	5.984167	0.949726
C	1.511739	2.595249	-3.866839
H	1.148301	2.543518	-4.888733
C	6.032901	3.972048	1.369662
C	7.322742	3.285128	1.827288
C	1.418895	1.463282	-3.058161
C	-5.961952	5.300445	1.561083
H	-6.800036	5.886343	1.929085
C	-3.341189	2.180606	-3.521219
C	-5.978771	3.914949	1.712790
C	1.863261	-0.932216	-3.670734
H	2.667392	-0.624950	-4.350954
H	1.419101	-1.856352	-4.056213
H	2.299504	-1.167429	-2.699427
C	-7.171913	3.207797	2.360036
C	-4.190573	1.166689	-4.296205
C	6.989659	2.283963	2.945395
H	6.570049	2.806328	3.812027
H	7.894542	1.753583	3.269041
H	6.258192	1.552271	2.600316
C	-1.273536	5.317197	-4.235340
H	-1.945544	6.173065	-4.388941
H	-0.933045	4.992041	-5.224535
H	-0.400239	5.679501	-3.685799
C	2.282745	4.946722	-4.383429
H	2.166311	5.914385	-3.883695
H	1.575118	4.913236	-5.217294
H	3.294088	4.928226	-4.813086
C	-7.851285	2.319259	1.306173
H	-8.265436	2.933661	0.499699
H	-8.670466	1.738991	1.751486
H	-7.124285	1.634484	0.866881
C	-4.951990	7.476066	0.766740
H	-5.321614	7.757545	-0.228669
H	-3.956346	7.920011	0.874638
H	-5.610921	7.950189	1.502611
C	4.593731	7.515558	1.216016
H	4.790040	7.989910	0.244524
H	5.314837	7.931252	1.928528
H	3.593104	7.832661	1.529182
C	7.980996	2.542283	0.657364
H	7.291446	1.799273	0.259054
H	8.897979	2.037400	0.987269
H	8.244560	3.242823	-0.143831
C	8.349279	4.277086	2.380906
H	8.669199	5.002088	1.623624
H	9.237942	3.728027	2.712981
H	7.957187	4.829946	3.241423
C	-0.319370	-0.284359	-2.590398
H	0.064579	-0.432986	-1.581293
H	-0.752511	-1.230658	-2.932875
H	-1.114202	0.466621	-2.553229
C	-8.227607	4.189259	2.877740
H	-7.816314	4.862376	3.638142
H	-9.049213	3.626974	3.336953
H	-8.651837	4.799049	2.072540
C	-6.708884	2.362682	3.557926
H	-5.958435	1.633276	3.250959
H	-7.564150	1.839087	4.006395
H	-6.267942	3.008599	4.325313

C	0.154041	0.338481	-4.939610
H	-0.613529	1.120295	-4.927607
H	-0.325652	-0.601805	-5.232176
H	0.895376	0.582906	-5.710480
C	-5.653306	1.294252	-3.839302
H	-6.035375	2.298482	-4.055092
H	-5.733998	1.118644	-2.765379
H	-6.282839	0.563483	-4.362416
C	-3.701963	-0.272761	-4.071477
H	-4.341161	-0.973442	-4.623250
H	-3.729785	-0.543431	-3.016364
H	-2.675408	-0.391711	-4.428755
C	-4.154677	1.422824	-5.806114
H	-4.537981	2.416596	-6.063855
H	-4.783656	0.680750	-6.310902
H	-3.140016	1.328358	-6.209044
O	4.851122	-1.839073	-1.347506
O	-1.985833	-0.484085	0.939447
O	-5.043367	-1.898406	-0.689208
O	3.835567	-1.131050	1.437386
C	-1.171912	-3.473923	-0.884718
C	2.540251	-3.117116	1.399944
C	-1.916158	-1.550700	1.724000
C	-4.937526	-3.199552	-0.886318
C	-3.698398	-3.853690	-0.647335
C	-1.130887	-4.037214	-2.164406
H	-2.057517	-4.216784	-2.701121
C	-3.606208	-5.237240	-0.764473
H	-2.642881	-5.710579	-0.583546
C	3.790416	-3.846115	-0.626705
C	0.035697	-3.227622	-0.229966
H	0.024826	-2.767138	0.751071
C	4.873187	-3.154802	-1.227653
C	3.256866	-2.117798	2.104714
C	1.271392	-3.540699	-0.802307
C	-5.881686	-5.355920	-1.463477
H	-6.716397	-5.957999	-1.812577
C	0.090117	-4.365353	-2.742316
H	0.112701	-4.807059	-3.736046
C	2.563370	-3.104637	-0.119654
H	2.665413	-2.058714	-0.425016
C	-2.497591	-3.013522	-0.271496
H	-2.654855	-2.027972	-0.728945
C	-4.695599	-6.017038	-1.144565
C	1.899327	-4.130065	2.104896
H	1.323314	-4.870257	1.553526
C	1.285465	-4.125381	-2.069867
H	2.234732	-4.373104	-2.534116
C	3.835947	-5.230228	-0.492106
H	2.992366	-5.729855	-0.019380
C	-2.436108	-3.901636	2.093800
H	-2.808920	-4.845527	1.701682
C	-2.341797	-2.813140	1.229378
C	1.948502	-4.199221	3.493674
C	2.675567	-3.221111	4.171801
H	2.717298	-3.283105	5.255706
C	-2.065917	-3.803567	3.430206
C	-0.789804	-0.161711	3.557005
C	4.910445	-5.984264	-0.949631
C	-1.511576	-2.594950	3.866425
H	-1.147955	-2.543287	4.888258
C	-6.033046	-3.971980	-1.369832
C	-7.322982	-3.285130	-1.827285
C	-1.418691	-1.462985	3.057752
C	5.962058	-5.300511	-1.560508
H	6.800288	-5.886389	-1.928209
C	3.341242	-2.181088	3.521151
C	5.978958	-3.915009	-1.712123
C	-1.862518	0.932629	3.670229
H	-2.666684	0.625594	4.350514
H	-1.418145	1.856706	4.055606
H	-2.298747	1.167859	2.698920
C	7.172377	-3.207884	-2.358893
C	4.190700	-1.167270	4.296179
C	-6.990061	-2.283732	-2.945230
H	-6.570446	-2.805899	-3.811977
H	-7.895011	-1.753380	-3.268735
H	-6.258646	-1.552032	-2.600062
C	1.273583	-5.317720	4.235108
H	1.945514	-6.173715	4.388332
H	0.933403	-4.992743	5.224469
H	0.400096	-5.679786	3.685709
C	-2.282890	-4.946294	4.383128
H	-2.166926	-5.913973	3.883317
H	-1.574981	-4.913058	5.216764
H	-3.294086	-4.927494	4.813117
C	7.851322	-2.319295	-1.304797
H	8.265134	-2.933656	-0.498119
H	8.670695	-1.739064	-1.749804
H	7.124163	-1.634486	-0.865826
C	4.951716	-7.476182	-0.766774
H	5.321118	-7.757781	0.228683
H	3.956067	-7.920055	-0.874920
H	5.610770	-7.950278	-1.502554
C	-4.593478	-7.515356	-1.216762
H	-4.789049	-7.989841	-0.245186
H	-5.315018	-7.931060	-1.928825
H	-3.593024	-7.832301	-1.530649
C	-7.981243	-2.542562	-0.657192
H	-7.291730	-1.799566	-0.258796
H	-8.898293	-2.037708	-0.986958
H	-8.244686	-3.243269	0.143896
C	-8.349441	-4.277102	-2.381023
H	-8.669260	-5.002254	-1.623842
H	-9.238172	-3.728085	-2.712984
H	-7.957320	-4.829790	-3.241638
C	0.319998	0.284252	2.589957
H	-0.063917	0.432979	1.580853
H	0.753384	1.230441	2.932436
H	1.114639	-0.466932	2.552800
C	8.228297	-4.189385	-2.876061
H	7.817346	-4.862562	-3.636596

H	9.050100	-3.627130	-3.334958
H	8.652172	-4.799115	-2.070628
C	6.709859	-2.362876	-3.557059
H	5.959229	-1.633489	-3.250494
H	7.565297	-1.839259	-4.005177
H	6.269314	-3.008882	-4.324598
C	-0.153616	-0.338400	4.939179
H	0.613677	-1.120489	4.927275
H	0.326402	0.601746	5.231660
H	-0.895053	-0.582492	5.710056
C	5.653400	-1.294771	3.839150
H	6.035482	-2.299035	4.054761
H	5.734027	-1.119003	2.765249
H	6.282968	-0.564083	4.362332
C	3.702057	0.272205	4.071686
H	4.341322	0.972822	4.623461
H	3.729733	0.543014	3.016606
H	2.675546	0.391110	4.429110
C	4.154916	-1.423615	5.806053
H	4.538152	-2.417461	6.063611
H	4.784002	-0.681670	6.310898
H	3.140297	-1.329119	6.209084
H	3.881644	1.770104	-3.480880
C	4.959018	1.929999	-3.458201
H	5.379736	1.734824	-4.454868
H	5.159625	2.969098	-3.169509
O	5.514870	1.032139	-2.515987
C	6.919597	1.115772	-2.483216
H	7.283772	0.407129	-1.738829
H	7.245813	2.127931	-2.211769
H	7.342881	0.842831	-3.460172
H	-5.379381	-1.732550	4.455440
C	-4.959332	-1.929149	3.458774
H	-3.881856	-1.769839	3.480654
H	-5.160687	-2.968480	3.171425
O	-5.515196	-1.032116	2.515793
C	-6.919958	-1.115294	2.483538
H	-7.246596	-2.127548	2.212946
H	-7.284135	-0.407101	1.738724
H	-7.342839	-0.841464	3.460416

K^+-Bound Starting Complex – Triplet (Complex 1)

SCF Energy (a.u.): -7094.647865

Ce	-4.818522	0.248110	-0.274001
Ce	4.818439	-0.247882	0.274189
O	4.874296	-2.455897	0.736761
O	-2.957758	-0.272631	-1.560570
O	-5.381121	-1.830400	0.396925
O	3.781186	-0.667274	-1.627163
C	-1.377687	-2.882715	0.623965
C	2.197238	-2.411279	-1.937985
C	-2.984064	-1.451448	-2.203388
C	-5.134332	-3.086433	0.744882
C	-3.818023	-3.584001	0.613233
C	-1.211588	-3.158906	1.985418
H	-2.086656	-3.283517	2.612543
C	-3.525227	-4.906937	0.939214
H	-2.502780	-5.265432	0.834751
C	3.268582	-3.926661	-0.206211
C	-0.234522	-2.760477	-0.173798
H	-0.378471	-2.617444	-1.238616
C	4.503033	-3.700212	0.447373
C	3.002749	-1.353398	-2.447364
C	1.055499	-2.924581	0.336243
C	-5.795530	-5.262757	1.565180
H	-6.557838	-5.932870	1.950504
C	0.068767	-3.322232	2.516316
H	0.188559	-3.556500	3.571545
C	2.332562	-2.758668	-0.470680
H	2.811844	-1.893793	-0.008440
C	-2.764236	-2.654057	0.049127
H	-3.028079	-1.643611	0.384752
C	-4.504011	-5.771782	1.412635
C	1.382881	-3.137330	-2.811465
H	0.800224	-3.971995	-2.428926
C	1.192622	-3.210085	1.703013
H	2.187733	-3.365231	2.110576
C	2.860662	-5.218378	-0.526587
H	1.896500	-5.362956	-1.009953
C	-2.783850	-3.875607	-2.144287
H	-2.683952	-4.786881	-1.559621
C	-2.825471	-2.657586	-1.472380
C	1.300178	-2.828674	-4.169894
C	2.099984	-1.786989	-4.648872
H	2.061129	-1.571766	-5.712138
C	-2.914887	-3.958856	-3.525653
C	-3.502389	-0.263047	-4.440791
C	3.641714	-6.324794	-0.223170
C	-3.124436	-2.771392	-4.227584
H	-3.269095	-2.843952	-5.300373
C	-6.144044	-3.950254	1.253326
C	-7.569784	-3.442935	1.471816
C	-3.175059	-1.516448	-3.614784
C	4.844215	-6.096623	0.449528
H	5.444561	-6.962336	0.710958
C	2.971878	-1.054068	-3.839262
C	5.297901	-4.827439	0.803407
C	-4.810149	0.371428	-3.934016
H	-5.591715	-0.390162	-3.835933
H	-5.166268	1.136498	-4.632604
H	-4.651610	0.879092	-2.978355
C	6.620479	-4.653628	1.554121
C	3.930380	-0.019624	-4.439224
C	-7.537281	-2.306427	2.504735
H	-7.195900	-2.686756	3.473332
H	-8.537690	-1.878136	2.644733
H	-6.850412	-1.519148	2.191856
C	0.403132	-3.604488	-5.093179
H	0.488624	-4.681400	-4.914525
H	0.660887	-3.419363	-6.139967
H	-0.649791	-3.336211	-4.952278

C	-2.852015	-5.283487	-4.231921
H	-3.460818	-6.035756	-3.720375
H	-1.826395	-5.669255	-4.271578
H	-3.210886	-5.203326	-5.261961
C	7.594259	-3.859058	0.673800
H	7.785836	-4.392677	-0.263125
H	8.554118	-3.725191	1.189995
H	7.172357	-2.881874	0.439698
C	3.219683	-7.714781	-0.607529
H	3.685388	-8.032449	-1.548900
H	2.135809	-7.777775	-0.744139
H	3.504095	-8.446362	0.155652
C	-4.194107	-7.205954	1.738526
H	-3.115286	-7.371203	1.813799
H	-4.576825	-7.887895	0.969000
H	-4.645680	-7.509997	2.688936
C	-8.156214	-2.951423	0.139142
H	-7.548757	-2.146744	-0.276708
H	-9.184425	-2.595363	0.285364
H	-8.186954	-3.771586	-0.585828
C	-8.505881	-4.528208	2.009848
H	-8.596576	-5.370695	1.316116
H	-9.506205	-4.104382	2.149720
H	-8.172605	-4.913400	2.979056
C	-2.387064	0.788210	-4.347110
H	-2.275948	1.134009	-3.317633
H	-2.632189	1.662113	-4.961023
H	-1.440826	0.382937	-4.730700
C	7.285747	-5.990268	1.892531
H	6.647934	-6.615488	2.526047
H	8.214611	-5.800697	2.441201
H	7.544150	-6.559929	0.993828
C	6.381634	-3.909991	2.877492
H	5.907368	-2.945055	2.696794
H	7.331968	-3.749994	3.401899
H	5.729825	-4.497970	3.532712
C	-3.697994	-0.588782	-5.925264
H	-2.797283	-1.027109	-6.367747
H	-3.919774	0.334220	-6.470172
H	-4.532330	-1.278299	-6.087446
C	5.377507	-0.475296	-4.186562
H	5.566836	-1.438887	-4.670707
H	5.566771	-0.583795	-3.117443
H	6.081502	0.260105	-4.591381
C	3.698095	1.363694	-3.818402
H	4.411290	2.090828	-4.222679
H	3.816306	1.343290	-2.735120
H	2.689304	1.716051	-4.062274
C	3.753724	0.123287	-5.953873
H	3.952638	-0.814273	-6.483297
H	4.461140	0.870591	-6.327086
H	2.746058	0.463627	-6.218374
O	-4.874272	2.456141	-0.736470
O	2.957463	0.272631	1.560600
O	5.381119	1.830470	-0.397197
O	-3.781269	0.666987	1.627498
C	1.377448	2.882337	-0.624111
C	-2.197235	2.410981	1.938313
C	2.984045	1.451560	2.203239
C	5.134129	3.086416	-0.745323
C	3.817744	3.583816	-0.613776
C	1.211144	3.158264	-1.985591
H	2.086119	3.282775	-2.612865
C	3.524765	4.906660	-0.939974
H	2.502269	5.265027	-0.835572
C	-3.268492	3.926688	0.206685
C	0.234415	2.760225	0.173869
H	0.378527	2.617527	1.238717
C	-4.502915	3.700413	-0.447031
C	-3.002721	1.353061	2.447649
C	-1.055668	2.924256	-0.336028
C	5.795043	5.262728	-1.565893
H	6.557276	5.932902	-1.951256
C	-0.069285	3.321544	-2.516321
H	-0.189235	3.555648	-3.571569
C	-2.332648	2.758532	0.471067
H	-2.812102	1.893775	0.008801
C	2.764097	2.653844	-0.049453
H	3.027950	1.643372	-0.384999
C	4.503436	5.771576	-1.413500
C	-1.382741	3.136883	2.811788
H	-0.800124	3.971594	2.429286
C	-1.193005	3.209549	-1.702818
H	-2.188180	3.364656	-2.110237
C	-2.860454	5.218335	0.527148
H	-1.896325	5.362800	1.010612
C	2.783946	3.875721	2.143760
H	2.684001	4.786905	1.558961
C	2.825508	2.657598	1.472047
C	-1.299845	2.828033	4.170162
C	-2.099640	1.786324	4.649103
H	-2.060636	1.570940	5.712330
C	2.915032	3.959170	3.525114
C	3.502465	0.263510	4.440808
C	-3.641359	6.324855	0.223690
C	3.124664	2.771824	4.227201
H	3.269359	2.844541	5.299973
C	6.143735	3.950324	-1.253823
C	7.569567	3.443173	-1.472107
C	3.175213	1.516782	3.614591
C	-4.843806	6.096853	-0.449152
H	-5.444021	6.962645	-0.710626
C	-2.971696	1.053574	3.839509
C	-5.297603	4.827730	-0.803127
C	4.810051	-0.371290	3.933994
H	5.591715	0.390162	3.835619
H	5.166168	-1.136236	4.632719
H	4.651306	-0.879187	2.978488
C	-6.620089	4.654069	-1.554037
C	-3.930251	0.019175	4.439472
C	7.537292	2.306530	-2.504882
H	7.196005	2.686711	-3.473571

H	8.537752	1.878297	-2.644700
H	6.850443	1.519239	-2.191985
C	-0.402653	3.603723	5.093411
H	-0.488989	4.680727	4.915684
H	-0.659531	3.417594	6.140237
H	0.650341	3.336259	4.951531
C	2.852080	5.283900	4.231190
H	3.461991	6.035773	3.720369
H	1.826641	5.670282	4.269488
H	3.209588	5.203602	5.261692
C	-7.594106	3.859636	-0.673854
H	-7.785776	4.393306	0.263024
H	-8.553895	3.725863	-1.190204
H	-7.172348	2.882414	-0.439645
C	-3.219201	7.714776	0.608149
H	-3.685029	8.032495	1.549442
H	-2.135342	7.777614	0.744954
H	-3.503371	8.446412	-0.155070
C	4.193321	7.205636	-1.739685
H	3.114451	7.370854	-1.814303
H	4.576555	7.887843	-0.970654
H	4.644259	7.509352	-2.690503
C	8.155912	2.951895	-0.139309
H	7.548480	2.147231	0.276613
H	9.184167	2.595899	-0.285382
H	8.186519	3.772165	0.585545
C	8.505599	4.528485	-2.010177
H	8.596057	5.371109	-1.316581
H	9.506006	4.104776	-2.149806
H	8.172434	4.913456	-2.979512
C	2.386948	-0.787571	4.347492
H	2.275796	-1.133669	3.318118
H	2.631937	-1.661318	4.961679
H	1.440788	-0.381989	4.730936
C	-7.285140	5.990779	-1.892594
H	-6.647165	6.615885	-2.526059
H	-8.213960	5.801305	-2.441373
H	-7.543578	6.560515	-0.993949
C	-6.381109	3.910355	-2.877341
H	-5.906965	2.945378	-2.696530
H	-7.331375	3.750424	-3.401892
H	-5.729141	4.498245	-3.532482
C	3.698316	0.589526	5.925186
H	2.797727	1.028073	6.367697
H	3.920039	-0.333395	6.470256
H	4.532772	1.278959	6.087110
C	-5.377341	0.475129	4.187083
H	-5.566449	1.438671	4.671409
H	-5.566725	0.583827	3.118004
H	-6.081406	-0.260224	4.591876
C	-3.698347	-1.364120	3.818454
H	-4.411510	-2.091175	4.222931
H	-3.816905	-1.343630	2.735212
H	-2.689528	-1.716637	4.061968
C	-3.753390	-0.123962	5.954076
H	-3.952129	0.813543	6.483662
H	-4.460829	-0.871243	6.327291
H	-2.745719	-0.464444	6.218381
H	-7.438018	0.327438	-2.554092
C	-8.158470	0.414108	-1.738575
H	-8.736204	1.335568	-1.874519
H	-8.828473	-0.454127	-1.750346
O	-7.431489	0.460324	-0.525842
C	-8.272282	0.623819	0.603558
H	-7.635681	0.664633	1.489706
H	-8.954971	-0.226790	0.698389
H	-8.839048	1.558441	0.523139
H	8.736643	-1.334848	1.874747
C	8.158618	-0.413555	1.738906
H	7.438286	-0.327098	2.554549
H	8.828383	0.454868	1.750557
O	7.431438	-0.459991	0.526306
C	8.272087	-0.623345	-0.603222
H	8.954393	0.227533	-0.698365
H	7.635341	-0.664636	-1.489245
H	8.839263	-1.557712	-0.522719
K	0.168587	0.083732	2.202842
K	-0.168410	-0.084574	-2.203294

K^+-Free Complex Following Two-Electron Reduction (Electrochemical Reduction) – Triplet

SCF Energy (a.u.): -5693.961276

Ce	2.787920	-0.798928	-0.065870
Ce	-2.797207	0.810707	0.052271
O	-3.290595	2.263190	1.859707
O	3.228702	1.156881	-1.299038
O	4.704171	-0.104887	1.257682
O	-2.527119	2.764143	-1.261533
C	2.590150	3.265974	1.871379
C	-0.871100	4.325578	-0.537790
C	3.599101	2.415708	-1.406518
C	5.443653	0.830483	1.821662
C	4.995295	2.204379	1.861634
C	2.668045	3.864338	3.141160
H	3.600300	3.813506	3.711042
C	5.779901	3.188832	2.472016
H	5.421543	4.225306	2.469550
C	-2.297083	4.426703	1.542995
C	1.358633	3.296306	1.195490
H	1.282946	2.806064	0.219506
C	-3.341627	3.572078	2.040374
C	-1.675200	3.729473	-1.569471
C	0.218254	3.920191	1.721838
C	7.467711	1.569183	3.007325
H	8.443938	1.342464	3.452607
C	1.535004	4.494609	3.683275
H	1.600304	4.956689	4.676779
C	-1.061072	3.823731	0.890581
H	-1.232748	2.734434	0.817230
C	3.709696	2.533024	1.134812
H	3.271812	1.553391	0.894769

C	7.018036	2.898042	3.069645
C	0.042660	5.339999	-0.837324
H	0.672082	5.735924	-0.031644
C	0.318180	4.533519	2.984335
H	-0.562106	5.017473	3.417746
C	-2.395180	5.816052	1.672493
H	-1.597271	6.430773	1.236266
C	4.391655	4.493417	-0.349445
H	4.628902	5.053088	0.564095
C	3.940122	3.175754	-0.235168
C	0.214320	5.817776	-2.146962
C	-0.580560	5.247732	-3.152508
H	-0.442153	5.617031	-4.174921
C	4.529995	5.124493	-1.595100
C	3.062955	2.390414	-3.926200
C	-3.474083	6.431478	2.327112
C	4.115515	4.407021	-2.735238
H	4.157609	4.920812	-3.702612
C	6.735266	0.535309	2.400506
C	7.301519	-0.892711	2.327104
C	3.623007	3.095391	-2.679788
C	-4.460423	5.593039	2.875355
H	-5.290674	6.068667	3.411148
C	-1.516941	4.224535	-2.912502
C	-4.427926	4.193232	2.763440
C	3.912319	1.139192	-4.245328
H	4.952629	1.423294	-4.488377
H	3.491724	0.591894	-5.109140
H	3.927824	0.465914	-3.377552
C	-5.503639	3.319674	3.434426
C	-2.412869	3.699053	-4.047989
C	6.341766	-1.865188	3.044984
H	6.264580	-1.614105	4.117561
H	6.697805	-2.908322	2.957736
H	5.340093	-1.795342	2.601185
C	1.267145	6.852255	-2.466282
H	1.242941	7.702128	-1.758133
H	1.132050	7.259302	-3.484885
H	2.280062	6.413434	-2.409968
C	5.102708	6.517770	-1.711979
H	4.943228	7.093185	-0.782721
H	4.631495	7.084953	-2.536013
H	6.196094	6.520527	-1.905789
C	-6.243904	2.467208	2.378760
H	-6.737358	3.112330	1.632339
H	-7.014471	1.834051	2.856870
H	-5.530976	1.816912	1.855848
C	-3.588892	7.935700	2.411583
H	-4.031523	8.383317	1.498206
H	-2.600861	8.412469	2.545495
H	-4.227377	8.244533	3.259920
C	7.823305	3.968420	3.768377
H	7.780957	4.931033	3.225949
H	8.887172	3.679890	3.851777
H	7.466352	4.174457	4.798827
C	7.447254	-1.310407	0.845325
H	6.478290	-1.220203	0.336794
H	7.793854	-2.357656	0.764994
H	8.175148	-0.660890	0.328343
C	8.687337	-1.023763	2.988220
H	9.440298	-0.377122	2.502995
H	9.032650	-2.069734	2.900260
H	8.656414	-0.768395	4.062501
C	1.591916	1.979001	-3.665028
H	1.515553	1.311575	-2.795289
H	1.185144	1.451564	-4.548297
H	0.969206	2.867823	-3.471373
C	-6.563978	4.151792	4.182149
H	-6.115155	4.770233	4.979666
H	-7.294426	3.469505	4.653342
H	-7.118344	4.820561	3.499850
C	-4.820112	2.390164	4.464938
H	-4.034543	1.801943	3.971319
H	-5.552525	1.694256	4.915136
H	-4.360735	2.985847	5.273576
C	3.066999	3.304425	-5.167108
H	2.454867	4.208156	-5.002344
H	2.634861	2.754597	-6.022222
H	4.088081	3.619653	-5.451175
C	-3.864147	4.132335	-3.736435
H	-3.941500	5.234488	-3.735059
H	-4.154305	3.759834	-2.743852
H	-4.571290	3.730938	-4.486166
C	-2.337081	2.158745	-4.167120
H	-2.983927	1.807131	-4.992755
H	-2.666424	1.684209	-3.234538
H	-1.302907	1.836512	-4.371007
C	-2.026148	4.278114	-5.423719
H	-2.125935	5.377764	-5.456843
H	-2.695594	3.856635	-6.195429
H	-0.988050	4.017645	-5.694082
O	3.281335	-2.251484	-1.873236
O	-3.237484	-1.145546	1.285023
O	-4.713772	0.117082	-1.270927
O	2.517727	-2.752568	1.247691
C	-2.599578	-3.253701	-1.885770
C	0.861351	-4.313604	0.523885
C	-3.608673	-2.404166	1.392095
C	-5.453220	-0.818070	-1.835361
C	-5.004697	-2.191886	-1.876128
C	-2.677257	-3.851821	-3.155677
H	-3.609376	-3.800813	-3.725765
C	-5.789170	-3.176054	-2.487149
H	-5.430688	-4.212486	-2.485354
C	2.287538	-4.414887	-1.556697
C	-1.368176	-3.284229	-1.209659
H	-1.292637	-2.794140	-0.233588
C	3.332322	-3.560398	-2.053792
C	1.665579	-3.717716	1.555579
C	-0.227734	-3.908086	-1.735906
C	-7.477218	-1.556292	-3.021389
H	-8.453495	-1.329430	-3.466485

C	-1.544155	-4.482083	-3.697686
H	-1.609308	-4.943980	-4.691284
C	1.051491	-3.811772	-0.904475
H	1.223301	-2.722496	-0.831103
C	-3.719197	-2.520803	-1.149267
H	-3.281264	-1.541266	-0.908942
C	-7.027339	-2.885038	-3.084598
C	-0.052623	-5.327851	0.823389
H	-0.682136	-5.723611	0.017701
C	-0.327467	-4.521200	-2.998525
H	0.552871	-5.005135	-3.431851
C	2.385463	-5.804247	-1.686207
H	1.587346	-6.418862	-1.250214
C	-4.402232	-4.481212	0.334532
H	-4.639898	-5.040516	-0.579122
C	-3.949935	-3.163751	0.220567
C	-0.224365	-5.805631	2.133007
C	0.570670	-5.235819	3.138571
H	0.432212	-5.605137	4.160972
C	-4.541050	-5.112515	1.579967
C	-3.073500	-2.379468	3.912005
C	3.464477	-6.419808	-2.340516
C	-4.126434	-4.395471	2.720387
H	-4.168970	-4.909386	3.687676
C	-6.744899	-0.522703	-2.413922
C	-7.311381	0.905174	-2.339486
C	-3.633326	-3.084086	2.665284
C	4.451129	-5.581501	-2.888390
H	5.281498	-6.057245	-3.423897
C	1.507259	-4.212819	2.898588
C	4.418800	-4.181688	-2.776454
C	-3.922591	-1.128002	4.230922
H	-4.963094	-1.411789	4.473502
H	-3.502179	-0.580939	5.094971
H	-3.937509	-0.454601	3.363229
C	5.494885	-3.308280	-3.447038
C	2.403227	-3.687453	4.034086
C	-6.351834	1.878317	-3.056731
H	-6.274679	1.628016	-4.129491
H	-6.708024	2.921336	-2.968717
H	-5.350119	1.808288	-2.613053
C	-1.277538	-6.839739	2.452396
H	-1.254550	-7.688936	1.743415
H	-1.141746	-7.247803	3.470501
H	-2.290226	-6.400199	2.397405
C	-5.114146	-6.505665	1.696475
H	-4.965375	-7.076458	0.762650
H	-4.634874	-7.077739	2.512518
H	-6.205349	-6.508040	1.902170
C	6.234840	-2.455849	-2.391122
H	6.727810	-3.100981	-1.644392
H	7.005765	-1.822919	-2.868955
H	5.521817	-1.805325	-1.868619
C	3.579052	-7.924047	-2.425063
H	4.020380	-8.371891	-1.511172
H	2.591101	-8.400607	-2.560351
H	4.218580	-8.232863	-3.272616
C	-7.832435	-3.955063	-3.784073
H	-7.789636	-4.918130	-3.242490
H	-8.896417	-3.666810	-3.866968
H	-7.475662	-4.160079	-4.814788
C	-7.457064	1.321768	-0.857392
H	-6.488043	1.231361	-0.349001
H	-7.803826	2.368902	-0.776264
H	-8.184808	0.671754	-0.340825
C	-8.697271	1.036469	-3.000404
H	-9.450103	0.389399	-2.515552
H	-9.042726	2.082332	-2.911723
H	-8.666396	0.781823	-4.074858
C	-1.602225	-1.968492	3.651496
H	-1.525307	-1.300953	2.781896
H	-1.195654	-1.441342	4.535029
H	-0.979716	-2.857478	3.457939
C	6.555426	-4.140558	-4.194295
H	6.106857	-4.758979	-4.991970
H	7.286148	-3.458380	-4.665220
H	7.109429	-4.809364	-3.511736
C	4.811879	-2.378729	-4.477859
H	4.026167	-1.790421	-3.984574
H	5.544542	-1.682902	-4.927777
H	4.352773	-2.974385	-5.286672
C	-3.078360	-3.293611	5.152814
H	-2.466571	-4.197592	4.988152
H	-2.646271	-2.744063	6.008133
H	-4.099669	-3.608423	5.436516
C	3.854532	-4.120570	3.722447
H	3.931956	-5.222719	3.720883
H	4.144663	-3.747876	2.729926
H	4.561637	-3.719263	4.472259
C	2.327246	-2.147160	4.153352
H	2.974130	-1.795495	4.978934
H	2.656419	-1.672524	3.220757
H	1.293044	-1.825097	4.357361
C	2.016610	-4.266704	5.409763
H	2.116363	-5.366364	5.442706
H	2.686144	-3.845359	6.181470
H	0.978547	-4.006240	5.680261
N	-0.585085	0.192632	0.005801
N	0.575958	-0.180450	-0.018942

K^+-Free Complex Following Two-Electron Reduction (Electrochemical Reduction) – Quintet

SCF Energy (a.u.): -5693.963313

Ce	-2.926599	-0.451467	0.185233
Ce	2.926590	0.451483	-0.185293
O	3.485891	1.848392	-2.003299
O	-3.051999	1.544151	1.438146
O	-4.759456	0.483021	-1.091576
O	2.890319	2.399820	1.165627
C	-2.243105	3.551411	-1.766444
C	1.417492	4.160334	0.503548

C	-3.248101	2.840917	1.552253
C	-5.389368	1.515102	-1.619323
C	-4.764727	2.817953	-1.667708
C	-2.292275	4.143302	-3.041829
H	-3.244244	4.206445	-3.576753
C	-5.434267	3.902353	-2.245076
H	-4.941326	4.881875	-2.253051
C	2.759095	4.108473	-1.634935
C	-0.993040	3.430643	-1.135556
H	-0.944583	2.943320	-0.156224
C	3.680099	3.145631	-2.176053
C	2.174571	3.460145	1.505173
C	0.197734	3.898820	-1.711593
C	-7.340142	2.524957	-2.724569
H	-8.353066	2.433133	-3.134769
C	-1.109401	4.618788	-3.632671
H	-1.152541	5.076536	-4.629475
C	1.488500	3.647746	-0.932597
H	1.539452	2.545191	-0.859697
C	-3.421705	2.972363	-0.985808
H	-3.109142	1.943499	-0.754794
C	-6.721013	3.783208	-2.797168
C	0.650578	5.280082	0.838173
H	0.048884	5.757980	0.056076
C	0.127830	4.508752	-2.979129
H	1.044756	4.873723	-3.451196
C	3.010146	5.478482	-1.765929
H	2.304008	6.177115	-1.299115
C	-3.789086	5.006125	0.511243
H	-3.976117	5.592982	-0.396848
C	-3.520271	3.640165	0.388233
C	0.584627	5.765676	2.154542
C	1.332270	5.090480	3.130938
H	1.274699	5.465410	4.159099
C	-3.805569	5.650183	1.757905
C	-2.650601	2.745522	4.057353
C	4.127047	5.971671	-2.459015
C	-3.457631	4.883491	2.888425
H	-3.402784	5.398173	3.854733
C	-6.728496	1.397757	-2.150960
C	-7.472369	0.054013	-2.068133
C	-3.146033	3.518115	2.823557
C	4.992842	5.031044	-3.043232
H	5.852891	5.413073	-3.606193
C	2.122324	3.958745	2.855380
C	4.805432	3.643209	-2.933013
C	-3.643825	1.611686	4.400015
H	-4.632239	2.026180	4.670560
H	-3.273975	1.012973	5.252970
H	-3.768698	0.948595	3.533214
C	5.754782	2.656468	-3.637400
C	2.975277	3.308702	3.958989
C	-6.674115	-1.023405	-2.833030
H	-6.610545	-0.770462	-3.906068
H	-7.155158	-2.014496	-2.738082
H	-5.654087	-1.085559	-2.432027
C	-0.316300	6.923637	2.512308
H	-0.193902	7.776266	1.817547
H	-0.109102	7.290350	3.534065
H	-1.379006	6.622576	2.471119
C	-4.184101	7.107243	1.886244
H	-3.979976	7.655793	0.949494
H	-3.615152	7.607504	2.691817
H	-5.260578	7.255776	2.115239
C	6.429320	1.724501	-2.604784
H	7.011400	2.308832	-1.872253
H	7.112302	1.013723	-3.106287
H	5.665894	1.152139	-2.062361
C	4.406543	7.454120	-2.546340
H	4.912501	7.847687	-1.641199
H	3.475476	8.038178	-2.662330
H	5.059736	7.691016	-3.406387
C	-7.402647	4.957611	-3.459485
H	-7.225976	5.898422	-2.905961
H	-8.496046	4.805912	-3.517534
H	-7.048550	5.134025	-4.496310
C	-7.616466	-0.363311	-0.585875
H	-6.626200	-0.407182	-0.113524
H	-8.093504	-1.357741	-0.502751
H	-8.234199	0.367429	-0.035093
C	-8.887363	0.112809	-2.675715
H	-9.530707	0.845305	-2.156024
H	-9.362473	-0.880546	-2.583113
H	-8.863829	0.376396	-3.748152
C	-1.250445	2.152324	3.759890
H	-1.281955	1.488543	2.884899
H	-0.892745	1.570054	4.629886
H	-0.524464	2.956096	3.554120
C	6.876712	3.367800	-4.419267
H	6.473953	4.035388	-5.201584
H	7.510686	2.610150	-4.914311
H	7.524186	3.968053	-3.755523
C	4.941130	1.810311	-4.645206
H	4.112348	1.309042	-4.126849
H	5.578930	1.040865	-5.119101
H	4.523650	2.455279	-5.438565
C	-2.507902	3.650169	5.296921
H	-1.789228	4.468330	5.116330
H	-2.129738	3.048128	6.142426
H	-3.473112	4.093419	5.604226
C	4.461663	3.543484	3.603379
H	4.688546	4.624812	3.604757
H	4.667054	3.143961	2.600204
H	5.130391	3.042883	4.328278
C	2.694654	1.791865	4.072638
H	3.315288	1.346693	4.872797
H	2.924975	1.287514	3.125980
H	1.633741	1.611062	4.310983
C	2.713821	3.922651	5.348937
H	2.961052	4.998771	5.382727
H	3.345262	3.409149	6.096584
H	1.659495	3.801029	5.652559

O	-3.485974	-1.848374	2.003220
O	3.051980	-1.544177	-1.438132
O	4.759451	-0.483017	1.091497
O	-2.890280	-2.399830	-1.165664
C	2.243071	-3.551369	1.766501
C	-1.417497	-4.160351	-0.503498
C	3.248117	-2.840941	-1.552213
C	5.389359	-1.515075	1.619292
C	4.764695	-2.817914	1.667756
C	2.292230	-4.143201	3.041913
H	3.244194	-4.206318	3.576848
C	5.434214	-3.902289	2.245196
H	4.941253	-4.881800	2.253239
C	-2.759128	-4.108455	1.634963
C	0.993012	-3.430632	1.135595
H	0.944563	-2.943353	0.156241
C	-3.680167	-3.145609	2.176012
C	-2.174544	-3.460178	-1.505159
C	-0.197768	-3.898777	1.711646
C	7.340119	-2.524896	2.724588
H	8.353047	-2.433066	3.134777
C	1.109349	-4.618659	3.632767
H	1.152481	-5.076362	4.629592
C	-1.488528	-3.647730	0.932632
H	-1.539489	-2.545179	0.859712
C	3.421673	-2.972337	0.985859
H	3.109111	-1.943479	0.754823
C	6.720965	-3.783131	2.797275
C	-0.650590	-5.280119	-0.838073
H	-0.048917	-5.758000	-0.055949
C	-0.127875	-4.508650	2.979210
H	-1.044805	-4.873600	3.451285
C	-3.010151	-5.478464	1.766015
H	-2.303984	-6.177104	1.299254
C	3.789069	-5.006130	-0.511145
H	3.976073	-5.592969	0.396963
C	3.520257	-3.640166	-0.388169
C	-0.584623	-5.765759	-2.154423
C	-1.332241	-5.090586	-3.130854
H	-1.274661	-5.465554	-4.159000
C	3.805582	-5.650213	-1.757793
C	2.650744	-2.745584	-4.057345
C	-4.127060	-5.971647	2.459094
C	3.457702	-4.883538	-2.888341
H	3.402895	-5.398235	-3.854643
C	6.728490	-1.397721	2.150913
C	7.472388	-0.053997	2.067991
C	3.146107	-3.518158	-2.823510
C	-4.992892	-5.031011	3.043241
H	-5.852950	-5.413033	3.606194
C	-2.122276	-3.958826	-2.855350
C	-4.805509	-3.643178	2.932964
C	3.643983	-1.611750	-4.399964
H	4.632417	-2.026243	-4.670438
H	3.274184	-1.013055	-5.252953
H	3.768797	-0.948640	-3.533169
C	-5.754903	-2.656421	3.637271
C	-2.975199	-3.308807	-3.958997
C	6.674183	1.023486	2.832849
H	6.610646	0.770611	3.905904
H	7.155241	2.014562	2.737822
H	5.654141	1.085631	2.431881
C	0.316305	-6.923735	-2.512140
H	0.194017	-7.776270	-1.817247
H	0.109003	-7.290595	-3.533824
H	1.379007	-6.622635	-2.471112
C	4.184086	-7.107283	-1.886089
H	3.979912	-7.655810	-0.949336
H	3.615153	-7.607547	-2.691673
H	5.260567	-7.255847	-2.115042
C	-6.429444	-1.724538	2.604582
H	-7.011496	-2.308931	1.872078
H	-7.112454	-1.013744	3.106025
H	-5.666022	-1.152194	2.062135
C	-4.406525	-7.454098	2.546478
H	-4.912484	-7.847710	1.641358
H	-3.475445	-8.038131	2.662483
H	-5.059706	-7.690974	3.406540
C	7.402578	-4.957501	3.459668
H	7.225922	-5.898341	2.906188
H	8.495976	-4.805802	3.517739
H	7.048453	-5.133863	4.496493
C	7.616452	0.363235	0.585703
H	6.626172	0.407100	0.113379
H	8.093508	1.357649	0.502504
H	8.234152	-0.367552	0.034947
C	8.887398	-0.112792	2.675536
H	9.530701	-0.845356	2.155887
H	9.362542	0.880538	2.582835
H	8.863886	-0.376287	3.747996
C	1.250566	-2.152389	-3.759979
H	1.282018	-1.488598	-2.884993
H	0.892919	-1.570129	-4.630004
H	0.524575	-2.956160	-3.554246
C	-6.876830	-3.367735	4.419160
H	-6.474070	-4.035254	5.201535
H	-7.510841	-2.610069	4.914134
H	-7.524267	-3.968055	3.755441
C	-4.941296	-1.810176	4.645039
H	-4.112522	-1.308911	4.126665
H	-5.579128	-1.040723	5.118879
H	-4.523806	-2.455082	5.438444
C	2.508126	-3.650249	-5.296910
H	1.789435	-4.468403	-5.116356
H	2.130024	-3.048219	-6.142450
H	3.473355	-4.093509	-5.604141
C	-4.461595	-3.543476	-3.603357
H	-4.688535	-4.624792	-3.604629
H	-4.666961	-3.143843	-2.600220
H	-5.130298	-3.042910	-4.328303
C	-2.694483	-1.791996	-4.072754
H	-3.315108	-1.346838	-4.872928

H	-2.924748	-1.287568	-3.126123
H	-1.633564	-1.611276	-4.311137
C	-2.713793	-3.922868	-5.348905
H	-2.961079	-4.998978	-5.382617
H	-3.345218	-3.409386	-6.096580
H	-1.659466	-3.801319	-5.652552
N	0.595487	0.100942	-0.032251
N	-0.595500	-0.100902	0.032188

K^+-Bound Complex Following Two-Electron Reduction (Electrochemical Reduction) – Triplet

SCF Energy (a.u.): -6893.682235

Ce	2.812552	-0.694020	-0.203250
Ce	-2.846628	0.873740	-0.026660
O	-2.732789	2.117820	2.005888
O	3.189121	1.219431	-1.476362
O	4.796953	-0.151696	0.891381
O	-2.314348	2.527129	-1.560909
C	2.622726	3.129592	1.724034
C	-0.742611	4.202684	-0.909688
C	3.698828	2.449056	-1.528160
C	5.516093	0.721932	1.592315
C	5.026324	2.060188	1.786758
C	2.535925	3.429181	3.096035
H	3.390832	3.234235	3.749761
C	5.743776	2.974856	2.565997
H	5.348063	3.989693	2.696167
C	-2.205432	4.305497	1.170478
C	1.488828	3.341550	0.917976
H	1.535087	3.059296	-0.137245
C	-3.022141	3.431412	1.957205
C	-1.487806	3.507038	-1.919614
C	0.278127	3.829558	1.427315
C	7.467044	1.340950	2.923948
H	8.437716	1.085716	3.361533
C	1.341098	3.965730	3.616010
H	1.283509	4.217354	4.681491
C	-0.950272	3.750477	0.522555
H	-1.090899	2.653137	0.434598
C	3.783614	2.440700	1.018399
H	3.342250	1.477359	0.725877
C	6.962703	2.628957	3.170635
C	0.142916	5.227745	-1.254648
H	0.728327	5.710521	-0.463185
C	0.217061	4.171296	2.796376
H	-0.718005	4.559897	3.211746
C	-2.508063	5.667145	1.061061
H	-1.868097	6.292656	0.427218
C	4.612406	4.410295	-0.353105
H	4.884487	4.893678	0.592688
C	4.074346	3.119433	-0.319756
C	0.335031	5.612312	-2.591735
C	-0.405697	4.937405	-3.575840
H	-0.251037	5.236148	-4.617673
C	4.802026	5.097433	-1.558352
C	3.414015	2.517903	-4.096614
C	-3.604905	6.227982	1.729229
C	4.411384	4.447430	-2.743823
H	4.545415	4.986637	-3.687093
C	6.798694	0.381897	2.143325
C	7.446159	-0.979052	1.828920
C	3.854736	3.159736	-2.770545
C	-4.381396	5.376082	2.534185
H	-5.226624	5.818308	3.070867
C	-1.304148	3.891849	-3.289515
C	-4.129972	4.000043	2.674979
C	4.260126	1.254748	-4.359585
H	5.331948	1.508772	-4.424891
H	3.958271	0.775704	-5.308525
H	4.124257	0.531826	-3.544826
C	-5.005778	3.127367	3.590554
C	-2.089554	3.187322	-4.410522
C	6.550474	-2.131073	2.333962
H	6.426435	-2.077022	3.428619
H	7.000144	-3.109408	2.085061
H	5.557113	-2.068755	1.871443
C	1.357095	6.662111	-2.957882
H	1.295200	7.544586	-2.296544
H	1.223120	7.008907	-3.996732
H	2.383164	6.259721	-2.867775
C	5.349283	6.505397	-1.588886
H	5.861385	6.754885	-0.644765
H	4.548994	7.256245	-1.735035
H	6.072991	6.646728	-2.411246
C	-5.732377	2.049486	2.753213
H	-6.380320	2.521181	1.996383
H	-6.361709	1.410835	3.398089
H	-5.012600	1.398597	2.238787
C	-3.960777	7.687379	1.567553
H	-4.609169	7.859621	0.687443
H	-3.060472	8.309312	1.426678
H	-4.503426	8.071702	2.448406
C	7.701034	3.602019	4.059612
H	7.576850	4.642457	3.712162
H	8.782538	3.383524	4.084614
H	7.342460	3.570883	5.106999
C	7.631014	-1.100789	0.296922
H	6.665416	-0.979642	-0.212994
H	8.049644	-2.089795	0.035210
H	8.320192	-0.323043	-0.073601
C	8.831715	-1.140776	2.482883
H	9.543630	-0.370705	2.139102
H	9.246866	-2.127106	2.212446
H	8.774964	-1.091894	3.584146
C	1.919690	2.131388	-4.004150
H	1.772408	1.532508	-3.094125
H	1.620784	1.553291	-4.900407
H	1.278132	3.022907	-3.929138
C	-6.088194	3.941287	4.326432
H	-5.649766	4.731328	4.960148
H	-6.666060	3.265714	4.980319

H	-6.796847	4.413773	3.625103
C	-4.113323	2.463345	4.665931
H	-3.332473	1.857994	4.185518
H	-4.715633	1.809246	5.320849
H	-3.632764	3.236138	5.291479
C	3.569349	3.465462	-5.300530
H	2.977983	4.387766	-5.170971
H	3.205872	2.955964	-6.210139
H	4.622514	3.746355	-5.473852
C	-3.598592	3.437615	-4.196227
H	-3.821795	4.515243	-4.272293
H	-3.900648	3.087746	-3.200808
H	-4.197509	2.902773	-4.955532
C	-1.815399	1.661849	-4.387014
H	-2.440565	1.143489	-5.136257
H	-2.056444	1.264077	-3.388944
H	-0.754972	1.473198	-4.632542
C	-1.709134	3.696763	-5.813503
H	-1.931270	4.770543	-5.933767
H	-2.294393	3.147264	-6.571231
H	-0.638476	3.539199	-6.030698
O	2.698407	-1.938028	-2.235837
O	-3.223282	-1.039594	1.246567
O	-4.830921	0.331392	-1.121504
O	2.280433	-2.347346	1.331053
C	-2.657077	-2.950112	-1.953535
C	0.708566	-4.022857	0.680036
C	-3.732914	-2.269241	1.298583
C	-5.550231	-0.542321	-1.822163
C	-5.060666	-1.880698	-2.016296
C	-2.570385	-3.249927	-3.325490
H	-3.425369	-3.055138	-3.979165
C	-5.778278	-2.795451	-2.795287
H	-5.382701	-3.810368	-2.925246
C	2.171188	-4.125683	-1.400257
C	-1.523101	-3.161883	-1.147534
H	-1.569281	-2.879452	-0.092356
C	2.987803	-3.251616	-2.187108
C	1.453925	-3.327246	1.689864
C	-0.312422	-3.649918	-1.656899
C	-7.501336	-1.161389	-3.153545
H	-8.471994	-0.906124	-3.591142
C	-1.375574	-3.786482	-3.845485
H	-1.318057	-4.038262	-4.910933
C	0.916058	-3.570684	-0.752249
H	1.056623	-2.473328	-0.664391
C	-3.817953	-2.261173	-1.247929
H	-3.376615	-1.297789	-0.955515
C	-6.997189	-2.449527	-3.399945
C	-0.176938	-5.047896	1.025119
H	-0.762479	-5.530648	0.233739
C	-0.251454	-3.991847	-3.025917
H	0.683597	-4.380455	-3.441313
C	2.473867	-5.487315	-1.290814
H	1.833971	-6.112816	-0.656890
C	-4.646658	-4.230616	0.123909
H	-4.918888	-4.714122	-0.821778
C	-4.108598	-2.939762	0.090313
C	-0.368856	-5.432474	2.362232
C	0.372038	-4.757603	3.346235
H	0.217522	-5.056353	4.388087
C	-4.836087	-4.917603	1.329279
C	-3.447394	-2.337818	3.866929
C	3.570648	-6.048158	-1.959081
C	-4.445200	-4.267482	2.514605
H	-4.579029	-4.806590	3.457961
C	-6.832806	-0.202237	-2.373195
C	-7.480014	1.158916	-2.059151
C	-3.888530	-2.979791	2.541069
C	4.347037	-5.196277	-2.764149
H	5.192200	-5.638517	-3.300922
C	1.270471	-3.712062	3.059787
C	4.095578	-3.820243	-2.904959
C	-4.293288	-1.074534	4.129959
H	-5.365124	-1.328422	4.195566
H	-3.991141	-0.595422	5.078773
H	-4.157540	-0.351716	3.315089
C	4.971268	-2.947574	-3.820649
C	2.056073	-3.007565	4.180676
C	-6.584056	2.310602	-2.564471
H	-6.460000	2.256236	-3.659110
H	-7.033500	3.289109	-2.315835
H	-5.590725	2.248167	-2.101905
C	-1.390874	-6.482271	2.728516
H	-1.328863	-7.364891	2.067379
H	-1.256957	-6.828830	3.767452
H	-2.416963	-6.079973	2.638241
C	-5.383368	-6.325553	1.360069
H	-5.895803	-6.575076	0.416137
H	-4.583050	-7.076417	1.505978
H	-6.106794	-6.466821	2.182687
C	5.698027	-1.869760	-2.983361
H	6.346044	-2.341515	-2.226635
H	6.327295	-1.231098	-3.628287
H	4.978345	-1.218854	-2.468819
C	3.926523	-7.507555	-1.797413
H	4.574058	-7.679936	-0.916702
H	3.026160	-8.129649	-1.657577
H	4.470078	-7.891579	-2.677833
C	-7.735705	-3.422702	-4.288645
H	-7.611710	-4.463067	-3.940908
H	-8.817169	-3.204015	-4.313698
H	-7.377133	-3.391923	-5.336043
C	-7.664876	1.281098	-0.527190
H	-6.699312	1.159888	-0.017223
H	-8.083307	2.270258	-0.265748
H	-8.354218	0.503590	-0.156472
C	-8.865523	1.320764	-2.713187
H	-9.577593	0.550904	-2.369256
H	-9.280489	2.307233	-2.442972
H	-8.808755	1.271635	-3.814438
C	-1.953046	-1.951497	3.773940

H	-1.805877	-1.353184	2.863517
H	-1.653904	-1.372922	4.669814
H	-1.311591	-2.843120	3.699325
C	6.053547	-3.761510	-4.556712
H	5.614993	-4.551581	-5.190305
H	6.631278	-3.085960	-5.210740
H	6.762345	-4.233963	-3.855509
C	4.078695	-2.283470	-4.895880
H	3.297963	-1.678072	-4.415337
H	4.680961	-1.629413	-5.550880
H	3.597988	-3.056223	-5.521363
C	-3.602477	-3.285180	5.071031
H	-3.011289	-4.207588	4.941413
H	-3.238628	-2.775605	5.980450
H	-4.655629	-3.565890	5.244736
C	3.565074	-3.257847	3.966089
H	3.788288	-4.335482	4.042030
H	3.866953	-2.907900	2.970644
H	4.164124	-2.723065	4.725331
C	1.781939	-1.482087	4.157299
H	2.407389	-0.963770	4.906335
H	2.022658	-1.084270	3.159168
H	0.721609	-1.293375	4.403200
C	1.675925	-3.517066	5.583709
H	1.898211	-4.590819	5.703933
H	2.261228	-2.967500	6.341354
H	0.605280	-3.359636	5.801064
N	-0.624759	0.239839	-0.140242
N	0.590673	-0.060124	-0.089569
K	0.147535	-0.594219	-2.756114
K	-0.181418	0.774079	2.526321

K^+-Bound Complex Following Two-Electron Reduction (Electrochemical Reduction) – Quintet

SCF Energy (a.u.): -6893.672352

Ce	2.916103	-0.686434	-0.217464
Ce	-2.948345	0.865120	-0.011310
O	-2.729798	2.084179	2.022155
O	3.293274	1.243155	-1.491483
O	4.864742	-0.122383	0.940002
O	-2.342275	2.494424	-1.572267
C	2.623210	3.110668	1.718035
C	-0.757704	4.160899	-0.917688
C	3.752362	2.491247	-1.529295
C	5.564108	0.775045	1.629497
C	5.053007	2.109439	1.798526
C	2.525985	3.389774	3.094167
H	3.383525	3.203109	3.746856
C	5.748345	3.044949	2.573270
H	5.334245	4.054361	2.687764
C	-2.213295	4.266443	1.165979
C	1.488676	3.311097	0.908899
H	1.545577	3.046025	-0.150398
C	-3.032480	3.395900	1.953603
C	-1.509132	3.468263	-1.927308
C	0.268654	3.778133	1.419168
C	7.492967	1.443642	2.971277
H	8.462728	1.209451	3.422542
C	1.321488	3.901082	3.616101
H	1.255864	4.140161	4.684107
C	-0.960024	3.706256	0.515171
H	-1.114117	2.611714	0.417105
C	3.811142	2.465013	1.015208
H	3.405901	1.493123	0.702725
C	6.966528	2.727230	3.194434
C	0.124204	5.189293	-1.261702
H	0.710513	5.670732	-0.470000
C	0.199212	4.102601	2.793151
H	-0.740519	4.479950	3.208525
C	-2.520329	5.626053	1.048368
H	-1.878717	6.250847	0.415636
C	4.591497	4.473881	-0.333346
H	4.840005	4.960334	0.617329
C	4.095030	3.166230	-0.312622
C	0.311339	5.580790	-2.597748
C	-0.426684	4.904010	-3.582417
H	-0.273986	5.205406	-4.623845
C	4.768710	5.175146	-1.532657
C	3.455750	2.579217	-4.095302
C	-3.626699	6.184856	1.703471
C	4.401735	4.523661	-2.725261
H	4.520456	5.075476	-3.663417
C	6.846285	0.463223	2.199447
C	7.512397	-0.896406	1.919991
C	3.884601	3.220171	-2.764558
C	-4.412388	5.332934	2.498698
H	-5.268582	5.773328	3.019116
C	-1.321785	3.855338	-3.297112
C	-4.157032	3.957985	2.647780
C	4.341051	1.347552	-4.380210
H	5.401836	1.640601	-4.461184
H	4.041214	0.862595	-5.327071
H	4.244110	0.617298	-3.566384
C	-5.050689	3.080024	3.541510
C	-2.098781	3.144487	-4.419723
C	6.625797	-2.046150	2.446624
H	6.495628	-1.968505	3.539249
H	7.086255	-3.025472	2.222247
H	5.634224	-2.003316	1.978255
C	1.321307	6.643293	-2.960600
H	1.222625	7.540288	-2.323242
H	1.208009	6.962663	-4.010652
H	2.352600	6.265689	-2.833450
C	5.276782	6.598012	-1.549796
H	5.751463	6.862884	-0.590442
H	4.461313	7.326408	-1.723307
H	6.022670	6.758801	-2.348676
C	-5.751344	1.998238	2.686298
H	-6.363523	2.464420	1.896917
H	-6.412358	1.372288	3.311527
H	-5.017062	1.331319	2.213553

C	-3.983353	7.643288	1.533997
H	-4.570454	7.819913	0.612911
H	-3.081501	8.275030	1.462403
H	-4.588577	8.011828	2.379844
C	7.680358	3.723961	4.077168
H	7.536498	4.758065	3.718633
H	8.766082	3.528240	4.109425
H	7.317740	3.696021	5.123336
C	7.709828	-1.052488	0.392614
H	6.746652	-0.951956	-0.126454
H	8.140032	-2.043137	0.157061
H	8.394111	-0.276786	0.008956
C	8.895161	-1.026823	2.586611
H	9.599546	-0.254930	2.231558
H	9.324822	-2.013290	2.340159
H	8.830066	-0.955404	3.686164
C	1.975080	2.142847	-3.992615
H	1.862938	1.529125	-3.087130
H	1.685156	1.565593	-4.892781
H	1.305732	3.012302	-3.900065
C	-6.155763	3.889464	4.248303
H	-5.737394	4.682025	4.892265
H	-6.747219	3.211925	4.887731
H	-6.848057	4.358139	3.528388
C	-4.186262	2.416014	4.639585
H	-3.393877	1.810091	4.179133
H	-4.805514	1.761668	5.278204
H	-3.721544	3.188113	5.277756
C	3.568038	3.545681	-5.288725
H	2.947644	4.445957	-5.141601
H	3.213309	3.035775	-6.201654
H	4.609606	3.863756	-5.467836
C	-3.611724	3.374294	-4.209696
H	-3.848567	4.448962	-4.286283
H	-3.911077	3.020403	-3.214787
H	-4.201573	2.832003	-4.970775
C	-1.802885	1.623069	-4.392928
H	-2.422776	1.091184	-5.136991
H	-2.035107	1.228063	-3.391460
H	-0.740074	1.451625	-4.642867
C	-1.721784	3.657337	-5.822222
H	-1.955838	4.728536	-5.942822
H	-2.299385	3.101140	-6.581008
H	-0.648893	3.512438	-6.037425
O	2.697322	-1.905410	-2.250963
O	-3.325252	-1.064487	1.262757
O	-4.897250	0.301252	-1.168402
O	2.310131	-2.316248	1.342976
C	-2.655983	-2.931855	-1.946789
C	0.725227	-3.982431	0.688484
C	-3.784664	-2.312461	1.300645
C	-5.596682	-0.596057	-1.857985
C	-5.085722	-1.930501	-2.027059
C	-2.558899	-3.210865	-3.322951
H	-3.416496	-3.024129	-3.975543
C	-5.781172	-2.865923	-2.801807
H	-5.367185	-3.875379	-2.916318
C	2.180555	-4.087827	-1.395350
C	-1.521368	-3.132362	-1.137781
H	-1.578149	-2.867353	-0.078461
C	2.999853	-3.217177	-2.182731
C	1.476890	-3.289984	1.698056
C	-0.301404	-3.599386	-1.648212
C	-7.525592	-1.264395	-3.199816
H	-8.495313	-1.030073	-3.651103
C	-1.354467	-3.722148	-3.845045
H	-1.288953	-3.961140	-4.913077
C	0.927385	-3.527639	-0.744349
H	1.081605	-2.433126	-0.646180
C	-3.843834	-2.286188	-1.243829
H	-3.438533	-1.314325	-0.931350
C	-6.999320	-2.548053	-3.422963
C	-0.156750	-5.010755	1.032530
H	-0.743232	-5.492052	0.240868
C	-0.232111	-3.923752	-3.022224
H	0.707566	-4.301098	-3.437723
C	2.487405	-5.447509	-1.278109
H	1.845708	-6.072389	-0.645547
C	-4.624389	-4.294921	0.104830
H	-4.873143	-4.781329	-0.845803
C	-4.127650	-2.987376	0.084023
C	-0.343735	-5.402355	2.368567
C	0.394488	-4.725730	3.353194
H	0.241886	-5.027182	4.394620
C	-4.801585	-4.996134	1.304176
C	-3.487666	-2.400463	3.866592
C	3.593703	-6.006283	-1.933358
C	-4.434332	-4.344709	2.496727
H	-4.553052	-4.896485	3.434907
C	-6.878796	-0.284059	-2.427976
C	-7.544733	1.075657	-2.148530
C	-3.916922	-3.041326	2.535938
C	4.379525	-5.154241	-2.728328
H	5.235671	-5.594606	-3.248852
C	1.289648	-3.677119	3.067856
C	4.124356	-3.779218	-2.877032
C	-4.372359	-1.168380	4.151569
H	-5.433283	-1.460904	4.232612
H	-4.072224	-0.683592	5.098423
H	-4.275123	-0.438164	3.337748
C	5.018155	-2.901143	-3.770512
C	2.066793	-2.966365	4.190423
C	-6.657924	2.225313	-2.675007
H	-6.527637	2.147709	-3.767621
H	-7.118293	3.204677	-2.450633
H	-5.666408	2.182345	-2.206528
C	-1.353788	-6.464762	2.731469
H	-1.255289	-7.361730	2.094046
H	-1.240404	-6.784209	3.781489
H	-2.385053	-6.087030	2.604462
C	-5.309945	-6.418896	1.321399
H	-5.784711	-6.683717	0.362073

H	-4.494616	-7.147447	1.494918
H	-6.055841	-6.579500	2.120310
C	5.718972	-1.819680	-2.915016
H	6.330917	-2.286140	-2.125616
H	6.380237	-1.193800	-3.540047
H	4.984776	-1.152647	-2.442297
C	3.950153	-7.464812	-1.764294
H	4.537216	-7.641785	-0.843249
H	3.048214	-8.096451	-1.692896
H	4.555340	-7.833194	-2.610237
C	-7.713275	-3.544692	-4.305700
H	-7.569534	-4.578816	-3.947176
H	-8.798977	-3.348842	-4.337945
H	-7.350663	-3.516785	-5.351871
C	-7.742295	1.231682	-0.621162
H	-6.779179	1.130989	-0.102012
H	-8.172382	2.222379	-0.385593
H	-8.426724	0.456054	-0.237614
C	-8.927407	1.206303	-2.815292
H	-9.631925	0.434464	-2.460388
H	-9.356976	2.192799	-2.568797
H	-8.862194	1.134976	-3.914843
C	-2.006809	-1.964778	3.763690
H	-1.894349	-1.351406	2.858003
H	-1.716575	-1.387386	4.663672
H	-1.337835	-2.834541	3.671378
C	6.123111	-3.710570	-4.477495
H	5.704623	-4.502826	-5.121755
H	6.714757	-3.032943	-5.116653
H	6.815249	-4.179637	-3.757684
C	4.153856	-2.236692	-4.868423
H	3.361611	-1.630705	-4.407813
H	4.773242	-1.582330	-5.506895
H	3.688967	-3.008541	-5.506771
C	-3.600252	-3.366801	5.060088
H	-2.980189	-4.267313	4.913018
H	-3.245306	-2.856960	5.972969
H	-4.641931	-3.684488	5.239246
C	3.579694	-3.196335	3.980277
H	3.816425	-4.271027	4.056891
H	3.878992	-2.842522	2.985324
H	4.169672	-2.654072	4.741274
C	1.771031	-1.444920	4.163676
H	2.391028	-0.913091	4.907691
H	2.003163	-1.049889	3.162197
H	0.708254	-1.273393	4.413713
C	1.689855	-3.479203	5.592944
H	1.923850	-4.550418	5.713523
H	2.267541	-2.923048	6.351695
H	0.616986	-3.334239	5.808216
N	-0.623820	0.205474	-0.129255
N	0.591644	-0.026693	-0.099241
K	0.231666	-0.575077	-2.813574
K	-0.264238	0.753893	2.585094

K^+-Bound Complex Following Two-Electron Reduction (K^0 as Redundant) – Triplet (Complex 2)

SCF Energy (a.u.): -8713.296093

Ce	2.746979	-1.187277	0.167575
Ce	-2.746999	1.187285	-0.167574
O	-2.672877	2.153578	1.972555
O	3.626433	0.762318	-0.879456
O	4.798177	-0.918322	1.363004
O	-1.723585	2.771671	-1.405748
C	2.755928	2.426726	2.427088
C	-0.072458	4.154602	-0.427423
C	4.132180	1.976769	-0.730194
C	5.414048	-0.236585	2.322891
C	5.008116	1.099157	2.620319
C	2.543194	2.619251	3.793241
H	3.271176	2.265631	4.516135
C	5.661084	1.835755	3.603641
H	5.341549	2.857576	3.799117
C	-1.745353	4.289745	1.468349
C	1.766007	2.843690	1.534261
H	1.903768	2.658457	0.473407
C	-2.764893	3.489791	2.040205
C	-0.755525	3.662851	-1.570993
C	0.585129	3.449073	1.947357
C	7.118861	0.000186	4.031935
H	7.949841	-0.412294	4.595544
C	1.379721	3.266363	4.224576
H	1.228977	3.438403	5.287505
C	-0.513024	3.617894	0.912382
H	-0.785512	2.574399	0.704157
C	3.908860	1.685433	1.775046
H	3.419414	0.822014	1.331017
C	6.716404	1.300978	4.338190
C	0.954559	5.080098	-0.561810
H	1.482213	5.416656	0.328700
C	0.406043	3.685691	3.316912
H	-0.502806	4.169735	3.662940
C	-1.830874	5.677533	1.490241
H	-1.035412	6.253550	1.021798
C	4.987915	3.724193	0.751786
H	5.150510	4.086222	1.765486
C	4.399927	2.476563	0.573346
C	1.338340	5.560553	-1.812673
C	0.662385	5.071247	-2.929888
H	0.967760	5.441739	-3.903944
C	5.339526	4.526411	-0.329385
C	4.124866	2.350003	-3.270908
C	-2.904939	6.328857	2.086782
C	5.045634	4.046189	-1.608488
H	5.281545	4.687076	-2.452306
C	6.514077	-0.785228	3.046589
C	7.012502	-2.207856	2.768035
C	4.445697	2.809157	-1.846810
C	-3.893118	5.537317	2.674196
H	-4.725911	6.044996	3.151330

C	-0.368538	4.129596	-2.854376
C	-3.862149	4.142066	2.668458
C	4.982396	1.124483	-3.615395
H	6.048936	1.364266	-3.518987
H	4.802271	0.802454	-4.647752
H	4.728473	0.287598	-2.961206
C	-4.984413	3.330798	3.315637
C	-1.086826	3.640541	-4.114867
C	5.887371	-3.210419	3.056012
H	5.590231	-3.162694	4.107981
H	6.217909	-4.233257	2.840444
H	5.013687	-2.988799	2.442752
C	2.431380	6.583119	-1.944820
H	2.079517	7.589648	-1.685637
H	2.813760	6.626373	-2.969679
H	3.270844	6.347437	-1.283672
C	6.006319	5.859548	-0.130644
H	5.620030	6.370010	0.757168
H	5.845590	6.516946	-0.990387
H	7.091819	5.759798	0.003560
C	-5.666642	2.482204	2.234100
H	-6.046946	3.120478	1.429701
H	-6.507557	1.919363	2.654580
H	-4.934381	1.782604	1.823186
C	-3.015644	7.827570	2.075351
H	-3.531537	8.185785	1.175668
H	-2.028875	8.300324	2.090215
H	-3.577778	8.194670	2.939845
C	7.386640	2.086384	5.430597
H	7.364146	3.160884	5.222540
H	8.433101	1.789908	5.552904
H	6.893442	1.935231	6.399048
C	7.444158	-2.349558	1.299737
H	6.580500	-2.221059	0.645746
H	7.855986	-3.348633	1.116786
H	8.224192	-1.618339	1.049497
C	8.216860	-2.585366	3.634685
H	9.074416	-1.926388	3.457527
H	8.526422	-3.607459	3.393459
H	7.976052	-2.558690	4.702111
C	2.639338	1.977363	-3.372951
H	2.417202	1.224282	-2.615278
H	2.422958	1.583127	-4.375045
H	2.005455	2.850102	-3.194212
C	-6.061141	4.210666	3.954702
H	-5.650536	4.845794	4.746017
H	-6.826741	3.571218	4.408691
H	-6.556186	4.853434	3.219110
C	-4.408860	2.420581	4.410437
H	-3.647690	1.759679	3.992600
H	-5.200954	1.808795	4.859773
H	-3.956007	3.025176	5.203481
C	4.399839	3.435870	-4.312985
H	3.814609	4.338832	-4.111242
H	4.113097	3.065711	-5.303086
H	5.459929	3.709364	-4.358245
C	-2.555300	4.080594	-4.048315
H	-2.623347	5.173138	-4.035251
H	-3.026496	3.695704	-3.144072
H	-3.110136	3.711579	-4.919386
C	-1.015809	2.106867	-4.222879
H	-1.596894	1.757335	-5.084454
H	-1.423964	1.653101	-3.316397
H	0.025901	1.795776	-4.368212
C	-0.475377	4.210067	-5.397360
H	-0.549662	5.301503	-5.434692
H	-1.016638	3.813358	-6.263104
H	0.579478	3.932743	-5.504849
O	2.672876	-2.153581	-1.972546
O	-3.626466	-0.762308	0.879456
O	-4.798204	0.918339	-1.363011
O	1.723571	-2.771665	1.405739
C	-2.755942	-2.426705	-2.427095
C	0.072431	-4.154581	0.427421
C	-4.132206	-1.976759	0.730178
C	-5.414058	0.236612	-2.322916
C	-5.008096	-1.099116	-2.620365
C	-2.543215	-2.619239	-3.793247
H	-3.271205	-2.265627	-4.516138
C	-5.660985	-1.835686	-3.603759
H	-5.341406	-2.857486	-3.799269
C	1.745327	-4.289741	-1.468352
C	-1.766023	-2.843667	-1.534267
H	-1.903782	-2.658432	-0.473413
C	2.764881	-3.489794	-2.040198
C	0.755509	-3.662840	1.570986
C	-0.585149	-3.449057	-1.947363
C	-7.118792	-0.000140	-4.032043
H	-7.949758	0.412342	-4.595674
C	-1.379744	-3.266353	-4.224583
H	-1.229003	-3.438400	-5.287511
C	0.513001	-3.617881	-0.912388
H	0.785499	-2.574388	-0.704167
C	-3.908870	-1.685404	-1.775062
H	-3.419425	-0.821989	-1.331023
C	-6.716278	-1.300903	-4.338343
C	-0.954601	-5.080060	0.561816
H	-1.482272	-5.416605	-0.328689
C	-0.406064	-3.685677	-3.316918
H	0.502783	-4.169724	-3.662946
C	1.830838	-5.677530	-1.490249
H	1.035367	-6.253543	-1.021814
C	-4.987909	-3.724184	-0.751816
H	-5.150493	-4.086210	-1.765519
C	-4.399954	-2.476539	-0.573368
C	-1.338378	-5.560509	1.812682
C	-0.662394	-5.071228	2.929892
H	-0.967761	-5.441724	3.903949
C	-5.339479	-4.526430	0.329348
C	-4.124825	-2.350015	3.270876
C	2.904903	-6.328861	-2.086781
C	-5.045584	-4.046219	1.608456

H	-5.281452	-4.687133	2.452264
C	-6.514075	0.785253	-3.046640
C	-7.012563	2.207856	-2.768067
C	-4.445686	-2.809170	1.846785
C	3.893096	-5.537329	-2.674180
H	4.725893	-6.045014	-3.151301
C	0.368543	-4.129593	2.854371
C	3.862140	-4.142077	-2.668437
C	-4.982381	-1.124523	3.615398
H	-6.048917	-1.364336	3.519007
H	-4.802244	-0.802505	4.647756
H	-4.728494	-0.287622	2.961216
C	4.984427	-3.330817	-3.315587
C	1.086890	-3.640564	4.114840
C	-5.887557	3.210495	-3.056268
H	-5.590576	3.162739	-4.108279
H	-6.218144	4.233318	-2.840703
H	-5.013763	2.988976	-2.443130
C	-2.431425	-6.583066	1.944838
H	-2.079508	-7.589635	1.685879
H	-2.813962	-6.626156	2.969645
H	-3.270794	-6.347507	1.283523
C	-6.006222	-5.859590	0.130593
H	-5.619799	-6.370104	-0.757131
H	-5.845606	-6.516930	0.990401
H	-7.091704	-5.759863	-0.003774
C	5.666633	-2.482231	-2.234028
H	6.046909	-3.120512	-1.429621
H	6.507565	-1.919394	-2.654480
H	4.934366	-1.782628	-1.823130
C	3.015595	-7.827575	-2.075353
H	3.531483	-8.185797	-1.175670
H	2.028822	-8.300321	-2.090221
H	3.577728	-8.194679	-2.939847
C	-7.386434	-2.086279	-5.430821
H	-7.363914	-3.160788	-5.222814
H	-8.432898	-1.789832	-5.553166
H	-6.893193	-1.935064	-6.399240
C	-7.444006	2.349588	-1.299710
H	-6.580234	2.221207	-0.645846
H	-7.855902	3.348632	-1.116745
H	-8.223929	1.618306	-1.049312
C	-8.217081	2.585230	-3.634552
H	-9.074570	1.926216	-3.457204
H	-8.526663	3.607323	-3.393355
H	-7.976442	2.558482	-4.702014
C	-2.639309	-1.977315	3.372849
H	-2.417241	-1.224229	2.615161
H	-2.422897	-1.583063	4.374929
H	-2.005401	-2.850029	3.194081
C	6.061165	-4.210690	-3.954626
H	5.650575	-4.845813	-4.745954
H	6.826782	-3.571248	-4.408594
H	6.556186	-4.853464	-3.219023
C	4.408908	-2.420593	-4.410399
H	3.647729	-1.759689	-3.992581
H	5.201016	-1.808809	-4.859712
H	3.956073	-3.025184	-5.203457
C	-4.399714	-3.435890	4.312967
H	-3.814452	-4.338828	4.111209
H	-4.112952	-3.065714	5.303056
H	-5.459790	-3.709428	4.358268
C	2.555370	-4.080581	4.048189
H	2.623445	-5.173123	4.035088
H	3.026504	-3.695651	3.143929
H	3.110249	-3.711577	4.919238
C	1.015863	-2.106893	4.222890
H	1.596993	-1.757374	5.084440
H	1.423961	-1.653106	3.316392
H	-0.025842	-1.795817	4.368288
C	0.475529	-4.210128	5.397359
H	0.549844	-5.301563	5.434668
H	1.016831	-3.813421	6.263079
H	-0.579327	-3.932832	5.504916
N	-0.573554	0.194891	-0.071000
N	0.573533	-0.194885	0.070995
K	0.364135	-0.543089	-2.661171
K	-0.364151	0.543097	2.661169
K	-6.421052	-0.186687	0.611420
K	6.421001	0.186682	-0.611363
O	8.428931	1.821516	0.081775
C	8.670196	2.821718	-0.884864
H	9.625032	3.332417	-0.693261
H	7.859251	3.561979	-0.896427
H	8.716922	2.322865	-1.855832
C	8.385482	2.344010	1.395458
H	9.351664	2.793298	1.667158
H	8.163133	1.518139	2.073754
H	7.594012	3.097759	1.491194
O	8.465930	-0.177338	-2.495127
C	8.486059	-0.568561	-3.848983
H	9.301120	-0.067793	-4.390780
H	7.530615	-0.280209	-4.291289
H	8.613057	-1.656165	-3.949778
C	9.661607	-0.527263	-1.829301
H	10.536547	-0.110036	-2.347988
H	9.776242	-1.618955	-1.767888
H	9.610634	-0.098460	-0.826474
O	-8.428977	-1.821577	-0.081629
C	-8.385566	-2.344114	-1.395295
H	-9.351754	-2.793417	-1.666950
H	-7.594093	-3.097861	-1.491033
H	-8.163245	-1.518263	-2.073624
C	-8.670216	-2.821749	0.885047
H	-8.716922	-2.322864	1.856000
H	-7.859270	-3.562008	0.896617
H	-9.625056	-3.332456	0.693483
O	-8.465930	0.177293	2.495236
C	-9.661636	0.527182	1.829441
H	-9.776303	1.618870	1.768024
H	-10.536549	0.109934	2.348156
H	-9.610679	0.098372	0.826616

C	-8.486028	0.568530	3.849088
H	-8.613048	1.656132	3.949876
H	-7.530565	0.280203	4.291369
H	-9.301062	0.067749	4.390914

K^+-Bound Complex Following Two-Electron Reduction (K^0 as Redundant) – Quintet (Complex 2)

SCF Energy (a.u.): -8713.296093

Ce	2.746979	-1.187277	0.167575
Ce	-2.746999	1.187285	-0.167574
O	-2.672877	2.153578	1.972555
O	3.626433	0.762318	-0.879456
O	4.798177	-0.918322	1.363004
O	-1.723585	2.771671	-1.405748
C	2.755928	2.426726	2.427088
C	-0.072458	4.154602	-0.427423
C	4.132180	1.976769	-0.730194
C	5.414048	-0.236585	2.322891
C	5.008116	1.099157	2.620319
C	2.543194	2.619251	3.793241
H	3.271176	2.265631	4.516135
C	5.661084	1.835755	3.603641
H	5.341549	2.857576	3.799117
C	-1.745353	4.289745	1.468349
C	1.766007	2.843690	1.534261
H	1.903768	2.658457	0.473407
C	-2.764893	3.489791	2.040205
C	-0.755525	3.662851	-1.570993
C	0.585129	3.449073	1.947357
C	7.118861	0.000186	4.031935
H	7.949841	-0.412294	4.595544
C	1.379721	3.266363	4.224576
H	1.228977	3.438403	5.287505
C	-0.513024	3.617894	0.912382
H	-0.785512	2.574399	0.704157
C	3.908860	1.685433	1.775046
H	3.419414	0.822014	1.331017
C	6.716404	1.300978	4.338190
C	0.954559	5.080098	-0.561810
H	1.482213	5.416656	0.328700
C	0.406043	3.685691	3.316912
H	-0.502806	4.169735	3.662940
C	-1.830874	5.677533	1.490241
H	-1.035412	6.253550	1.021798
C	4.987915	3.724193	0.751786
H	5.150510	4.086222	1.765486
C	4.399927	2.476563	0.573346
C	1.338340	5.560553	-1.812673
C	0.662385	5.071247	-2.929888
H	0.967760	5.441739	-3.903944
C	5.339526	4.526411	-0.329385
C	4.124866	2.350003	-3.270908
C	-2.904939	6.328857	2.086782
C	5.045634	4.046189	-1.608488
H	5.281545	4.687076	-2.452306
C	6.514077	-0.785228	3.046589
C	7.012502	-2.207856	2.768035
C	4.445697	2.809157	-1.846810
C	-3.893118	5.537317	2.674196
H	-4.725911	6.044996	3.151330
C	-0.368538	4.129596	-2.854376
C	-3.862149	4.142066	2.668458
C	4.982396	1.124483	-3.615395
H	6.048936	1.364266	-3.518987
H	4.802271	0.802454	-4.647752
H	4.728473	0.287598	-2.961206
C	-4.984413	3.330798	3.315637
C	-1.086826	3.640541	-4.114867
C	5.887371	-3.210419	3.056012
H	5.590231	-3.162694	4.107981
H	6.217909	-4.233257	2.840444
H	5.013687	-2.988799	2.442752
C	2.431380	6.583119	-1.944820
H	2.079517	7.589648	-1.685637
H	2.813760	6.626373	-2.969679
H	3.270844	6.347437	-1.283672
C	6.006319	5.859548	-0.130644
H	5.620030	6.370010	0.757168
H	5.845590	6.516946	-0.990387
H	7.091819	5.759798	0.003560
C	-5.666642	2.482204	2.234100
H	-6.046946	3.120478	1.429701
H	-6.507557	1.919363	2.654580
H	-4.934381	1.782604	1.823186
C	-3.015644	7.827570	2.075351
H	-3.531537	8.185785	1.175668
H	-2.028875	8.300324	2.090215
H	-3.577778	8.194670	2.939845
C	7.386640	2.086384	5.430597
H	7.364146	3.160884	5.222540
H	8.433101	1.789908	5.552904
H	6.893442	1.935231	6.399048
C	7.444158	-2.349558	1.299737
H	6.580500	-2.221059	0.645746
H	7.855986	-3.348633	1.116786
H	8.224192	-1.618339	1.049497
C	8.216860	-2.585366	3.634685
H	9.074416	-1.926388	3.457527
H	8.526422	-3.607459	3.393459
H	7.976052	-2.558690	4.702111
C	2.639338	1.977363	-3.372951
H	2.417202	1.224282	-2.615278
H	2.422958	1.583127	-4.375045
H	2.005455	2.850102	-3.194212
C	-6.061141	4.210666	3.954702
H	-5.650536	4.845794	4.746017
H	-6.826741	3.571218	4.408691
H	-6.556186	4.853434	3.219110
C	-4.408860	2.420581	4.410437
H	-3.647690	1.759679	3.992600
H	-5.200954	1.808795	4.859773

H	-3.956007	3.025176	5.203481
C	4.399839	3.435870	-4.312985
H	3.814609	4.338832	-4.111242
H	4.113097	3.065711	-5.303086
H	5.459929	3.709364	-4.358245
C	-2.555300	4.080594	-4.048315
H	-2.623347	5.173138	-4.035251
H	-3.026496	3.695704	-3.144072
H	-3.110136	3.711579	-4.919386
C	-1.015809	2.106867	-4.222879
H	-1.596894	1.757335	-5.084454
H	-1.423964	1.653101	-3.316397
H	0.025901	1.795776	-4.368212
C	-0.475377	4.210067	-5.397360
H	-0.549662	5.301503	-5.434692
H	-1.016638	3.813358	-6.263104
H	0.579478	3.932743	-5.504849
O	2.672876	-2.153581	-1.972546
O	-3.626466	-0.762308	0.879456
O	-4.798204	0.918339	-1.363011
O	1.723571	-2.771665	1.405739
C	-2.755942	-2.426705	-2.427095
C	0.072431	-4.154581	0.427421
C	-4.132206	-1.976759	0.730178
C	-5.414058	0.236612	-2.322916
C	-5.008096	-1.099116	-2.620365
C	-2.543215	-2.619239	-3.793247
H	-3.271205	-2.265627	-4.516138
C	-5.660985	-1.835686	-3.603759
H	-5.341406	-2.857486	-3.799269
C	1.745327	-4.289741	-1.468352
C	-1.766023	-2.843667	-1.534267
H	-1.903782	-2.658432	-0.473413
C	2.764881	-3.489794	-2.040198
C	0.755509	-3.662840	1.570986
C	-0.585149	-3.449057	-1.947363
C	-7.118792	-0.000140	-4.032043
H	-7.949758	0.412342	-4.595674
C	-1.379744	-3.266353	-4.224583
H	-1.229003	-3.438400	-5.287511
C	0.513001	-3.617881	-0.912388
H	0.785499	-2.574388	-0.704167
C	-3.908870	-1.685404	-1.775062
H	-3.419425	-0.821989	-1.331023
C	-6.716278	-1.300903	-4.338343
C	-0.954601	-5.080060	0.561816
H	-1.482272	-5.416605	-0.328689
C	-0.406064	-3.685677	-3.316918
H	0.502783	-4.169724	-3.662946
C	1.830838	-5.677530	-1.490249
H	1.035367	-6.253543	-1.021814
C	-4.987909	-3.724184	-0.751816
H	-5.150493	-4.086210	-1.765519
C	-4.399954	-2.476539	-0.573368
C	-1.338378	-5.560509	1.812682
C	-0.662394	-5.071228	2.929892
H	-0.967761	-5.441724	3.903949
C	-5.339479	-4.526430	0.329348
C	-4.124825	-2.350015	3.270876
C	2.904903	-6.328861	-2.086781
C	-5.045584	-4.046219	1.608456
H	-5.281452	-4.687133	2.452264
C	-6.514075	0.785253	-3.046640
C	-7.012563	2.207856	-2.768067
C	-4.445686	-2.809170	1.846785
C	3.893096	-5.537329	-2.674180
H	4.725893	-6.045014	-3.151301
C	0.368543	-4.129593	2.854371
C	3.862140	-4.142077	-2.668437
C	-4.982381	-1.124523	3.615398
H	-6.048917	-1.364336	3.519007
H	-4.802244	-0.802505	4.647756
H	-4.728494	-0.287622	2.961216
C	4.984427	-3.330817	-3.315587
C	1.086890	-3.640564	4.114840
C	-5.887557	3.210495	-3.056268
H	-5.590576	3.162739	-4.108279
H	-6.218144	4.233318	-2.840703
H	-5.013763	2.988976	-2.443130
C	-2.431425	-6.583066	1.944838
H	-2.079508	-7.589635	1.685879
H	-2.813962	-6.626156	2.969645
H	-3.270794	-6.347507	1.283523
C	-6.006222	-5.859590	0.130593
H	-5.619799	-6.370104	-0.757131
H	-5.845606	-6.516930	0.990401
H	-7.091704	-5.759863	-0.003774
C	5.666633	-2.482231	-2.234028
H	6.046909	-3.120512	-1.429621
H	6.507565	-1.919394	-2.654480
H	4.934366	-1.782628	-1.823130
C	3.015595	-7.827575	-2.075353
H	3.531483	-8.185797	-1.175670
H	2.028822	-8.300321	-2.090221
H	3.577728	-8.194679	-2.939847
C	-7.386434	-2.086279	-5.430821
H	-7.363914	-3.160788	-5.222814
H	-8.432898	-1.789832	-5.553166
H	-6.893193	-1.935064	-6.399240
C	-7.444006	2.349588	-1.299710
H	-6.580234	2.221207	-0.645846
H	-7.855902	3.348632	-1.116745
H	-8.223929	1.618306	-1.049312
C	-8.217081	2.585230	-3.634552
H	-9.074570	1.926216	-3.457204
H	-8.526663	3.607323	-3.393355
H	-7.976442	2.558482	-4.702014
C	-2.639309	-1.977315	3.372849
H	-2.417241	-1.224229	2.615161
H	-2.422897	-1.583063	4.374929
H	-2.005401	-2.850029	3.194081
C	6.061165	-4.210690	-3.954626

H	5.650575	-4.845813	-4.745954
H	6.826782	-3.571248	-4.408594
H	6.556186	-4.853464	-3.219023
C	4.408908	-2.420593	-4.410399
H	3.647729	-1.759689	-3.992581
H	5.201016	-1.808809	-4.859712
H	3.956073	-3.025184	-5.203457
C	-4.399714	-3.435890	4.312967
H	-3.814452	-4.338828	4.111209
H	-4.112952	-3.065714	5.303056
H	-5.459790	-3.709428	4.358268
C	2.555370	-4.080581	4.048189
H	2.623445	-5.173123	4.035088
H	3.026504	-3.695651	3.143929
H	3.110249	-3.711577	4.919238
C	1.015863	-2.106893	4.222890
H	1.596993	-1.757374	5.084440
H	1.423961	-1.653106	3.316392
H	-0.025842	-1.795817	4.368288
C	0.475529	-4.210128	5.397359
H	0.549844	-5.301563	5.434668
H	1.016831	-3.813421	6.263079
H	-0.579327	-3.932832	5.504916
N	-0.573554	0.194891	-0.071000
N	0.573533	-0.194885	0.070995
K	0.364135	-0.543089	-2.661171
K	-0.364151	0.543097	2.661169
K	-6.421052	-0.186687	0.611420
K	6.421001	0.186682	-0.611363
O	8.428931	1.821516	0.081775
C	8.670196	2.821718	-0.884864
H	9.625032	3.332417	-0.693261
H	7.859251	3.561979	-0.896427
H	8.716922	2.322865	-1.855832
C	8.385482	2.344010	1.395458
H	9.351664	2.793298	1.667158
H	8.163133	1.518139	2.073754
H	7.594012	3.097759	1.491194
O	8.465930	-0.177338	-2.495127
C	8.486059	-0.568561	-3.848983
H	9.301120	-0.067793	-4.390780
H	7.530615	-0.280209	-4.291289
H	8.613057	-1.656165	-3.949778
C	9.661607	-0.527263	-1.829301
H	10.536547	-0.110036	-2.347988
H	9.776242	-1.618955	-1.767888
H	9.610634	-0.098460	-0.826474
O	-8.428977	-1.821577	-0.081629
C	-8.385566	-2.344114	-1.395295
H	-9.351754	-2.793417	-1.666950
H	-7.594093	-3.097861	-1.491033
H	-8.163245	-1.518263	-2.073624
C	-8.670216	-2.821749	0.885047
H	-8.716922	-2.322864	1.856000
H	-7.859270	-3.562008	0.896617
H	-9.625056	-3.332456	0.693483
O	-8.465930	0.177293	2.495236
C	-9.661636	0.527182	1.829441
H	-9.776303	1.618870	1.768024
H	-10.536549	0.109934	2.348156
H	-9.610679	0.098372	0.826616
C	-8.486028	0.568530	3.849088
H	-8.613048	1.656132	3.949876
H	-7.530565	0.280203	4.291369
H	-9.301062	0.067749	4.390914

K^+-Free Complex Following Four-Electron Reduction (Electrochemical Reduction) – Triplet

SCF Energy (a.u.): -5693.317191

Ce	2.679609	-0.742881	-0.055687
Ce	-2.689141	0.754633	0.041943
O	-3.249528	2.242836	1.899450
O	3.312132	1.205215	-1.326685
O	4.674969	-0.081384	1.365409
O	-2.532046	2.807647	-1.286915
C	2.632497	3.339824	1.855246
C	-0.858229	4.348111	-0.534628
C	3.691390	2.458486	-1.422794
C	5.447609	0.862818	1.862187
C	5.029621	2.251358	1.853469
C	2.748948	4.054674	3.058713
H	3.703791	4.058320	3.594774
C	5.874385	3.250878	2.383195
H	5.545736	4.296184	2.341019
C	-2.281846	4.416990	1.549656
C	1.377088	3.289543	1.217516
H	1.273659	2.699299	0.300561
C	-3.314342	3.548256	2.060777
C	-1.679045	3.770677	-1.571046
C	0.249173	3.975153	1.712911
C	7.541014	1.608036	2.959397
H	8.525591	1.380230	3.390840
C	1.625809	4.739482	3.574868
H	1.719344	5.304470	4.513857
C	-1.036813	3.835441	0.896381
H	-1.175641	2.738376	0.814317
C	3.745758	2.586815	1.127975
H	3.302196	1.609892	0.886061
C	7.122305	2.948179	2.961059
C	0.062433	5.356708	-0.829746
H	0.704717	5.725571	-0.020829
C	0.386540	4.710663	2.903174
H	-0.482599	5.241299	3.306212
C	-2.408609	5.812031	1.660132
H	-1.627974	6.434435	1.203679
C	4.435923	4.553534	-0.346182
H	4.593587	5.130357	0.574487
C	3.985841	3.231140	-0.241152
C	0.231386	5.859661	-2.132148
C	-0.584616	5.323929	-3.140063
H	-0.451302	5.711122	-4.158459

C	4.624585	5.178112	-1.594782
C	3.212974	2.441662	-3.954474
C	-3.492485	6.417558	2.324734
C	4.265091	4.452711	-2.746622
H	4.353066	4.961459	-3.715943
C	6.754164	0.561082	2.417533
C	7.276281	-0.883489	2.394748
C	3.766773	3.136912	-2.700259
C	-4.466261	5.573432	2.886451
H	-5.302869	6.045695	3.419918
C	-1.529305	4.306200	-2.905823
C	-4.413445	4.167419	2.780706
C	4.015222	1.152933	-4.245989
H	5.072596	1.392006	-4.469016
H	3.591317	0.609421	-5.112323
H	3.983121	0.495866	-3.365699
C	-5.472108	3.282330	3.461046
C	-2.439140	3.805409	-4.040545
C	6.317010	-1.797598	3.187851
H	6.283666	-1.494469	4.250307
H	6.632927	-2.857952	3.136482
H	5.305500	-1.706098	2.767760
C	1.320099	6.858754	-2.446170
H	1.367609	7.673319	-1.696440
H	1.162999	7.325310	-3.438539
H	2.316207	6.374729	-2.455177
C	5.189758	6.574678	-1.695577
H	4.797231	7.229624	-0.893155
H	4.922568	7.046261	-2.661130
H	6.300862	6.616678	-1.613555
C	-6.195737	2.398875	2.417770
H	-6.713260	3.024076	1.669872
H	-6.942473	1.739813	2.902825
H	-5.459355	1.774111	1.894901
C	-3.631350	7.920027	2.393122
H	-4.041053	8.370752	1.461591
H	-2.655601	8.415175	2.567200
H	-4.309046	8.224717	3.215712
C	7.973267	4.026702	3.589551
H	7.955261	4.961440	2.993798
H	9.031671	3.707263	3.670191
H	7.649089	4.313019	4.616020
C	7.357551	-1.384475	0.932206
H	6.369570	-1.279382	0.462668
H	7.665349	-2.448403	0.885944
H	8.084164	-0.782981	0.357113
C	8.680961	-1.025878	3.014700
H	9.431857	-0.419462	2.475131
H	8.997282	-2.085614	2.965883
H	8.693348	-0.715479	4.075961
C	1.720529	2.089884	-3.723358
H	1.605039	1.441874	-2.842497
H	1.308455	1.561015	-4.605022
H	1.127862	3.004221	-3.552873
C	-6.550206	4.101119	4.199709
H	-6.112872	4.737413	4.991124
H	-7.271746	3.410122	4.676014
H	-7.111911	4.755553	3.508131
C	-4.773663	2.375969	4.502639
H	-3.978869	1.802133	4.005097
H	-5.488687	1.666823	4.964148
H	-4.320885	2.990733	5.302012
C	3.282757	3.340503	-5.205342
H	2.698589	4.267157	-5.066148
H	2.856828	2.795672	-6.068627
H	4.323409	3.619654	-5.460613
C	-3.893985	4.190563	-3.686293
H	-3.995602	5.290885	-3.637747
H	-4.146702	3.768460	-2.702602
H	-4.609388	3.801809	-4.436416
C	-2.327518	2.272075	-4.208362
H	-2.995170	1.919513	-5.018560
H	-2.608105	1.771417	-3.272742
H	-1.291056	1.986101	-4.453236
C	-2.097893	4.439211	-5.404440
H	-2.210419	5.539376	-5.392013
H	-2.783345	4.036206	-6.174257
H	-1.063326	4.203741	-5.710355
O	3.239325	-2.230899	-1.913559
O	-3.321811	-1.193491	1.312853
O	-4.684695	0.093332	-1.379289
O	2.522617	-2.796019	1.273095
C	-2.642251	-3.328053	-1.869044
C	0.848476	-4.336245	0.521064
C	-3.701237	-2.446710	1.408896
C	-5.457326	-0.850796	-1.876163
C	-5.039303	-2.239393	-1.867565
C	-2.758638	-4.043020	-3.072455
H	-3.713409	-4.046647	-3.608636
C	-5.884078	-3.238759	-2.397494
H	-5.555444	-4.284094	-2.355534
C	2.272086	-4.405137	-1.563195
C	-1.386892	-3.277766	-1.231233
H	-1.283513	-2.687447	-0.314322
C	3.304412	-3.536340	-2.074558
C	1.669480	-3.758883	1.557381
C	-0.258945	-3.963426	-1.726502
C	-7.550776	-1.595919	-2.973469
H	-8.535402	-1.368062	-3.404746
C	-1.635484	-4.727918	-3.588461
H	-1.728985	-5.293021	-4.527386
C	1.027014	-3.823616	-0.909964
H	1.165790	-2.726527	-0.827949
C	-3.755556	-2.574959	-1.141914
H	-3.311962	-1.598059	-0.899952
C	-7.131931	-2.936083	-2.975347
C	-0.072291	-5.344706	0.816307
H	-0.714692	-5.713521	0.007462
C	-0.396261	-4.699054	-2.916701
H	0.472900	-5.229731	-3.319639
C	2.399063	-5.800168	-1.673398
H	1.618529	-6.422603	-1.216808

C	-4.446018	-4.541620	0.332215
H	-4.603876	-5.118365	-0.588473
C	-3.995781	-3.219275	0.227204
C	-0.241194	-5.847574	2.118755
C	0.574951	-5.311887	3.126571
H	0.441651	-5.698992	4.145002
C	-4.634713	-5.166242	1.580771
C	-3.222867	-2.429998	3.940573
C	3.483023	-6.405671	-2.337882
C	-4.275123	-4.440938	2.732657
H	-4.363117	-4.949717	3.701958
C	-6.763882	-0.549066	-2.431418
C	-7.286060	0.895496	-2.408354
C	-3.776687	-3.125183	2.686326
C	4.456678	-5.561501	-2.899770
H	5.293360	-6.033738	-3.433144
C	1.519752	-4.294287	2.892203
C	4.403623	-4.155480	-2.794329
C	-4.025047	-1.141218	4.232052
H	-5.082428	-1.380232	4.455103
H	-3.601103	-0.597692	5.098358
H	-3.992931	-0.484187	3.351735
C	5.462152	-3.270349	-3.474827
C	2.429667	-3.793507	4.026862
C	-6.326785	1.809762	-3.201260
H	-6.293414	1.506836	-4.263774
H	-6.642724	2.870100	-3.149700
H	-5.315288	1.718198	-2.781156
C	-1.329919	-6.846624	2.432886
H	-1.376713	-7.661951	1.683923
H	-1.173424	-7.312181	3.425813
H	-2.326133	-6.362803	2.440738
C	-5.200132	-6.562714	1.681514
H	-4.808902	-7.217212	0.878108
H	-4.931721	-7.035009	2.646386
H	-6.311366	-6.604383	1.601052
C	6.185552	-2.386498	-2.431721
H	6.703099	-3.011408	-1.683596
H	6.932231	-1.727462	-2.916896
H	5.449036	-1.761679	-1.909104
C	3.622153	-7.908129	-2.405909
H	4.032710	-8.358501	-1.474578
H	2.646356	-8.403499	-2.579044
H	4.299245	-8.212962	-3.228951
C	-7.982435	-4.014502	-3.604638
H	-7.957844	-4.951804	-3.013302
H	-9.042451	-3.698564	-3.678222
H	-7.662898	-4.294775	-4.634255
C	-7.367381	1.396181	-0.945721
H	-6.379408	1.291030	-0.476181
H	-7.675215	2.460086	-0.899264
H	-8.093994	0.794550	-0.370771
C	-8.690726	1.037959	-3.028321
H	-9.441608	0.431383	-2.488912
H	-9.007099	2.097669	-2.979283
H	-8.703057	0.727785	-4.089648
C	-1.730386	-2.078325	3.709526
H	-1.614825	-1.430290	2.828692
H	-1.318309	-1.549518	4.591223
H	-1.137774	-2.992693	3.539031
C	6.540456	-4.089103	-4.213229
H	6.103295	-4.725707	-5.004492
H	7.261863	-3.398076	-4.689692
H	7.102272	-4.743227	-3.521450
C	4.763580	-2.364378	-4.516673
H	3.968638	-1.790589	-4.019311
H	5.478486	-1.655197	-4.978313
H	4.310974	-2.979429	-5.315924
C	-3.292765	-3.328838	5.191435
H	-2.708596	-4.255501	5.052295
H	-2.866902	-2.784010	6.054753
H	-4.333444	-3.607975	5.446616
C	3.884480	-4.178798	3.672615
H	3.985996	-5.279133	3.624125
H	4.137220	-3.756773	2.688896
H	4.599923	-3.790073	4.422713
C	2.318139	-2.260157	4.194586
H	2.985791	-1.907574	5.004774
H	2.598791	-1.759576	3.258945
H	1.281685	-1.974107	4.439411
C	2.088401	-4.427196	5.390802
H	2.200846	-5.527371	5.378444
H	2.773902	-4.024191	6.160576
H	1.053859	-4.191629	5.696724
N	-0.608906	0.198870	0.019958
N	0.599302	-0.187303	-0.033894

K^+- Free Complex Following Four-Electron Reduction (Electrochemical Reduction) – Quintet

SCF Energy (a.u.): -5693.314056

Ce	2.835347	-0.503660	-0.143550
Ce	-2.835340	0.503658	0.143556
O	-3.461326	1.970742	1.962809
O	3.123380	1.495631	-1.416370
O	4.757691	0.364504	1.143788
O	-2.818828	2.511433	-1.214159
C	2.332272	3.544472	1.802383
C	-1.292844	4.224100	-0.522867
C	3.404882	2.778946	-1.515705
C	5.423838	1.379468	1.671954
C	4.828031	2.702838	1.729363
C	2.402565	4.206328	3.039705
H	3.355283	4.255012	3.575802
C	5.560466	3.776999	2.282690
H	5.097744	4.771776	2.306711
C	-2.660358	4.211864	1.605938
C	1.082251	3.427239	1.168023
H	1.025978	2.889162	0.216171
C	-3.612023	3.271781	2.137878
C	-2.069526	3.550572	-1.532628
C	-0.100186	3.979496	1.706366

C	7.438199	2.336910	2.751289
H	8.458749	2.219406	3.138698
C	1.227270	4.772000	3.592670
H	1.281878	5.302376	4.554633
C	-1.390835	3.726682	0.921537
H	-1.454368	2.622361	0.861426
C	3.496954	2.906430	1.040706
H	3.143261	1.890858	0.810392
C	6.849983	3.615293	2.812639
C	-0.477475	5.309183	-0.856314
H	0.142349	5.752431	-0.067349
C	-0.010262	4.664855	2.932067
H	-0.918265	5.093141	3.369888
C	-2.881708	5.597392	1.730360
H	-2.159391	6.276516	1.259940
C	3.977152	4.927822	-0.442994
H	4.113470	5.512520	0.476229
C	3.642420	3.569123	-0.330597
C	-0.378257	5.795370	-2.171430
C	-1.157006	5.163105	-3.153266
H	-1.078006	5.538324	-4.181598
C	4.093763	5.567709	-1.686884
C	2.953678	2.706871	-4.049063
C	-3.989378	6.116661	2.429319
C	3.796175	4.815949	-2.843310
H	3.834886	5.328649	-3.812836
C	6.762485	1.219648	2.188384
C	7.454217	-0.151391	2.106943
C	3.424818	3.455544	-2.790610
C	-4.882315	5.203060	3.012268
H	-5.736070	5.611670	3.570510
C	-1.996286	4.066058	-2.880384
C	-4.730531	3.802448	2.897326
C	3.876591	1.497840	-4.324882
H	4.909373	1.834556	-4.535396
H	3.517399	0.913842	-5.194298
H	3.896130	0.842735	-3.442900
C	-5.701088	2.840237	3.602482
C	-2.866624	3.448501	-3.988500
C	6.622283	-1.200611	2.875926
H	6.571481	-0.941863	3.949131
H	7.058695	-2.214737	2.781526
H	5.599586	-1.213157	2.474088
C	0.614277	6.875965	-2.531541
H	0.659816	7.669499	-1.760889
H	0.355890	7.356416	-3.495932
H	1.638024	6.462026	-2.624294
C	4.517210	7.014068	-1.787380
H	4.357465	7.537238	-0.826614
H	3.937293	7.561077	-2.558774
H	5.592316	7.148667	-2.047887
C	-6.400235	1.921475	2.573512
H	-6.987332	2.518395	1.854376
H	-7.080775	1.204211	3.073188
H	-5.641440	1.358045	2.014366
C	-4.230762	7.605088	2.520325
H	-4.583487	8.051993	1.564758
H	-3.309752	8.160190	2.791953
H	-4.996397	7.839942	3.285778
C	7.573892	4.771106	3.462560
H	7.150554	5.738742	3.134832
H	8.655203	4.778498	3.205932
H	7.525155	4.763800	4.575955
C	7.576246	-0.583449	0.626375
H	6.577535	-0.580427	0.167969
H	8.009269	-1.599744	0.535324
H	8.218253	0.123001	0.070134
C	8.873930	-0.146048	2.709061
H	9.540885	0.560708	2.181636
H	9.312049	-1.159283	2.624458
H	8.861966	0.133090	3.778720
C	1.497445	2.219636	-3.835818
H	1.435230	1.564268	-2.955119
H	1.144375	1.655463	-4.721314
H	0.822053	3.076095	-3.671295
C	-6.804991	3.576253	4.388888
H	-6.382865	4.234839	5.170119
H	-7.458934	2.833198	4.884176
H	-7.436179	4.196031	3.725838
C	-4.909318	1.970614	4.608904
H	-4.096101	1.455163	4.078574
H	-5.559932	1.211245	5.086549
H	-4.469682	2.605703	5.399499
C	2.957717	3.602880	-5.304078
H	2.290357	4.473485	-5.177786
H	2.595298	3.017632	-6.169963
H	3.971911	3.974798	-5.545955
C	-4.349186	3.679354	-3.615544
H	-4.572960	4.762303	-3.593069
H	-4.538308	3.259326	-2.617212
H	-5.028985	3.192803	-4.341248
C	-2.590008	1.933567	-4.131062
H	-3.227657	1.494267	-4.922613
H	-2.799281	1.422801	-3.182401
H	-1.532537	1.757631	-4.389524
C	-2.618667	4.089058	-5.369153
H	-2.845538	5.171455	-5.371855
H	-3.272398	3.602727	-6.118004
H	-1.571190	3.957004	-5.692527
O	3.461294	-1.970752	-1.962813
O	-3.123384	-1.495637	1.416365
O	-4.757664	-0.364512	-1.143819
O	2.818847	-2.511429	1.214194
C	-2.332267	-3.544509	-1.802357
C	1.292855	-4.224099	0.522917
C	-3.404894	-2.778951	1.515712
C	-5.423811	-1.379475	-1.671984
C	-4.828020	-2.702852	-1.729376
C	-2.402549	-4.206367	-3.039679
H	-3.355261	-4.255050	-3.575786
C	-5.560457	-3.777006	-2.282716
H	-5.097743	-4.771788	-2.306730

C	2.660360	-4.211876	-1.605897
C	-1.082252	-3.427276	-1.167985
H	-1.025989	-2.889192	-0.216136
C	3.612006	-3.271791	-2.137870
C	2.069542	-3.550563	1.532670
C	0.100192	-3.979527	-1.706318
C	-7.438161	-2.336892	-2.751357
H	-8.458701	-2.219376	-3.138788
C	-1.227249	-4.772045	-3.592629
H	-1.281847	-5.302425	-4.554590
C	1.390839	-3.726694	-0.921492
H	1.454365	-2.622372	-0.861394
C	-3.496955	-2.906454	-1.040699
H	-3.143256	-1.890883	-0.810387
C	-6.849963	-3.615282	-2.812692
C	0.477483	-5.309176	0.856374
H	-0.142343	-5.752429	0.067413
C	0.010277	-4.664895	-2.932016
H	0.918285	-5.093181	-3.369827
C	2.881717	-5.597402	-1.730307
H	2.159412	-6.276527	-1.259868
C	-3.977210	-4.927822	0.443017
H	-4.113550	-5.512524	-0.476201
C	-3.642444	-3.569133	0.330607
C	0.378262	-5.795349	2.171495
C	1.157010	-5.163074	3.153326
H	1.078005	-5.538280	4.181661
C	-4.093842	-5.567697	1.686909
C	-2.953701	-2.706873	4.049075
C	3.989376	-6.116672	-2.429284
C	-3.796235	-4.815936	2.843332
H	-3.834955	-5.328626	3.812862
C	-6.762444	-1.219637	-2.188441
C	-7.454137	0.151422	-2.107026
C	-3.424845	-3.455540	2.790621
C	4.882287	-5.203072	-3.012271
H	5.736029	-5.611681	-3.570535
C	1.996296	-4.066035	2.880432
C	4.730494	-3.802460	-2.897348
C	-3.876612	-1.497843	4.324908
H	-4.909396	-1.834559	4.535408
H	-3.517424	-0.913862	5.194336
H	-3.896141	-0.842721	3.442937
C	5.701017	-2.840264	-3.602570
C	2.866635	-3.448466	3.988542
C	-6.622074	1.200633	-2.875884
H	-6.571190	0.941934	-3.949097
H	-7.058436	2.214780	-2.781474
H	-5.599412	1.213100	-2.473954
C	-0.614276	-6.875936	2.531619
H	-0.659799	-7.669494	1.760990
H	-0.355906	-7.356357	3.496029
H	-1.638024	-6.461994	2.624342
C	-4.517300	-7.014053	1.787412
H	-4.357841	-7.537142	0.826556
H	-3.937183	-7.561151	2.558596
H	-5.592335	-7.148639	2.048218
C	6.400189	-1.921451	-2.573663
H	6.987306	-2.518334	-1.854512
H	7.080716	-1.204211	-3.073393
H	5.641410	-1.357992	-2.014526
C	4.230772	-7.605099	-2.520270
H	4.583578	-8.051976	-1.564719
H	3.309747	-8.160217	-2.791811
H	4.996349	-7.839964	-3.285777
C	-7.573869	-4.771080	-3.462644
H	-7.150673	-5.738732	-3.134776
H	-8.655219	-4.778350	-3.206183
H	-7.524951	-4.763866	-4.576031
C	-7.576295	0.583437	-0.626456
H	-6.577631	0.580352	-0.167949
H	-8.009280	1.599749	-0.535413
H	-8.218390	-0.123003	-0.070304
C	-8.873789	0.146163	-2.709290
H	-9.540821	-0.560605	-2.181977
H	-9.311884	1.159407	-2.624667
H	-8.861726	-0.132907	-3.778965
C	-1.497465	-2.219641	3.835833
H	-1.435245	-1.564273	2.955136
H	-1.144395	-1.655471	4.721331
H	-0.822076	-3.076103	3.671311
C	6.804903	-3.576309	-4.388971
H	6.382758	-4.234949	-5.170148
H	7.458818	-2.833275	-4.884326
H	7.436123	-4.196039	-3.725907
C	4.909213	-1.970696	-4.609015
H	4.096010	-1.455220	-4.078688
H	5.559811	-1.211350	-5.086717
H	4.469558	-2.605829	-5.399564
C	-2.957738	-3.602893	5.304082
H	-2.290344	-4.473473	5.177798
H	-2.595362	-3.017640	6.169982
H	-3.971926	-3.974850	5.545930
C	4.349194	-3.679364	3.615603
H	4.572943	-4.762319	3.593166
H	4.538331	-3.259374	2.617259
H	5.028999	-3.192804	4.341294
C	2.590053	-1.933521	4.131056
H	3.227705	-1.494213	4.922600
H	2.799350	-1.422789	3.182382
H	1.532584	-1.757553	4.389501
C	2.618654	-4.088975	5.369212
H	2.845527	-5.171372	5.371957
H	3.272372	-3.602618	6.118058
H	1.571171	-3.956912	5.692563
N	-0.601291	0.123225	0.047371
N	0.601298	-0.123230	-0.047356

K^+-Bound Complex Following Four-Electron Reduction (Electrochemical Reduction) – Quintet

SCF Energy (a.u.): -6893.384569

Ce	2.787767	-0.678597	-0.119434
Ce	-2.820003	0.857400	-0.109296
O	-2.827759	2.149218	1.916902
O	3.190279	1.246338	-1.425001
O	4.827058	-0.072318	1.001617
O	-2.395939	2.660958	-1.552807
C	2.607240	3.208979	1.731700
C	-0.776464	4.285126	-0.892714
C	3.697097	2.467312	-1.502742
C	5.529325	0.833038	1.664672
C	5.024854	2.176108	1.818796
C	2.511935	3.499479	3.105264
H	3.355879	3.289150	3.769082
C	5.729645	3.121978	2.569279
H	5.308306	4.128965	2.679987
C	-2.240781	4.351191	1.167546
C	1.470630	3.407347	0.923779
H	1.515423	3.114472	-0.128811
C	-3.102158	3.459174	1.887986
C	-1.563574	3.634295	-1.902699
C	0.256225	3.890308	1.434488
C	7.482783	1.531479	2.971047
H	8.458353	1.304437	3.416416
C	1.312410	4.019857	3.627000
H	1.235972	4.226687	4.700883
C	-0.973113	3.805202	0.532173
H	-1.110203	2.708071	0.434125
C	3.777550	2.519902	1.040657
H	3.355020	1.542133	0.764582
C	6.959427	2.818225	3.177538
C	0.126116	5.297945	-1.227932
H	0.745608	5.735634	-0.435976
C	0.191701	4.228160	2.803747
H	-0.749145	4.593121	3.228800
C	-2.529882	5.716829	1.084665
H	-1.855951	6.353296	0.497853
C	4.626418	4.452896	-0.378171
H	4.903195	4.957634	0.555642
C	4.076854	3.168466	-0.310076
C	0.296544	5.719023	-2.557296
C	-0.491080	5.098930	-3.541090
H	-0.352452	5.421376	-4.578754
C	4.821228	5.109058	-1.600746
C	3.317140	2.511997	-4.054159
C	-3.656531	6.268623	1.711496
C	4.411346	4.438368	-2.769673
H	4.533545	4.957423	-3.726967
C	6.822286	0.536914	2.228931
C	7.475259	-0.834202	1.981980
C	3.840825	3.157544	-2.762103
C	-4.479373	5.400928	2.450118
H	-5.348155	5.835318	2.956638
C	-1.409388	4.068740	-3.263675
C	-4.241598	4.020223	2.566689
C	4.046221	1.178031	-4.321987
H	5.131440	1.342745	-4.447664
H	3.657787	0.702371	-5.240499
H	3.899110	0.488709	-3.480362
C	-5.150236	3.133390	3.435754
C	-2.244116	3.423838	-4.383045
C	6.580750	-1.952406	2.558551
H	6.477497	-1.843090	3.651518
H	7.010124	-2.949469	2.347048
H	5.579667	-1.892794	2.112616
C	1.353442	6.736162	-2.919490
H	1.348281	7.601715	-2.231276
H	1.207664	7.119074	-3.945200
H	2.364674	6.289703	-2.868901
C	5.387423	6.508736	-1.665862
H	5.839064	6.798258	-0.701452
H	4.610819	7.263333	-1.901824
H	6.169170	6.606080	-2.443001
C	-5.800441	2.021506	2.580648
H	-6.404269	2.459350	1.768252
H	-6.460472	1.389188	3.201859
H	-5.035007	1.371784	2.136885
C	-3.993382	7.735129	1.572281
H	-4.544463	7.954225	0.636030
H	-3.083014	8.360406	1.555995
H	-4.626246	8.084539	2.407852
C	7.680208	3.830463	4.036560
H	7.611095	4.849113	3.612912
H	8.752231	3.581635	4.135717
H	7.265857	3.887741	5.063069
C	7.646003	-1.042298	0.458360
H	6.672915	-0.943372	-0.042037
H	8.057067	-2.046740	0.244474
H	8.332969	-0.287368	0.037947
C	8.866467	-0.958965	2.632199
H	9.572998	-0.203897	2.244092
H	9.282474	-1.957929	2.409391
H	8.817449	-0.852190	3.730210
C	1.799720	2.256750	-3.891943
H	1.625138	1.710682	-2.952829
H	1.417051	1.680596	-4.756449
H	1.239114	3.202264	-3.830132
C	-6.296460	3.927589	4.093989
H	-5.916855	4.727712	4.753075
H	-6.901036	3.240636	4.712092
H	-6.966109	4.384017	3.343448
C	-4.302969	2.512365	4.570454
H	-3.465376	1.937089	4.153953
H	-4.913191	1.833169	5.193188
H	-3.886897	3.302021	5.219157
C	3.498590	3.411550	-5.291251
H	2.970578	4.374025	-5.175981
H	3.075623	2.897488	-6.172179
H	4.564290	3.618769	-5.498064
C	-3.737469	3.708435	-4.106666
H	-3.934798	4.794289	-4.152460
H	-4.007365	3.345926	-3.105858
H	-4.378658	3.203468	-4.851863

C	-2.000931	1.895030	-4.428311
H	-2.647771	1.414224	-5.183374
H	-2.215310	1.451472	-3.444549
H	-0.954097	1.691113	-4.712124
C	-1.899724	3.978572	-5.778567
H	-2.095120	5.063694	-5.850382
H	-2.522818	3.469790	-6.534646
H	-0.843436	3.795348	-6.040410
O	2.795631	-1.970348	-2.145700
O	-3.222375	-1.067608	1.196027
O	-4.859816	0.251521	-1.229601
O	2.363540	-2.482857	1.323215
C	-2.640248	-3.029705	-1.960940
C	0.743596	-4.106483	0.662917
C	-3.729456	-2.288469	1.273719
C	-5.562202	-0.653550	-1.892905
C	-5.057824	-1.996605	-2.047548
C	-2.545124	-3.320065	-3.334545
H	-3.389151	-3.109657	-3.998233
C	-5.762761	-2.942175	-2.798269
H	-5.341521	-3.949165	-2.909336
C	2.207819	-4.172422	-1.397286
C	-1.503530	-3.228177	-1.153193
H	-1.548175	-2.935427	-0.100563
C	3.069734	-3.280370	-2.117034
C	1.531047	-3.456147	1.672956
C	-0.289199	-3.711116	-1.664112
C	-7.515815	-1.351396	-3.199348
H	-8.491406	-1.124132	-3.644559
C	-1.345678	-3.840402	-3.856497
H	-1.269406	-4.047151	-4.930408
C	0.940218	-3.626293	-0.761890
H	1.077578	-2.529215	-0.663633
C	-3.810447	-2.340680	-1.269654
H	-3.387814	-1.362989	-0.993469
C	-6.992572	-2.638111	-3.406323
C	-0.159165	-5.119194	0.997973
H	-0.778898	-5.556489	0.205989
C	-0.224859	-4.048816	-3.033416
H	0.715921	-4.413770	-3.458626
C	2.496487	-5.538177	-1.314828
H	1.822136	-6.174677	-0.728533
C	-4.659471	-4.273692	0.149116
H	-4.936603	-4.778248	-0.784691
C	-4.109619	-2.989384	0.081046
C	-0.329442	-5.540675	2.327226
C	0.458554	-4.921126	3.311060
H	0.320071	-5.243899	4.348641
C	-4.854151	-4.929942	1.371670
C	-3.348840	-2.333460	3.824991
C	3.623265	-6.090050	-1.941352
C	-4.443845	-4.259486	2.540589
H	-4.565933	-4.778630	3.497848
C	-6.855193	-0.357135	-2.456932
C	-7.508105	1.013895	-2.209315
C	-3.873038	-2.978790	2.533033
C	4.446756	-5.222276	-2.679152
H	5.315713	-5.656698	-3.185341
C	1.377058	-3.891066	3.033807
C	4.209423	-3.841457	-2.795290
C	-4.077433	-0.999268	4.093067
H	-5.162664	-1.163651	4.219069
H	-3.688588	-0.523728	5.011473
H	-3.930385	-0.309972	3.251409
C	5.118822	-2.954523	-3.663457
C	2.212269	-3.246888	4.153229
C	-6.613637	2.132420	-2.785344
H	-6.510295	2.023601	-3.878350
H	-7.043130	3.129343	-2.573423
H	-5.612580	2.072707	-2.339359
C	-1.386519	-6.557676	2.689284
H	-1.381637	-7.423047	2.000837
H	-1.240689	-6.940895	3.714872
H	-2.397660	-6.110985	2.638943
C	-5.420685	-6.329484	1.436761
H	-5.872424	-6.618864	0.472354
H	-4.644257	-7.084277	1.672678
H	-6.202437	-6.426668	2.213917
C	5.768438	-1.842819	-2.807670
H	6.371498	-2.280828	-1.994793
H	6.429104	-1.210537	-3.428240
H	5.002716	-1.193022	-2.364519
C	3.959603	-7.556718	-1.802599
H	4.509715	-7.776460	-0.865931
H	3.049064	-8.181782	-1.787536
H	4.593185	-7.905831	-2.637748
C	-7.713497	-3.649993	-4.265644
H	-7.644391	-4.668803	-3.842381
H	-8.785518	-3.401074	-4.364595
H	-7.299260	-3.706914	-5.292220
C	-7.678787	1.221234	-0.685582
H	-6.705681	1.122041	-0.185271
H	-8.089818	2.225579	-0.471181
H	-8.365754	0.466110	-0.265520
C	-8.899338	1.138987	-2.859422
H	-9.605875	0.383768	-2.471623
H	-9.315308	2.137863	-2.636152
H	-8.850364	1.032697	-3.957482
C	-1.831378	-2.078696	3.662387
H	-1.656822	-1.532554	2.723310
H	-1.448272	-1.502820	4.526881
H	-1.271107	-3.024387	3.600299
C	6.265527	-3.748661	-4.320935
H	5.886412	-4.548593	-4.980534
H	6.870673	-3.061610	-4.938371
H	6.934508	-4.205324	-3.569943
C	4.272457	-2.333271	-4.798700
H	3.434514	-1.758093	-4.382759
H	4.883167	-1.653946	-5.420816
H	3.856950	-3.122839	-5.447869
C	-3.530264	-3.233020	5.062082
H	-3.002616	-4.195671	4.946609

H	-3.106882	-2.719158	5.942927
H	-4.595979	-3.439883	5.269173
C	3.705426	-3.532062	3.876391
H	3.902269	-4.618020	3.921827
H	3.975225	-3.169404	2.875608
H	4.347045	-3.027598	4.621556
C	1.969699	-1.718004	4.199133
H	2.616850	-1.237745	4.954278
H	2.184062	-1.274101	3.215530
H	0.922992	-1.513777	4.483189
C	1.867972	-3.802003	5.548625
H	2.063000	-4.887217	5.620022
H	2.491405	-3.293710	6.304756
H	0.811801	-3.618502	5.810747
N	-0.622451	0.256610	-0.153469
N	0.590255	-0.077694	-0.075179
K	0.258709	-0.638003	-2.921595
K	-0.291007	0.816839	2.693035

Complex 3 – Quartet

SCF Energy (a.u.): -9467.916649

Ce	2.654133	-1.093245	0.023044
Ce	-2.626209	1.193524	-0.153186
O	-2.770978	2.253354	1.992592
O	3.517841	1.094056	-0.759936
O	4.597815	-0.805918	1.478708
O	-1.535569	2.796758	-1.446935
C	2.463620	2.480829	2.650884
C	-0.131997	4.338211	-0.315385
C	3.973982	2.297247	-0.451616
C	5.174178	-0.163375	2.483556
C	4.699353	1.128121	2.871982
C	2.203792	2.697902	4.006817
H	2.881810	2.319335	4.764611
C	5.288667	1.814324	3.929275
H	4.919010	2.802898	4.192338
C	-1.943679	4.414610	1.447058
C	1.530740	2.939788	1.721233
H	1.699111	2.736309	0.668215
C	-2.948123	3.578463	1.998792
C	-0.686408	3.811877	-1.515366
C	0.366908	3.604040	2.077593
C	6.849600	0.045086	4.234630
H	7.701201	-0.359112	4.772858
C	1.057731	3.411688	4.383399
H	0.874811	3.604347	5.437918
C	-0.659558	3.776865	0.978424
H	-0.888932	2.732693	0.735557
C	3.627706	1.744644	2.015747
H	3.156493	0.913837	1.491208
C	6.356393	1.281878	4.647622
C	0.818324	5.349179	-0.346482
H	1.245781	5.699150	0.591793
C	0.141264	3.869034	3.433787
H	-0.760465	4.394214	3.735967
C	-2.101946	5.794437	1.399075
H	-1.314534	6.392260	0.944993
C	4.730927	3.867962	1.284716
H	4.837405	4.094649	2.343714
C	4.174167	2.647372	0.916349
C	1.237764	5.910591	-1.551156
C	0.650209	5.432358	-2.721397
H	0.952230	5.893428	-3.656743
C	5.115788	4.810276	0.341227
C	4.207804	3.049335	-2.941507
C	-3.242726	6.410464	1.903284
C	4.898760	4.484136	-0.997693
H	5.184430	5.221175	-1.741273
C	6.311851	-0.687674	3.172171
C	6.906114	-2.049199	2.800610
C	4.332270	3.283739	-1.430779
C	-4.216341	5.590472	2.473557
H	-5.099950	6.071657	2.881745
C	-0.304109	4.408601	-2.749336
C	-4.110489	4.199598	2.538704
C	5.428190	2.237801	-3.394432
H	6.354265	2.753226	-3.114138
H	5.425695	2.101276	-4.482084
H	5.418540	1.243759	-2.941868
C	-5.213396	3.366917	3.191213
C	-1.015334	4.042170	-4.056373
C	5.868193	-3.133587	3.104016
H	5.613219	-3.130249	4.169044
H	6.262617	-4.123079	2.848605
H	4.958397	-2.961132	2.528793
C	2.268752	7.003296	-1.576331
H	1.972910	7.851474	-0.947961
H	2.421825	7.381777	-2.591705
H	3.235106	6.644144	-1.204351
C	5.674528	6.147965	0.739000
H	4.883118	6.902194	0.833053
H	6.388463	6.523895	-0.001645
H	6.188163	6.096317	1.704386
C	-5.800623	2.403521	2.151735
H	-6.174697	2.962004	1.285570
H	-6.634196	1.839887	2.594640
H	-5.024697	1.704096	1.829253
C	-3.433642	7.898265	1.811068
H	-3.853241	8.191022	0.840382
H	-2.484094	8.430940	1.923552
H	-4.117127	8.262879	2.584338
C	6.955415	2.012397	5.816607
H	6.914371	3.097491	5.674924
H	8.002953	1.733644	5.968047
H	6.424355	1.790328	6.750953
C	7.275489	-2.110923	1.309662
H	6.385112	-1.970604	0.694126
H	7.704137	-3.089089	1.064433
H	8.032906	-1.353432	1.066787
C	8.177518	-2.373348	3.590568
H	8.962893	-1.626173	3.428697
H	8.565544	-3.343450	3.262974
H	7.986587	-2.444687	4.665966
C	2.921607	2.298330	-3.303056
H	2.946633	1.303841	-2.858539
H	2.836641	2.208267	-4.392648
H	2.055333	2.863216	-2.937548
C	-6.366296	4.218797	3.727399
H	-6.030290	4.927614	4.490762

H	-7.112694	3.563594	4.191187
H	-6.862962	4.783904	2.930815
C	-4.627696	2.569713	4.365681
H	-3.808392	1.939308	4.017045
H	-5.395307	1.935549	4.825772
H	-4.246289	3.253892	5.131223
C	4.188688	4.361238	-3.737787
H	3.392884	5.022687	-3.384348
H	3.998680	4.133798	-4.792205
H	5.140702	4.899621	-3.695432
C	-2.483771	4.470438	-3.918193
H	-2.549474	5.553349	-3.770809
H	-2.942925	3.975555	-3.060045
H	-3.051747	4.208548	-4.818679
C	-0.959893	2.535600	-4.352978
H	-1.478865	2.315799	-5.292795
H	-1.454778	1.978270	-3.555396
H	0.081532	2.209075	-4.473607
C	-0.416032	4.758913	-5.269467
H	-0.505531	5.846668	-5.189094
H	-0.953829	4.451179	-6.172536
H	0.642464	4.509147	-5.406606
O	2.660166	-1.532562	-2.311563
O	-4.303129	0.972621	-1.858128
C	-2.925983	-2.481712	-2.517847
C	-5.263376	0.183903	-2.278873
C	-5.146882	-1.230794	-2.131726
C	-3.259658	-3.140026	-3.697594
H	-4.274586	-3.092519	-4.081355
C	-6.208683	-2.077438	-2.438870
H	-6.090802	-3.146964	-2.267992
C	1.890409	-3.748561	-2.735552
C	-1.605975	-2.535062	-2.078355
H	-1.339168	-1.941032	-1.204102
C	2.854786	-2.723750	-2.886430
C	-0.634331	-3.315398	-2.689811
C	-7.516350	-0.202535	-3.117438
H	-8.450399	0.185254	-3.514233
C	-2.271091	-3.851820	-4.383936
H	-2.524108	-4.349092	-5.316685
C	0.654577	-3.478622	-1.917786
H	0.811864	-2.517621	-1.414812
C	-3.860309	-1.769692	-1.568656
H	-3.296912	-0.885042	-1.279673
C	-7.418584	-1.584947	-2.927308
C	-0.975194	-3.963588	-3.881146
H	-0.229344	-4.551124	-4.407546
C	2.084715	-5.014345	-3.281634
H	1.343133	-5.786481	-3.085069
C	3.213316	-5.322325	-4.028690
C	-6.487355	0.695000	-2.818482
C	-6.654453	2.197287	-3.055181
C	4.156438	-4.309739	-4.194222
H	5.044587	-4.543425	-4.772634
C	4.021919	-3.034171	-3.645112
C	5.104310	-1.987250	-3.889560
C	-5.549508	2.672131	-4.008632
H	-5.660908	2.191875	-4.986726
H	-5.605981	3.757389	-4.151153
H	-4.567401	2.423208	-3.606940
C	5.601727	-1.428766	-2.547545
H	5.876224	-2.248412	-1.872199
H	6.491646	-0.808694	-2.702849
H	4.809549	-0.829918	-2.091042
C	3.437201	-6.697634	-4.591367
H	4.043696	-7.317049	-3.918394
H	2.489735	-7.222763	-4.746905
H	3.959990	-6.658289	-5.552751
C	-8.559099	-2.503531	-3.268197
H	-8.595965	-3.362590	-2.589835
H	-9.521795	-1.985246	-3.205905
H	-8.473241	-2.900764	-4.287231
C	-6.557765	2.957259	-1.722854
H	-5.600417	2.760526	-1.237444
H	-6.640169	4.037567	-1.887442
H	-7.375728	2.661751	-1.052869
C	-8.003025	2.548393	-3.687545
H	-8.846672	2.283652	-3.038908
H	-8.048213	3.628781	-3.859451
H	-8.143328	2.052350	-4.653467
C	6.324122	-2.550519	-4.624488
H	6.067164	-2.926010	-5.619660
H	7.061466	-1.751536	-4.759159
H	6.802205	-3.360434	-4.062771
C	4.510370	-0.868263	-4.755284
H	3.668709	-0.397606	-4.244139
H	5.260208	-0.102511	-4.980852
H	4.153934	-1.284022	-5.703379
N	-0.723112	0.028386	0.201195
N	0.502138	-0.412445	0.329995
K	0.495083	0.504028	-2.256548
K	-0.445160	0.805695	2.786753
K	-6.652429	0.021513	0.297501
K	6.334037	0.635586	-0.262000
O	8.220374	2.337965	0.648994
C	8.527669	3.410049	-0.215663
H	9.488622	3.870930	0.056970
H	7.739478	4.173632	-0.189574
H	8.599909	2.995013	-1.223142
C	8.146869	2.747041	1.999124
H	9.113255	3.150096	2.336555
H	7.886606	1.872256	2.597463
H	7.369065	3.508746	2.135868
O	8.582712	0.598675	-1.970271
C	8.768303	0.467215	-3.360816
H	9.606722	1.089863	-3.705272
H	7.851300	0.800460	-3.850257
H	8.966301	-0.576904	-3.641859
C	9.726329	0.196298	-1.247531
H	10.618118	0.741967	-1.588220
H	9.909416	-0.881957	-1.359503
H	9.548891	0.441982	-0.198931
O	-8.101283	-2.084593	1.071626
C	-7.578026	-3.382433	0.879347
H	-8.322618	-4.037937	0.405084
H	-7.262159	-3.825443	1.833076
H	-6.702840	-3.295018	0.233690
C	-9.205720	-2.071437	1.942299
H	-9.534596	-1.033810	2.031869
H	-8.933103	-2.453568	2.937175

H	-10.031418	-2.682023	1.548217
O	-9.135409	1.101403	0.497787
C	-10.007153	0.517153	-0.446103
H	-10.082932	1.134831	-1.351250
H	-11.012774	0.382155	-0.022176
H	-9.595272	-0.458026	-0.714992
C	-9.569830	2.379731	0.904648
H	-9.621532	3.071250	0.051942
H	-8.844015	2.759722	1.626251
H	-10.559864	2.328102	1.379556
C	1.495800	-5.516051	1.189337
C	-0.333536	-5.615688	-0.942122
C	1.432147	-4.426548	0.269943
C	0.613487	-6.584078	1.019944
C	-0.319380	-6.656993	-0.017199
C	0.534373	-4.530459	-0.829444
H	0.657908	-7.416586	1.716446
H	-1.021262	-5.651778	-1.784681
O	2.156705	-3.332786	0.413958
C	2.586089	-5.561388	2.259541
C	2.510989	-6.822943	3.124754
H	3.318944	-6.798955	3.863452
H	2.631249	-7.735773	2.532503
H	1.564448	-6.893374	3.673481
C	2.485736	-4.353358	3.201009
H	3.267821	-4.395778	3.967165
H	1.512654	-4.351121	3.700635
H	2.586602	-3.419145	2.648165
C	3.942425	-5.580373	1.537062
H	4.761545	-5.648049	2.260048
H	4.073997	-4.678276	0.936586
H	3.999101	-6.448095	0.871694
C	-1.209712	-7.859319	-0.168121
H	-0.627965	-8.761842	-0.391340
H	-1.922771	-7.721390	-0.986132
H	-1.783685	-8.065761	0.742453
H	-3.951335	-4.476127	-1.233585
C	-4.064555	-3.952125	-0.286373
C	-4.244162	-2.566470	2.155224
C	-4.035024	-2.559835	-0.284044
C	-4.202622	-4.681541	0.894389
C	-4.281111	-3.962509	2.089440
C	-4.130748	-1.824860	0.935761
H	-4.374436	-4.530903	3.009858
O	-4.106968	-0.508121	0.907270
C	-4.339326	-1.850102	3.505521
C	-4.389422	-2.825178	4.683442
H	-3.505613	-3.468885	4.708147
H	-5.280391	-3.461309	4.652414
H	-4.421110	-2.258619	5.620111
C	-5.614397	-0.998271	3.550832
H	-5.541056	-0.191191	2.824378
H	-5.743504	-0.546368	4.540736
H	-6.495915	-1.609366	3.330016
C	-3.119280	-0.935914	3.702146
H	-3.087412	-0.195608	2.899100
H	-2.207429	-1.546619	3.707460
H	-3.184942	-0.413499	4.664438
C	-4.291840	-6.181608	0.885749
H	-5.330672	-6.526873	0.964226
H	-3.743379	-6.624041	1.724467
H	-3.877593	-6.596453	-0.036160
K	-0.886696	-2.740741	1.225138
O	-0.981027	-3.813178	3.773934
C	-1.325538	-5.181181	3.689847
H	-0.488300	-5.814026	4.011178
H	-1.551797	-5.409533	2.646875
H	-2.206192	-5.402307	4.309560
C	-0.625648	-3.442935	5.085866
H	0.223612	-4.036465	5.450319
H	-1.471493	-3.564520	5.776845
H	-0.333260	-2.390383	5.066756

K^+-Bound Complex Following Four-Electron Reduction (Reduced using K^0) – Triplet (Complex 4)

SCF Energy (a.u.): -10532.236219

Ce	3.023117	-1.073764	-0.816177
Ce	-2.559245	-0.066668	-0.524551
O	-2.594348	1.190204	1.551904
O	3.272467	0.866457	-2.091679
O	4.840075	-0.340621	0.479417
O	-2.623856	1.889439	-1.946834
C	2.551853	2.809122	1.071237
C	-1.024351	3.550096	-1.362172
C	3.583516	2.140449	-2.182851
C	5.548188	0.633201	1.013686
C	5.025149	1.959319	1.066553
C	2.527159	3.240397	2.398868
H	3.432971	3.203840	2.996565
C	5.745254	2.978928	1.690513
H	5.316632	3.978638	1.737332
C	-2.367572	3.423779	0.777883
C	1.357725	2.821533	0.345388
H	1.362885	2.436757	-0.671144
C	-3.045780	2.430314	1.544259
C	-1.799356	2.858128	-2.338572
C	0.153508	3.259779	0.889127
C	7.542242	1.470847	2.126155
H	8.538990	1.302472	2.522483
C	1.330417	3.704941	2.952967
H	1.318990	4.052748	3.983101
C	-1.099087	3.038663	0.058588
H	-1.108819	1.945807	-0.054791
C	3.733079	2.208465	0.336895
H	3.376201	1.212285	0.084164
C	7.001124	2.754945	2.250648
C	-0.205580	4.612399	-1.721605
H	0.391998	5.099301	-0.953922
C	0.148543	3.723410	2.210482
H	-0.778208	4.070141	2.658691
C	-2.831885	4.733529	0.728682
H	-2.278239	5.453716	0.128540
C	4.252334	4.231140	-1.094414
H	4.449802	4.777688	-0.173553
C	3.904872	2.883842	-1.013039
C	-0.095726	5.031375	-3.047868

C	-0.822779	4.326621	-4.004182
H	-0.712407	4.632720	-5.039688
C	4.308339	4.900958	-2.312661
C	3.054980	2.145969	-4.693428
C	-3.979767	5.133236	1.416691
C	3.928683	4.184401	-3.451264
H	3.923575	4.715504	-4.398618
C	6.865293	0.410095	1.522772
C	7.506723	-0.974338	1.408237
C	3.549882	2.844355	-3.427372
C	-4.633997	4.163813	2.182201
H	-5.506853	4.476825	2.749171
C	-1.660387	3.246185	-3.701092
C	-4.209727	2.831858	2.272357
C	3.967526	0.965336	-5.038462
H	4.995280	1.299521	-5.219691
H	3.613073	0.464165	-5.947115
H	3.980007	0.243458	-4.222659
C	-4.936148	1.836689	3.179032
C	-2.403263	2.510222	-4.820320
C	6.647880	-1.979132	2.183964
H	6.623193	-1.731337	3.250468
H	7.062837	-2.993259	2.092861
H	5.621387	-1.957489	1.812940
C	0.818050	6.161516	-3.427122
H	0.595184	7.072898	-2.860392
H	0.733475	6.400013	-4.491694
H	1.861065	5.896193	-3.222732
C	4.766080	6.327546	-2.419449
H	4.659528	6.855590	-1.466067
H	4.192280	6.880479	-3.171254
H	5.822046	6.374942	-2.713622
C	-5.442473	0.646969	2.350852
H	-6.181827	0.982560	1.611728
H	-5.913768	-0.096353	3.006683
H	-4.595798	0.181308	1.840850
C	-4.477544	6.549811	1.340049
H	-4.644499	6.852640	0.300087
H	-3.758930	7.255609	1.771932
H	-5.421599	6.669130	1.880586
C	7.757398	3.840436	2.962474
H	7.242028	4.801808	2.877033
H	8.765789	3.961497	2.551921
H	7.867237	3.622084	4.031537
C	7.584412	-1.388178	-0.069716
H	6.607057	-1.290066	-0.547793
H	7.931620	-2.425231	-0.162450
H	8.295552	-0.759750	-0.617851
C	8.925745	-1.018886	1.977611
H	9.597528	-0.332138	1.451292
H	9.330848	-2.030071	1.858849
H	8.945555	-0.780177	3.046637
C	1.627621	1.636359	-4.441992
H	1.615855	1.061127	-3.514049
H	1.298856	1.014374	-5.287469
H	0.927275	2.467934	-4.329750
C	-6.146025	2.446824	3.890688
H	-5.863149	3.283779	4.536817
H	-6.610921	1.684171	4.524810
H	-6.908061	2.798087	3.184929
C	-3.957290	1.341770	4.255140
H	-3.079615	0.892243	3.788967
H	-4.436191	0.593383	4.896974
H	-3.635434	2.179194	4.883024
C	3.001784	3.080867	-5.903479
H	2.346053	3.939997	-5.724692
H	2.606121	2.531077	-6.764821
H	3.994310	3.453314	-6.180654
C	-3.912720	2.724728	-4.653999
H	-4.153327	3.793897	-4.635977
H	-4.242576	2.260149	-3.726464
H	-4.469415	2.258954	-5.475691
C	-2.094549	1.003917	-4.772071
H	-2.682680	0.467355	-5.526086
H	-2.332675	0.599513	-3.786002
H	-1.033189	0.841610	-4.989511
C	-2.011490	3.008557	-6.214303
H	-2.282584	4.058484	-6.367885
H	-2.541228	2.418073	-6.969486
H	-0.937278	2.900088	-6.396897
O	2.977595	-2.335179	-2.883589
O	-3.001054	-1.991440	0.842859
O	-4.705664	-0.859394	-1.469518
O	3.034157	-3.094067	0.569658
C	-2.212257	-3.880455	-2.378205
C	1.381754	-4.698991	-0.004878
C	-3.172392	-3.294862	0.911059
C	-5.315671	-1.810621	-2.155576
C	-4.709797	-3.097983	-2.304607
C	-2.198717	-4.235267	-3.728261
H	-3.105738	-4.165520	-4.320533
C	-5.364411	-4.106334	-3.005044
H	-4.882318	-5.077309	-3.102988
C	2.709236	-4.574901	-2.147212
C	-1.012922	-3.931161	-1.663465
H	-1.002646	-3.605393	-0.627354
C	3.414214	-3.583781	-2.889095
C	2.191063	-4.036495	0.965885
C	0.187200	-4.341899	-2.238756
C	-7.216039	-2.660662	-3.413392
H	-8.196389	-2.508385	-3.856548
C	-1.006900	-4.669873	-4.315913
H	-1.003690	-4.959539	-5.363845
C	1.452650	-4.169109	-1.417627
H	1.495418	-3.079340	-1.288304
C	-3.394952	-3.324021	-1.603722
H	-3.067437	-2.324347	-1.331412
C	-6.619454	-3.911265	-3.580266
C	0.559280	-5.760523	0.348086
H	-0.050494	-6.232832	-0.419562
C	0.178823	-4.734109	-3.583048
H	1.102518	-5.060216	-4.052692

C	3.145042	-5.895461	-2.113016
H	2.573773	-6.613708	-1.527640
C	-3.824322	-5.383767	-0.181737
H	-4.068715	-5.921249	-1.096189
C	-3.510249	-4.029636	-0.260114
C	0.471554	-6.205140	1.667099
C	1.209464	-5.512911	2.624602
H	1.109372	-5.832025	3.657458
C	-3.816396	-6.065646	1.031445
C	-2.492366	-3.302918	3.380666
C	4.291786	-6.304173	-2.794976
C	-3.396339	-5.359344	2.165170
H	-3.314533	-5.908463	3.098881
C	-6.613028	-1.610046	-2.718696
C	-7.301974	-0.247920	-2.593824
C	-3.050442	-4.008983	2.143495
C	4.977301	-5.333266	-3.531339
H	5.854849	-5.651114	-4.087659
C	2.049997	-4.432911	2.328586
C	4.583960	-3.990724	-3.603744
C	-3.415111	-2.158886	3.820240
H	-4.425427	-2.516095	4.047965
H	-3.018172	-1.680959	4.723903
H	-3.475402	-1.404065	3.035855
C	5.362014	-2.990647	-4.460551
C	2.817965	-3.736951	3.457462
C	-6.425406	0.796586	-3.294459
H	-6.347959	0.585277	-4.365079
H	-6.848684	1.803427	-3.180512
H	-5.418768	0.762302	-2.872701
C	-0.389680	-7.380069	2.034626
H	0.099413	-8.334992	1.802530
H	-0.619942	-7.384561	3.104950
H	-1.337195	-7.354904	1.488727
C	-4.231151	-7.508138	1.124373
H	-4.041459	-8.038359	0.185913
H	-3.688637	-8.030599	1.918642
H	-5.302297	-7.613928	1.344190
C	5.911410	-1.856292	-3.582101
H	6.603277	-2.250865	-2.828660
H	6.471945	-1.131590	-4.183334
H	5.107524	-1.315143	-3.080580
C	4.777713	-7.724776	-2.719389
H	5.136377	-7.964731	-1.711207
H	3.981056	-8.437700	-2.958310
H	5.602003	-7.900692	-3.417067
C	-7.294124	-4.997587	-4.370982
H	-7.058197	-5.989905	-3.972563
H	-8.382739	-4.883036	-4.360969
H	-6.978484	-4.991107	-5.421701
C	-7.466868	0.151799	-1.118365
H	-6.486070	0.201239	-0.640838
H	-7.939157	1.137513	-1.037111
H	-8.102726	-0.566898	-0.586779
C	-8.690168	-0.222027	-3.235622
H	-9.372629	-0.938823	-2.765253
H	-9.125677	0.776718	-3.118706
H	-8.649044	-0.439596	-4.307313
C	-1.112465	-2.726666	3.027135
H	-1.203640	-2.092475	2.142582
H	-0.727391	-2.144685	3.876528
H	-0.397828	-3.521956	2.802040
C	6.557162	-3.626322	-5.177183
H	6.251741	-4.436090	-5.848513
H	7.056758	-2.863068	-5.781877
H	7.301282	-4.019063	-4.475396
C	4.422733	-2.433710	-5.541219
H	3.549025	-1.969256	-5.083295
H	4.941353	-1.683990	-6.148543
H	4.090348	-3.242051	-6.202414
C	-2.309555	-4.257327	4.562007
H	-1.638518	-5.085005	4.309884
H	-1.865186	-3.711089	5.401049
H	-3.262904	-4.672487	4.908992
C	4.297148	-4.129054	3.360729
H	4.414138	-5.215439	3.430859
H	4.707791	-3.789956	2.412107
H	4.883934	-3.661914	4.160245
C	2.680862	-2.207563	3.369984
H	3.257741	-1.729759	4.170399
H	3.039108	-1.835177	2.409688
H	1.628085	-1.929506	3.501275
C	2.318474	-4.149331	4.846919
H	2.499758	-5.208366	5.057359
H	2.854643	-3.570935	5.606874
H	1.247235	-3.953655	4.966384
N	-0.421897	-0.456736	-0.652917
N	0.840790	-0.711573	-0.620563
K	-4.789634	3.279479	-1.280036
K	-5.792116	-2.110351	0.811681
K	5.339329	-4.262869	-0.183577
K	7.643270	2.538240	-1.400710
C	9.862103	5.227761	0.076119
H	10.491977	4.352320	-0.101455
H	10.215194	6.056294	-0.556726
H	9.943612	5.529663	1.130589
O	8.539101	4.867058	-0.246613
C	7.631322	5.923502	-0.058084
H	7.862099	6.773455	-0.717826
H	7.639248	6.274735	0.983659
H	6.637140	5.545648	-0.302855
C	7.066187	3.880555	-4.709442
H	6.233346	3.210232	-4.490069
H	6.700313	4.699669	-5.347493
H	7.851342	3.329222	-5.246857
O	7.543609	4.374574	-3.478895
C	8.617418	5.267709	-3.655919
H	9.455183	4.788299	-4.181970
H	8.953469	5.567156	-2.661909
H	8.301065	6.156870	-4.223041
C	6.247022	-7.621931	1.035972
H	6.126072	-8.586073	0.519681

H	6.352222	-7.814922	2.113949
H	7.144867	-7.126545	0.661502
O	5.161788	-6.766631	0.773819
C	3.925073	-7.330553	1.157807
H	3.734529	-8.261470	0.604122
H	3.141519	-6.606820	0.932601
H	3.907338	-7.546871	2.235055
C	9.076024	-4.905144	0.504125
H	9.648088	-3.982336	0.337425
H	9.751018	-5.765829	0.391613
H	8.672374	-4.894931	1.519112
O	7.986068	-4.999720	-0.386428
C	8.406215	-4.995116	-1.735858
H	8.904169	-4.049799	-1.993005
H	7.514755	-5.113253	-2.356213
H	9.093976	-5.828508	-1.937270
C	-5.753196	6.656467	-2.497629
H	-6.669178	6.185818	-2.134352
H	-5.854785	6.877870	-3.570191
H	-5.600192	7.603356	-1.959102
O	-4.699160	5.758368	-2.257566
C	-3.442558	6.281565	-2.643468
H	-3.420625	6.499566	-3.719784
H	-2.683403	5.530717	-2.422752
H	-3.218407	7.202705	-2.086996
C	-7.908254	3.914575	0.300313
H	-7.026000	3.885540	0.943788
H	-8.566547	3.069235	0.547749
H	-8.451792	4.852363	0.482468
O	-7.461510	3.837767	-1.036064
C	-8.525403	3.913156	-1.956663
H	-8.098467	3.866637	-2.960649
H	-9.080201	4.855718	-1.844352
H	-9.225581	3.075524	-1.827319
C	-7.406341	-5.096900	-0.101696
H	-7.229110	-5.094808	-1.184104
H	-8.127663	-5.887638	0.152374
H	-6.458765	-5.293440	0.404741
O	-7.875063	-3.834785	0.334709
C	-9.077064	-3.480173	-0.307465
H	-8.931911	-3.382123	-1.391462
H	-9.397800	-2.517500	0.099832
H	-9.863810	-4.224422	-0.113581
C	-8.196366	-2.292880	3.542241
H	-8.421344	-2.464664	4.604580
H	-8.966724	-2.787998	2.932836
H	-8.219813	-1.216895	3.349086
O	-6.911419	-2.756200	3.209992
C	-6.771058	-4.141011	3.452232
H	-6.893408	-4.366168	4.521086
H	-5.764256	-4.429971	3.139196
H	-7.509144	-4.713450	2.874377
K	0.186901	0.230922	1.902391
K	0.369601	-1.272287	-3.240025

K^+- Bound Complex Following Four-Electron Reduction (Reduced using K^0) – Quintet (Complex 4)

SCF Energy (a.u.): -10532.236197

Ce	3.024228	-1.074619	-0.841080
Ce	-2.565094	-0.072977	-0.526907
O	-2.591107	1.189017	1.546599
O	3.316383	0.867301	-2.102691
O	4.831629	-0.354782	0.489865
O	-2.613385	1.872842	-1.957376
C	2.558616	2.800756	1.064571
C	-1.014760	3.535624	-1.375930
C	3.604357	2.146698	-2.188485
C	5.546334	0.618224	1.014824
C	5.031227	1.948464	1.063042
C	2.531283	3.229190	2.392885
H	3.436421	3.192392	2.991662
C	5.755716	2.965398	1.685591
H	5.333257	3.968022	1.727261
C	-2.360137	3.418775	0.762731
C	1.365943	2.814161	0.336122
H	1.373924	2.433105	-0.681792
C	-3.040004	2.430007	1.533642
C	-1.787797	2.839945	-2.351156
C	0.160382	3.250108	0.878410
C	7.546368	1.450167	2.122730
H	8.543559	1.278808	2.516646
C	1.332999	3.691514	2.945750
H	1.319260	4.037175	3.976575
C	-1.091436	3.028710	0.046356
H	-1.103649	1.935529	-0.063542
C	3.742201	2.204617	0.330241
H	3.385432	1.210577	0.069881
C	7.009460	2.735849	2.249084
C	-0.197836	4.598472	-1.737854
H	0.397639	5.089302	-0.971016
C	0.152579	3.710496	2.201046
H	-0.775337	4.055325	2.648316
C	-2.822631	4.728986	0.706760
H	-2.268277	5.445217	0.102515
C	4.242377	4.241500	-1.090065
H	4.432086	4.786424	-0.166542
C	3.914169	2.889136	-1.015065
C	-0.087801	5.013814	-3.065356
C	-0.809564	4.302589	-4.020837
H	-0.697808	4.604905	-5.057294
C	4.287158	4.917691	-2.305509
C	3.073783	2.154759	-4.698863
C	-3.969853	5.133784	1.392696
C	3.913092	4.201991	-3.446582
H	3.896216	4.738347	-4.390858
C	6.865439	0.392195	1.518194
C	7.506074	-0.991716	1.392752
C	3.554578	2.856269	-3.428980
C	-4.625292	4.169195	2.163428
H	-5.497530	4.486413	2.728996

C	-1.645777	3.221838	-3.715039
C	-4.203021	2.837229	2.260337
C	4.025038	1.008413	-5.055807
H	5.038808	1.381601	-5.239490
H	3.684137	0.499092	-5.965014
H	4.066956	0.283570	-4.243522
C	-4.929744	1.848360	3.173608
C	-2.383740	2.478459	-4.832554
C	6.652633	-2.001013	2.168245
H	6.634118	-1.758329	3.236029
H	7.067871	-3.014466	2.070240
H	5.623937	-1.977697	1.803611
C	0.815097	6.152306	-3.445400
H	0.554083	7.074268	-2.912706
H	0.761299	6.359739	-4.518424
H	1.855565	5.915115	-3.199587
C	4.727103	6.350383	-2.407739
H	4.615788	6.873730	-1.452262
H	4.145441	6.899160	-3.156548
H	5.782118	6.412123	-2.703134
C	-5.437757	0.653743	2.353692
H	-6.178554	0.984887	1.614020
H	-5.907385	-0.085859	3.014815
H	-4.591920	0.185339	1.844833
C	-4.463573	6.551599	1.312522
H	-4.591336	6.865436	0.270466
H	-3.761598	7.252394	1.778843
H	-5.427179	6.666106	1.818609
C	7.761262	3.814943	2.974949
H	7.331190	4.800151	2.770103
H	8.815771	3.836856	2.680077
H	7.733128	3.666508	4.061686
C	7.574318	-1.396435	-0.088359
H	6.593889	-1.295287	-0.559696
H	7.921801	-2.432528	-0.190446
H	8.281523	-0.764092	-0.637186
C	8.929026	-1.039702	1.951955
H	9.597238	-0.350121	1.424776
H	9.333154	-2.050238	1.824524
H	8.956334	-0.807100	3.022155
C	1.664300	1.596328	-4.448617
H	1.680267	1.000114	-3.534112
H	1.349050	0.982559	-5.305061
H	0.940558	2.404473	-4.313342
C	-6.138433	2.464012	3.882449
H	-5.854275	3.304346	4.523617
H	-6.603870	1.705593	4.521243
H	-6.900392	2.812066	3.174991
C	-3.950073	1.359340	4.251708
H	-3.073014	0.906663	3.787415
H	-4.428705	0.614896	4.898325
H	-3.627190	2.200208	4.874433
C	2.986385	3.098796	-5.899732
H	2.307857	3.937239	-5.707913
H	2.600834	2.546052	-6.763773
H	3.966031	3.501717	-6.179973
C	-3.894902	2.681491	-4.666500
H	-4.143700	3.748964	-4.652940
H	-4.220417	2.217941	-3.736842
H	-4.448152	2.208401	-5.486319
C	-2.062710	0.974842	-4.780325
H	-2.649353	0.430664	-5.530037
H	-2.293842	0.572567	-3.791533
H	-1.000710	0.821124	-5.001143
C	-1.995462	2.976729	-6.227437
H	-2.271939	4.025123	-6.382000
H	-2.522649	2.382574	-6.981518
H	-0.920832	2.873531	-6.410648
O	2.954557	-2.350323	-2.892687
O	-2.996396	-1.992516	0.847494
O	-4.714726	-0.865553	-1.458409
O	3.032974	-3.100205	0.551425
C	-2.229643	-3.895253	-2.367476
C	1.376650	-4.707259	-0.007941
C	-3.174183	-3.294727	0.922944
C	-5.327775	-1.817737	-2.141037
C	-4.724842	-3.106592	-2.287442
C	-2.222605	-4.255384	-3.716218
H	-3.132040	-4.186529	-4.304868
C	-5.383533	-4.116013	-2.982621
H	-4.903662	-5.088290	-3.078391
C	2.691903	-4.590785	-2.158794
C	-1.027226	-3.944880	-1.657813
H	-1.012067	-3.615857	-0.622755
C	3.392746	-3.598491	-2.902692
C	2.190984	-4.039639	0.955965
C	0.170126	-4.358887	-2.236734
C	-7.232633	-2.667419	-3.392053
H	-8.213451	-2.514429	-3.833855
C	-1.033980	-4.693995	-4.307266
H	-1.035778	-4.987962	-5.354011
C	1.439688	-4.183410	-1.422992
H	1.486896	-3.093359	-1.297302
C	-3.408065	-3.333240	-1.590438
H	-3.076756	-2.333378	-1.323294
C	-6.639562	-3.920184	-3.555344
C	0.556290	-5.767559	0.353003
H	-0.056536	-6.243288	-0.410149
C	0.154896	-4.756586	-3.579444
H	1.076086	-5.085634	-4.051927
C	3.128891	-5.910835	-2.127915
H	2.561321	-6.630214	-1.540316
C	-3.839189	-5.385667	-0.157790
H	-4.089663	-5.926409	-1.068638
C	-3.520159	-4.033121	-0.243513
C	0.474475	-6.206846	1.674289
C	1.216347	-5.510100	2.625106
H	1.121143	-5.824826	3.659786
C	-3.828743	-6.062015	1.058439
C	-2.483901	-3.293977	3.389920
C	4.273260	-6.317200	-2.815553
C	-3.401569	-5.352190	2.187400

H	-3.317977	-5.897454	3.123220
C	-6.625489	-1.615698	-2.702601
C	-7.310318	-0.251047	-2.582126
C	-3.050490	-4.003301	2.158324
C	4.953921	-5.345085	-3.554824
H	5.828768	-5.661751	-4.116041
C	2.054807	-4.430527	2.321015
C	4.558838	-4.002693	-3.623757
C	-3.398139	-2.142204	3.827104
H	-4.409544	-2.492054	4.061318
H	-2.994499	-1.661839	4.726490
H	-3.457454	-1.391167	3.039016
C	5.333291	-2.998629	-4.479274
C	2.827585	-3.731990	3.445047
C	-6.431302	0.788240	-3.287560
H	-6.356025	0.573125	-4.357574
H	-6.850923	1.796769	-3.175929
H	-5.424328	0.751742	-2.866889
C	-0.387015	-7.378763	2.050718
H	0.083892	-8.334667	1.787497
H	-0.582593	-7.398039	3.127732
H	-1.351312	-7.335245	1.535929
C	-4.248019	-7.502631	1.159861
H	-4.082392	-8.032566	0.216771
H	-3.689817	-8.028677	1.940860
H	-5.314213	-7.603529	1.404523
C	5.893330	-1.874463	-3.594453
H	6.587660	-2.278186	-2.848081
H	6.453093	-1.146352	-4.192200
H	5.094131	-1.334162	-3.084150
C	4.762893	-7.736612	-2.741515
H	5.141230	-7.970284	-1.738976
H	3.962864	-8.451993	-2.960832
H	5.573987	-7.915367	-3.453797
C	-7.318865	-5.008066	-4.339903
H	-7.093240	-5.998759	-3.931514
H	-8.406485	-4.884452	-4.336615
H	-6.997557	-5.013526	-5.388890
C	-7.472373	0.154673	-1.108010
H	-6.490681	0.205558	-0.632522
H	-7.943958	1.140995	-1.030104
H	-8.107681	-0.561527	-0.572471
C	-8.699038	-0.223335	-3.222726
H	-9.383198	-0.936360	-2.749126
H	-9.131501	0.777089	-3.108962
H	-8.659641	-0.444828	-4.293676
C	-1.102077	-2.727583	3.028020
H	-1.193585	-2.097372	2.140671
H	-0.709828	-2.143654	3.872790
H	-0.392926	-3.527958	2.803700
C	6.520039	-3.633116	-5.210796
H	6.205579	-4.437098	-5.884887
H	7.017100	-2.867394	-5.814454
H	7.268875	-4.033690	-4.518555
C	4.389181	-2.426159	-5.547574
H	3.526564	-1.952014	-5.078474
H	4.911063	-1.681213	-6.157890
H	4.039324	-3.227784	-6.207937
C	-2.302094	-4.243424	4.575341
H	-1.637022	-5.076401	4.324882
H	-1.851169	-3.695638	5.409859
H	-3.256537	-4.651076	4.928183
C	4.303073	-4.138455	3.351131
H	4.410041	-5.224573	3.438906
H	4.713609	-3.820317	2.395293
H	4.896746	-3.663493	4.140853
C	2.702726	-2.202324	3.347492
H	3.280862	-1.724070	4.146720
H	3.065282	-1.837074	2.386211
H	1.651549	-1.916062	3.475224
C	2.324603	-4.130335	4.837553
H	2.498994	-5.188660	5.057014
H	2.863958	-3.549303	5.593250
H	1.254520	-3.927014	4.954607
N	-0.425011	-0.462840	-0.665015
N	0.837814	-0.708299	-0.640460
K	-4.775333	3.281296	-1.305306
K	-5.793710	-2.106522	0.829363
K	5.344197	-4.255203	-0.205756
K	7.679057	2.547164	-1.363478
C	9.801602	5.276628	0.224177
H	10.454450	4.407809	0.108321
H	10.188712	6.098758	-0.397017
H	9.801200	5.598031	1.275510
O	8.510954	4.891153	-0.185359
C	7.579291	5.937924	-0.082161
H	7.846605	6.779808	-0.738387
H	7.508312	6.307099	0.951532
H	6.610192	5.542794	-0.391045
C	7.082884	3.961613	-4.631539
H	6.237960	3.306857	-4.411510
H	6.728621	4.795632	-5.256672
H	7.851137	3.400262	-5.182924
O	7.583027	4.430824	-3.400033
C	8.680075	5.295451	-3.577927
H	9.496487	4.799869	-4.122131
H	9.038266	5.569452	-2.584319
H	8.382470	6.201811	-4.127707
C	6.252086	-7.614208	1.011226
H	6.128746	-8.580644	0.499771
H	6.362075	-7.802462	2.089575
H	7.148374	-7.120671	0.630614
O	5.165839	-6.760010	0.750051
C	3.931034	-7.321743	1.143410
H	3.737112	-8.254979	0.594806
H	3.146467	-6.598708	0.919520
H	3.919340	-7.533391	2.221634
C	9.087990	-4.904057	0.445918
H	9.662695	-3.985670	0.264424
H	9.757188	-5.769246	0.333330
H	8.696181	-4.882638	1.465340
O	7.987282	-5.000891	-0.431141

C	8.391686	-5.008435	-1.785232
H	8.891359	-4.067559	-2.055062
H	7.492536	-5.126779	-2.394360
H	9.072926	-5.846734	-1.988482
C	-5.735971	6.658322	-2.518625
H	-6.651588	6.189234	-2.152462
H	-5.842496	6.884801	-3.589629
H	-5.576675	7.602194	-1.976697
O	-4.683857	5.755351	-2.288229
C	-3.427172	6.275367	-2.677931
H	-3.409284	6.497135	-3.753586
H	-2.669729	5.521058	-2.463016
H	-3.196976	7.193740	-2.119359
C	-7.891866	3.930069	0.277376
H	-7.009226	3.899138	0.920232
H	-8.555362	3.090549	0.530571
H	-8.429206	4.872441	0.454170
O	-7.446923	3.842171	-1.059002
C	-8.511522	3.918002	-1.978797
H	-8.086058	3.864170	-2.983031
H	-9.061511	4.863880	-1.870792
H	-9.215654	3.084541	-1.844193
C	-7.419549	-5.090117	-0.061619
H	-7.237745	-5.089786	-1.143289
H	-8.144768	-5.877985	0.190127
H	-6.474942	-5.289693	0.449170
O	-7.885570	-3.825866	0.371724
C	-9.085172	-3.468705	-0.273749
H	-8.937295	-3.372581	-1.357561
H	-9.404163	-2.504673	0.131696
H	-9.874355	-4.210546	-0.080703
C	-8.186793	-2.262690	3.572511
H	-8.408675	-2.429897	4.636213
H	-8.959926	-2.758845	2.967502
H	-8.208749	-1.187450	3.375180
O	-6.903692	-2.729776	3.238042
C	-6.765071	-4.113755	3.486355
H	-6.883317	-4.333535	4.556770
H	-5.760198	-4.406373	3.170517
H	-7.506727	-4.687439	2.914316
K	0.193558	0.221335	1.889868
K	0.345968	-1.300393	-3.246675

Complex 5 – Quartet

SCF Energy (a.u.): -9467.899144

Ce	-2.864624	1.139920	0.178187
Ce	2.323159	-1.722743	-0.053790
O	2.642471	-2.450370	2.140431
O	-3.876851	-0.851151	-0.788567
O	-4.585083	0.693125	1.759175
O	1.691460	-2.782570	-1.935803
C	-2.203458	-2.598859	2.361852
C	0.229297	-4.277853	-0.805882
C	-4.117068	-2.140431	-0.593543
C	-5.027830	-0.114198	2.715631
C	-4.476902	-1.421569	2.863557
C	-1.806079	-2.672514	3.705208
H	-2.439845	-2.293778	4.499733
C	-4.941245	-2.268240	3.865658
H	-4.497378	-3.256585	3.962379
C	2.182483	-4.379392	0.799028
C	-1.357788	-3.082384	1.369884
H	-1.691482	-3.013587	0.340405
C	3.017984	-3.675172	1.731605
C	0.730354	-3.704588	-2.010578
C	-0.068197	-3.608716	1.613260
C	-6.507224	-0.618342	4.575047
H	-7.304274	-0.323743	5.250849
C	-0.582594	-3.297411	3.992429
H	-0.284031	-3.427979	5.031418
C	0.824131	-3.897816	0.512088
H	-0.467272	-1.589706	-0.681231
C	-3.453599	-1.887580	1.856136
H	-3.060998	-0.987896	1.381685
C	-5.949805	-1.885270	4.746627
C	-0.798087	-5.221282	-0.891122
H	-1.176288	-5.652352	0.033882
C	0.264273	-3.756197	2.991397
H	1.197322	-4.235501	3.264686
C	2.733609	-5.490984	0.131764
H	2.124547	-5.978326	-0.625851
C	-4.458503	-4.000812	0.962989
H	-4.379459	-4.385658	1.977750
C	-4.066773	-2.688840	0.718776
C	-1.342156	-5.623037	-2.108439
C	-0.831396	-5.050579	-3.274492
H	-1.247669	-5.375071	-4.223998
C	-4.896287	-4.839349	-0.055358
C	-4.447162	-2.564238	-3.119104
C	3.983163	-5.998492	0.447464
C	-4.860701	-4.330273	-1.353779
H	-5.136880	-4.999895	-2.161736
C	-6.086700	0.278354	3.588469
C	-6.715061	1.671735	3.482845
C	-4.466684	-3.027026	-1.660689
C	4.689715	-5.411277	1.505478
H	5.625126	-5.870421	1.811900
C	0.194729	-4.100806	-3.263774
C	4.235011	-4.272683	2.164649
C	-5.651468	-1.644617	-3.357346
H	-6.582775	-2.167342	-3.109216
H	-5.703386	-1.329978	-4.406283
H	-5.566499	-0.744292	-2.744436
C	4.991358	-3.682713	3.355136
C	0.766202	-3.531130	-4.566400
C	-5.639095	2.724952	3.774857
H	-5.268235	2.617316	4.799819
H	-6.048548	3.735859	3.663582
H	-4.798404	2.610789	3.089970
C	-2.386582	-6.702475	-2.169056
H	-1.932580	-7.695975	-2.278913
H	-3.065419	-6.563494	-3.017360

H	-2.989666	-6.715266	-1.257716
C	-5.370017	-6.237216	0.229952
H	-4.707250	-6.749334	0.935640
H	-5.411762	-6.837110	-0.684031
H	-6.375467	-6.244733	0.671938
C	5.546931	-2.307374	2.976008
H	6.334109	-2.430202	2.223077
H	5.979472	-1.804882	3.849697
H	4.730670	-1.698357	2.580988
C	4.557350	-7.172811	-0.294929
H	5.300509	-6.855306	-1.037883
H	3.777785	-7.721164	-0.831235
H	5.058359	-7.873033	0.382559
C	-6.410748	-2.798574	5.848269
H	-6.409371	-3.845785	5.528202
H	-7.424607	-2.548767	6.176350
H	-5.759338	-2.732505	6.728806
C	-7.289125	1.917342	2.077244
H	-6.490348	1.888052	1.333566
H	-7.761126	2.905196	2.025595
H	-8.061074	1.173233	1.838560
C	-7.861232	1.875753	4.477403
H	-8.676071	1.160603	4.316905
H	-8.271116	2.883612	4.352830
H	-7.523203	1.784617	5.514425
C	-3.144369	-1.809709	-3.422679
H	-3.106452	-0.925011	-2.785002
H	-3.118355	-1.512838	-4.479369
H	-2.285358	-2.460132	-3.218051
C	6.168212	-4.553744	3.798978
H	5.841650	-5.559587	4.080612
H	6.646903	-4.100127	4.675180
H	6.927287	-4.648088	3.014461
C	4.033205	-3.537190	4.547767
H	3.181482	-2.909299	4.278605
H	4.553508	-3.090147	5.404702
H	3.658321	-4.519597	4.852761
C	-4.531228	-3.730622	-4.108132
H	-3.716254	-4.442073	-3.943745
H	-4.442626	-3.342568	-5.128822
H	-5.484504	-4.265952	-4.046734
C	2.254128	-3.899972	-4.668192
H	2.373567	-4.988229	-4.681962
H	2.799569	-3.502190	-3.811365
H	2.689660	-3.494872	-5.590569
C	0.627190	-1.999221	-4.593318
H	1.099848	-1.584025	-5.492116
H	1.118318	-1.581943	-3.709678
H	-0.436896	-1.730126	-4.619537
C	0.051284	-4.073876	-5.805738
H	0.155923	-5.160128	-5.890719
H	0.490386	-3.626709	-6.704595
H	-1.017758	-3.832246	-5.797404
O	-2.892065	1.906921	-2.077037
O	4.519978	-1.168462	-0.816791
C	2.558777	2.131729	-2.323806
C	5.132965	-0.627529	-1.852668
C	4.733363	0.667822	-2.292337
C	2.601817	2.387157	-3.699402
H	3.394228	1.970504	-4.307457
C	5.472303	1.328317	-3.273706
H	5.217075	2.350310	-3.544816
C	-2.020706	4.115221	-2.178087
C	1.439783	2.590476	-1.612835
H	1.295639	2.247988	-0.585979
C	-3.049033	3.178089	-2.443162
C	0.419410	3.341891	-2.213013
C	6.876069	-0.587132	-3.530197
H	7.702712	-1.068088	-4.044295
C	1.601876	3.146706	-4.307450
H	1.658674	3.339485	-5.375743
C	-0.811003	3.663048	-1.389431
H	-1.066827	2.698895	-0.939341
C	3.552850	1.266029	-1.559600
H	2.941580	0.414858	-1.255920
C	6.543916	0.713510	-3.917958
C	0.525263	3.641700	-3.574428
H	-0.263257	4.213805	-4.054236
C	-2.144203	5.441133	-2.585957
H	-1.350398	6.143670	-2.342804
C	-3.270934	5.898142	-3.257385
C	6.217924	-1.277915	-2.512658
C	6.620335	-2.706107	-2.129488
C	-4.301694	4.982270	-3.472932
H	-5.200342	5.344792	-3.962233
C	-4.235566	3.647043	-3.078124
C	-5.409923	2.704407	-3.336940
C	5.453123	-3.661846	-2.422609
H	5.225415	-3.669699	-3.492879
H	5.713962	-4.682148	-2.120262
H	4.548539	-3.375777	-1.884361
C	-5.839897	2.018743	-2.027772
H	-5.983123	2.759417	-1.232075
H	-6.789563	1.490659	-2.170031
H	-5.077043	1.297597	-1.725833
C	-3.384347	7.321082	-3.727334
H	-2.714240	7.978501	-3.164798
H	-3.125444	7.422492	-4.789220
H	-4.403460	7.703297	-3.608053
C	7.305177	1.414317	-5.008881
H	7.147512	2.496960	-4.972418
H	8.382360	1.230559	-4.933472
H	6.992406	1.074576	-6.003998
C	6.981772	-2.797758	-0.637674
H	6.101291	-2.609248	-0.023147
H	7.340341	-3.804509	-0.396619
H	7.785139	-2.088930	-0.388609
C	7.836153	-3.192574	-2.923183
H	8.720606	-2.569951	-2.743174
H	8.079353	-4.214639	-2.615915
H	7.640882	-3.212235	-4.000113
C	-6.637904	3.434128	-3.889320

H	-6.438121	3.899531	-4.859567
H	-7.449041	2.712389	-4.035526
H	-6.995610	4.208385	-3.202069
C	-4.981747	1.651663	-4.368238
H	-4.144504	1.063817	-3.986892
H	-5.808802	0.971399	-4.599292
H	-4.675816	2.141737	-5.298648
N	0.002177	-0.777625	-0.237623
N	-0.888600	0.152269	0.078212
K	-0.749220	0.309773	-2.733252
K	0.271261	-0.696958	2.539377
K	6.173526	0.060023	1.002994
K	-6.460614	-0.546853	0.021674
O	-8.184495	-2.461665	0.804469
C	-8.390960	-3.413679	-0.218115
H	-9.221762	-4.088593	0.035212
H	-7.483537	-4.006502	-0.395287
H	-8.642147	-2.858162	-1.124796
C	-7.875759	-3.071126	2.043457
H	-8.711525	-3.698490	2.386515
H	-7.694482	-2.275394	2.768500
H	-6.968586	-3.682989	1.963062
O	-8.743046	-0.305250	-1.552131
C	-8.987318	0.054576	-2.891824
H	-9.789035	-0.561367	-3.324272
H	-8.066078	-0.114459	-3.452362
H	-9.272451	1.113265	-2.977376
C	-9.888404	-0.143430	-0.742958
H	-10.743079	-0.696962	-1.157754
H	-10.165944	0.916626	-0.652815
H	-9.651952	-0.556167	0.239791
O	8.440763	1.260543	0.176163
C	8.469580	1.534339	-1.208274
H	9.179782	0.877666	-1.728990
H	8.749764	2.581751	-1.394130
H	7.472426	1.351635	-1.610212
C	9.689277	1.468812	0.790145
H	9.561635	1.253550	1.851743
H	10.023737	2.509444	0.663756
H	10.457171	0.804081	0.367905
O	7.897267	0.027082	3.169352
C	8.783656	-1.046574	3.398033
H	8.334361	-1.803865	4.053970
H	9.722473	-0.693814	3.848349
H	9.000929	-1.503785	2.430045
C	7.543009	0.690345	4.360272
H	7.024426	0.015592	5.056258
H	6.871208	1.508009	4.089142
H	8.428128	1.104535	4.864162
H	5.499872	3.072597	-1.188842
C	5.045323	2.806716	-0.236718
C	3.856073	2.098213	2.204431
C	3.998320	1.888447	-0.239664
C	5.552419	3.364234	0.939429
C	4.927626	2.996368	2.137803
C	3.388867	1.463933	0.993084
H	5.291676	3.448614	3.056867
O	2.446658	0.579126	1.001581
C	3.134863	1.828415	3.527108
C	3.276740	0.352051	3.922720
H	4.315590	0.131733	4.190216
H	2.999800	-0.333671	3.121378
H	2.667547	0.130453	4.808274
C	1.653948	2.219143	3.365745
H	1.528303	3.309166	3.378968
H	1.061415	1.844481	4.209141
H	1.228855	1.843974	2.431346
C	3.687836	2.660903	4.687263
H	3.618854	3.738263	4.497378
H	4.731823	2.416630	4.911800
H	3.103976	2.449691	5.588989
C	6.750691	4.270092	0.921500
H	6.767677	4.889435	0.019751
H	7.678336	3.685592	0.932260
H	6.767533	4.936338	1.789944
C	-1.078164	5.140871	2.110033
C	0.206267	5.724717	-0.324245
C	-1.286577	4.271377	0.987193
C	-0.248643	6.255534	1.955554
C	0.386337	6.594042	0.753460
C	-0.568749	4.573330	-0.213080
H	-0.114740	6.927282	2.799049
H	0.694963	5.938840	-1.275431
O	-2.098496	3.254802	1.019602
C	-1.882124	4.943268	3.396625
C	-1.468728	5.912183	4.508095
H	-2.051028	5.692826	5.408986
H	-1.660735	6.956893	4.242072
H	-0.407624	5.809483	4.765499
C	-1.725687	3.520658	3.954903
H	-2.416488	3.368712	4.791977
H	-0.707832	3.368103	4.328122
H	-1.937939	2.776238	3.187317
C	-3.355603	5.218412	3.056165
H	-3.984712	5.085446	3.943048
H	-3.701202	4.538361	2.276084
H	-3.475131	6.246797	2.698915
C	1.171277	7.870556	0.609699
H	0.529429	8.705561	0.301979
H	1.957032	7.770417	-0.146299
H	1.643781	8.164687	1.553827
K	2.492277	4.416007	0.821958
O	3.783101	5.984450	-0.954697
C	4.722729	7.014949	-0.773000
H	5.692627	6.754400	-1.220747
H	4.855835	7.159363	0.301637
H	4.372973	7.957059	-1.218990
C	3.564566	5.698729	-2.320815
H	4.489379	5.351270	-2.802633
H	3.197556	6.586929	-2.853873
H	2.815684	4.908350	-2.384132

Complex 6 – Triplet

SCF Energy (a.u.): -8522.521645

Ce	-2.936971	-1.202262	-0.299402
Ce	2.941627	0.972063	0.036593
O	3.309518	2.582049	-1.435201
O	-3.312795	0.863345	0.872326
O	-4.833231	-0.585055	-1.449060
O	1.718960	2.196884	1.540546
C	-2.510887	2.740030	-2.325779
C	0.294060	3.910551	0.718181
C	-3.883804	2.060498	0.795697
C	-5.362059	0.196173	-2.395767
C	-4.818162	1.493343	-2.622861
C	-2.369925	3.260174	-3.612084
H	-3.121302	3.079214	-4.371941
C	-5.416177	2.339381	-3.552847
H	-5.024295	3.343383	-3.687218
C	1.971881	4.514002	-1.088690
C	-1.471892	2.939044	-1.417850
H	-1.565624	2.516302	-0.422124
C	3.171116	3.905718	-1.521628
C	0.850529	3.169249	1.796712
C	-0.323784	3.654693	-1.726134
C	-7.026304	0.664089	-4.088462
H	-7.884082	0.355845	-4.677329
C	-1.231985	4.004637	-3.931882
H	-1.132523	4.416739	-4.932454
C	0.788775	3.655271	-0.691961
H	1.128496	2.614561	-0.717576
C	-3.665310	1.931578	-1.751369
H	-3.186764	1.013625	-1.412575
C	-6.514722	1.941375	-4.311059
C	-0.673785	4.878719	0.959445
H	-1.113444	5.400722	0.111781
C	-0.217313	4.214015	-3.002238
H	0.668816	4.780124	-3.270198
C	1.847442	5.900475	-1.113411
H	0.923447	6.348639	-0.754296
C	-4.753538	3.872284	-0.617606
H	-4.890071	4.281213	-1.616196
C	-4.139541	2.631991	-0.484195
C	-1.106757	5.179438	2.248176
C	-0.524563	4.478507	3.302227
H	-0.838247	4.735272	4.309137
C	-5.169801	4.602862	0.487682
C	-4.220531	2.290166	3.390198
C	2.866926	6.717264	-1.589483
C	-4.946232	4.033487	1.740200
H	-5.277189	4.596755	2.606378
C	-6.493126	-0.223471	-3.148934
C	-7.096420	-1.620450	-2.965540
C	-4.310343	2.804006	1.943571
C	4.022393	6.097943	-2.071213
H	4.806962	6.733451	-2.471005
C	0.447360	3.486225	3.127091
C	4.206960	4.716406	-2.056983
C	-5.462276	1.430187	3.661596
H	-6.377971	1.999116	3.461527
H	-5.486502	1.096823	4.705564
H	-5.450813	0.527863	3.043129
C	5.483920	4.076187	-2.606925
C	1.158819	2.877980	4.345134
C	-6.046712	-2.677907	-3.330939
H	-5.738886	-2.567603	-4.375381
H	-6.456505	-3.685446	-3.199980
H	-5.160170	-2.587113	-2.703345
C	-2.151008	6.233307	2.484913
H	-1.890695	7.173273	1.985558
H	-2.265932	6.446306	3.552264
H	-3.127043	5.917038	2.099703
C	-5.769404	5.974131	0.348915
H	-4.990731	6.746594	0.327810
H	-6.433710	6.211381	1.186410
H	-6.344930	6.072052	-0.577326
C	6.215621	3.353592	-1.467741
H	6.503986	4.060815	-0.684105
H	7.126730	2.864735	-1.835034
H	5.555832	2.607970	-1.019832
C	2.740722	8.214835	-1.573025
H	3.159110	8.644762	-0.654226
H	1.693299	8.526942	-1.627730
H	3.271704	8.671432	-2.414529
C	-7.116513	2.853381	-5.343190
H	-7.070392	3.900960	-5.028142
H	-8.164784	2.604828	-5.534309
H	-6.586391	2.782167	-6.300797
C	-7.552290	-1.834772	-1.513319
H	-6.699503	-1.792310	-0.834351
H	-8.017320	-2.820688	-1.401956
H	-8.301035	-1.084359	-1.227178
C	-8.319491	-1.847535	-3.859041
H	-9.126945	-1.139619	-3.640194
H	-8.706086	-2.857167	-3.687109
H	-8.069658	-1.768872	-4.921693
C	-2.966339	1.455356	3.663081
H	-2.987010	0.538662	3.073927
H	-2.925666	1.189363	4.725684
H	-2.076886	2.054737	3.434806
C	6.451939	5.107424	-3.191936
H	6.002068	5.662304	-4.021580
H	7.337848	4.591628	-3.579857
H	6.790320	5.826798	-2.438826
C	5.129223	3.082439	-3.724266
H	4.448758	2.310918	-3.361212
H	6.037508	2.602811	-4.110548
H	4.645864	3.604320	-4.556649
C	-4.202474	3.440106	4.409203
H	-3.399996	4.148579	4.184533
H	-4.025023	3.029100	5.408438
H	-5.148601	3.987233	4.456309
C	2.628099	3.316022	4.289572
H	2.703870	4.407182	4.329445

H	3.087096	2.971506	3.362892
H	3.189133	2.898334	5.133758
C	1.104743	1.342676	4.372485
H	1.675365	0.961433	5.226280
H	1.549804	0.918731	3.470377
H	0.072942	0.990702	4.506753
C	0.563874	3.362735	5.670751
H	0.656773	4.446505	5.789530
H	1.104640	2.893567	6.499418
H	-0.494561	3.093820	5.767226
O	-2.945971	-1.901701	1.859978
O	4.127370	-0.718737	-1.122634
O	4.890308	0.760873	1.394532
O	-2.352020	-3.227399	-1.046458
C	2.815775	-2.459853	2.176898
C	-0.487894	-4.334209	-0.093122
C	4.489519	-1.994731	-1.054317
C	5.538857	-0.065916	2.209615
C	5.167726	-1.439923	2.271411
C	2.703631	-2.432927	3.567976
H	3.543563	-2.104017	4.170622
C	5.850423	-2.332841	3.090529
H	5.532115	-3.373508	3.110882
C	-1.889564	-4.031212	1.899238
C	1.712135	-2.851003	1.417362
H	1.791332	-2.853023	0.332898
C	-2.984489	-3.200211	2.211982
C	-1.471476	-4.231452	-1.109242
C	0.506465	-3.221688	2.010901
C	7.293765	-0.582855	3.807084
H	8.132505	-0.265188	4.418134
C	1.507260	-2.809446	4.174226
H	1.425549	-2.792149	5.257883
C	-0.701814	-3.483363	1.136794
H	-0.973058	-2.486374	0.767780
C	4.007378	-1.902791	1.424545
H	3.623583	-0.978741	1.016391
C	6.921293	-1.926711	3.878983
C	0.543627	-5.256370	-0.195144
H	1.300455	-5.295889	0.584760
C	0.413369	-3.201553	3.407284
H	-0.518169	-3.493066	3.882665
C	-1.886893	-5.373528	2.262927
H	-1.029290	-5.983753	1.987737
C	4.732767	-4.034890	0.276238
H	4.615097	-4.542928	1.232013
C	4.418010	-2.684461	0.191988
C	0.632577	-6.118843	-1.286079
C	-0.401406	-6.087701	-2.217786
H	-0.362873	-6.799141	-3.036394
C	5.179045	-4.747793	-0.834071
C	5.097193	-2.026387	-3.570868
C	-2.961702	-5.947441	2.930397
C	5.298423	-4.054173	-2.039695
H	5.651143	-4.612344	-2.901261
C	6.646832	0.363025	3.007831
C	7.110391	1.825136	3.020657
C	4.974784	-2.702081	-2.195229
C	-4.050525	-5.125743	3.217974
H	-4.896549	-5.574838	3.728091
C	-1.473104	-5.190548	-2.152365
C	-4.101385	-3.772732	2.877267
C	5.954268	-0.753274	-3.509018
H	6.968011	-0.971400	-3.153328
H	6.048394	-0.322821	-4.512639
H	5.475884	-0.001303	-2.878705
C	-5.315065	-2.928154	3.264547
C	-2.623876	-5.273381	-3.157024
C	5.950613	2.725394	3.461662
H	5.623619	2.463193	4.472399
H	6.259484	3.777207	3.463694
H	5.105240	2.609035	2.784291
C	1.811372	-7.035526	-1.448635
H	2.088073	-7.508277	-0.499742
H	1.605184	-7.829706	-2.172372
H	2.691778	-6.483430	-1.800613
C	5.552925	-6.200197	-0.728670
H	4.847582	-6.748936	-0.096658
H	5.562047	-6.681330	-1.711102
H	6.550697	-6.332552	-0.290622
C	-5.858112	-2.174300	2.039912
H	-6.046542	-2.868638	1.213693
H	-6.802976	-1.673602	2.281737
H	-5.121546	-1.432567	1.721533
C	-2.970354	-7.407716	3.285054
H	-3.225990	-8.028972	2.417945
H	-1.989106	-7.739181	3.639385
H	-3.701605	-7.623850	4.069792
C	7.635268	-2.885339	4.790376
H	7.585191	-3.910266	4.409721
H	8.691134	-2.619944	4.903898
H	7.194540	-2.892309	5.795090
C	7.565407	2.259115	1.620943
H	6.724001	2.226112	0.928670
H	7.931411	3.291862	1.639580
H	8.388035	1.627210	1.260264
C	8.282874	2.062198	3.976478
H	9.171324	1.486367	3.693555
H	8.553820	3.122713	3.951745
H	8.024003	1.812231	5.010260
C	3.705039	-1.639425	-4.080521
H	3.206697	-0.980076	-3.368563
H	3.782332	-1.119407	-5.043187
H	3.090162	-2.531717	-4.220528
C	-6.468216	-3.770179	3.818468
H	-6.192998	-4.286215	4.743059
H	-7.313459	-3.113348	4.052857
H	-6.811073	-4.517286	3.094925
C	-4.883676	-1.938557	4.354750
H	-4.079082	-1.295616	3.992240
H	-5.724191	-1.309897	4.671744
H	-4.521466	-2.485125	5.231370

C	5.741322	-2.947479	-4.611883
H	5.143527	-3.846485	-4.790599
H	5.819576	-2.412787	-5.564187
H	6.751159	-3.256715	-4.318466
C	-3.935863	-5.472084	-2.381332
H	-3.901944	-6.408214	-1.814239
H	-4.101960	-4.653639	-1.678725
H	-4.784391	-5.520923	-3.073737
C	-2.693007	-3.995980	-4.001010
H	-3.523937	-4.050262	-4.714107
H	-2.838613	-3.126400	-3.363657
H	-1.765196	-3.856403	-4.566342
C	-2.475689	-6.454942	-4.119597
H	-2.424461	-7.411132	-3.588480
H	-3.346969	-6.487611	-4.782461
H	-1.585473	-6.361816	-4.750848
N	0.647590	-0.029225	-0.363334
N	-0.408741	-0.354610	-0.940374
K	-0.628720	0.262563	1.997835
K	6.762407	-0.016333	-0.542173
K	-6.480389	0.676949	0.445543
O	-8.369071	2.459116	-0.202712
C	-8.707228	3.355084	0.833585
H	-9.676832	3.835240	0.637850
H	-7.938471	4.129921	0.950436
H	-8.774642	2.768774	1.752885
C	-8.292547	3.097876	-1.461114
H	-9.259751	3.546837	-1.729046
H	-8.023363	2.341571	-2.200568
H	-7.520040	3.877489	-1.458846
O	-8.663396	0.228996	2.117127
C	-8.793009	-0.218407	3.447922
H	-9.605767	0.313123	3.963093
H	-7.850567	-0.015147	3.959077
H	-8.997311	-1.297731	3.488825
C	-9.837393	-0.007040	1.367635
H	-10.712357	0.444233	1.856735
H	-10.018909	-1.083847	1.243321
H	-9.699491	0.464782	0.392892
O	8.591472	-2.010108	-0.349377
C	8.346586	-2.895284	0.727091
H	9.212777	-3.552218	0.893541
H	7.455435	-3.508258	0.537738
H	8.174601	-2.290930	1.619382
C	8.846094	-2.702089	-1.552018
H	9.042266	-1.949982	-2.319601
H	7.980056	-3.310717	-1.847013
H	9.726140	-3.354147	-1.451338
O	8.927732	0.691051	-2.092436
C	10.128647	0.727769	-1.352027
H	10.347333	1.745306	-0.997897
H	10.975380	0.376520	-1.959069
H	10.004091	0.053453	-0.502174
C	9.020094	1.419814	-3.294592
H	9.224855	2.483352	-3.105348
H	8.061428	1.327969	-3.808191
H	9.814771	1.016786	-3.938735
Si	-0.208008	-0.558378	-2.783356
C	0.847687	0.808229	-3.496973
H	0.257945	1.714851	-3.653139
H	1.248980	0.488200	-4.464965
H	1.699086	1.070468	-2.862346
C	0.568284	-2.245321	-2.960952
H	-0.100639	-3.038273	-2.622974
H	1.488647	-2.304394	-2.372844
H	0.820897	-2.438889	-4.008254
C	-1.905369	-0.487231	-3.603497
H	-1.814171	-0.927453	-4.603280
H	-2.233910	0.547191	-3.728406
H	-2.714457	-1.047155	-3.122720

Complex 6 – Quintet

SCF Energy (a.u.): -8522.523143

Ce	-2.932668	1.169469	0.351576
Ce	2.925669	-0.918314	0.101051
O	3.308187	-2.518393	1.574857
O	-3.281160	-0.884833	-0.891180
O	-4.835896	0.499319	1.453193
O	1.727557	-1.998813	-1.517437
C	-2.469226	-2.807867	2.270974
C	0.404686	-3.839662	-0.785108
C	-3.839572	-2.088222	-0.841393
C	-5.348637	-0.304077	2.390031
C	-4.791534	-1.600655	2.587454
C	-2.306891	-3.310659	3.561348
H	-3.057346	-3.138043	4.324370
C	-5.373724	-2.468080	3.507506
H	-4.969516	-3.469999	3.621718
C	2.053227	-4.468737	1.053001
C	-1.433801	-2.994955	1.356167
H	-1.542458	-2.578489	0.360160
C	3.203855	-3.849512	1.591441
C	0.934329	-3.023611	-1.823265
C	-0.264590	-3.672980	1.665718
C	-6.990181	-0.814002	4.091252
H	-7.843080	-0.522785	4.695691
C	-1.150394	-4.025751	3.880597
H	-1.034216	-4.425598	4.884284
C	0.862373	-3.625367	0.645005
H	1.166411	-2.577024	0.710291
C	-3.634591	-2.009034	1.706745
H	-3.162651	-1.080843	1.387179
C	-6.468074	-2.092137	4.283354
C	-0.520201	-4.833267	-1.085748
H	-0.953223	-5.407109	-0.268778
C	-0.135939	-4.217204	2.947177
H	0.767210	-4.755097	3.216690
C	1.968276	-5.857771	1.008454
H	1.081821	-6.313514	0.572972
C	-4.687716	-3.943702	0.528360
H	-4.824283	-4.374771	1.517768
C	-4.095008	-2.690279	0.424877

C	-0.926639	-5.088432	-2.392839
C	-0.352490	-4.325051	-3.407696
H	-0.642010	-4.549820	-4.429245
C	-5.078440	-4.661068	-0.594940
C	-4.177977	-2.259279	-3.440600
C	2.978298	-6.667915	1.514529
C	-4.858015	-4.061508	-1.833994
H	-5.173065	-4.613202	-2.713537
C	-6.472431	0.095229	3.163661
C	-7.085760	1.492054	3.010836
C	-4.249512	-2.813611	-2.007543
C	4.081439	-6.040995	2.098547
H	4.856434	-6.673265	2.521321
C	0.576866	-3.303894	-3.173942
C	4.227100	-4.655963	2.156401
C	-5.436846	-1.413872	-3.677462
H	-6.340789	-2.002669	-3.481624
H	-5.478096	-1.054888	-4.712334
H	-5.432088	-0.526550	-3.037627
C	5.457724	-4.009446	2.797531
C	1.276340	-2.602717	-4.350657
C	-6.037186	2.553591	3.370230
H	-5.698161	2.424150	4.402726
H	-6.460574	3.559585	3.273237
H	-5.168347	2.488103	2.715374
C	-1.943515	-6.154254	-2.688172
H	-1.677785	-7.104198	-2.211419
H	-2.029410	-6.335381	-3.764017
H	-2.934048	-5.867228	-2.316258
C	-5.652252	-6.046249	-0.488563
H	-4.859702	-6.804690	-0.480199
H	-6.308850	-6.277587	-1.333793
H	-6.229808	-6.174366	0.432723
C	6.235948	-3.255277	1.711758
H	6.585807	-3.947170	0.939904
H	7.110782	-2.745702	2.134342
H	5.581719	-2.523198	1.233616
C	2.896838	-8.165993	1.425868
H	3.389323	-8.543485	0.520908
H	1.857608	-8.507135	1.394388
H	3.382108	-8.645447	2.282076
C	-7.053112	-3.027828	5.303944
H	-7.015114	-4.067606	4.962940
H	-8.097181	-2.782054	5.519833
H	-6.505547	-2.980921	6.253208
C	-7.569425	1.721146	1.569863
H	-6.727997	1.698607	0.875949
H	-8.047668	2.702966	1.480049
H	-8.313164	0.965207	1.285624
C	-8.293091	1.698763	3.930341
H	-9.100985	0.990309	3.715148
H	-8.687931	2.708880	3.781740
H	-8.022896	1.604105	4.986736
C	-2.942425	-1.393908	-3.705239
H	-2.963632	-0.497258	-3.085335
H	-2.925949	-1.089900	-4.758168
H	-2.039527	-1.988129	-3.519879
C	6.407616	-5.039786	3.413154
H	5.919040	-5.623143	4.200349
H	7.259808	-4.520030	3.865783
H	6.803145	-5.733842	2.664239
C	5.033136	-3.042560	3.914110
H	4.368752	-2.267183	3.530544
H	5.916701	-2.568264	4.359936
H	4.507448	-3.584423	4.707123
C	-4.149440	-3.379788	-4.491592
H	-3.332614	-4.080471	-4.294853
H	-3.988804	-2.937942	-5.480425
H	-5.086035	-3.942441	-4.545418
C	2.780820	-2.884417	-4.250624
H	2.975637	-3.961380	-4.270646
H	3.181204	-2.477328	-3.322283
H	3.312788	-2.420471	-5.089944
C	1.078928	-1.079101	-4.357676
H	1.610803	-0.637697	-5.207185
H	1.495009	-0.621654	-3.457845
H	0.021243	-0.812328	-4.483557
C	0.780715	-3.119619	-5.704613
H	0.960559	-4.192651	-5.822247
H	1.321774	-2.603852	-6.504679
H	-0.289016	-2.929767	-5.850622
O	-2.998904	1.879242	-1.806615
O	4.052737	0.873543	1.134059
O	4.890529	-0.828300	-1.221176
O	-2.410946	3.233411	1.027541
C	2.775543	2.351825	-2.260282
C	-0.484328	4.261012	0.103033
C	4.468821	2.122436	0.941158
C	5.497973	-0.100514	-2.156869
C	5.109336	1.255408	-2.365535
C	2.625913	2.325622	-3.646570
H	3.441018	1.979864	-4.273023
C	5.755391	2.048809	-3.307862
H	5.435244	3.081313	-3.433713
C	-1.900137	3.984316	-1.875271
C	1.695039	2.753701	-1.469965
H	1.800204	2.746154	-0.387915
C	-3.017839	3.175598	-2.163440
C	-1.502385	4.209833	1.091194
C	0.478675	3.141447	-2.028825
C	7.174909	0.228129	-3.880238
H	7.988748	-0.156072	-4.486298
C	1.418352	2.720035	-4.219376
H	1.305888	2.702341	-5.300245
C	-0.711115	3.414838	-1.130235
H	-0.989209	2.419111	-0.764275
C	3.986767	1.811730	-1.523780
H	3.597429	0.935162	-1.028491
C	6.790983	1.553179	-4.092193
C	0.573805	5.148837	0.225005
H	1.355252	5.154205	-0.531402
C	0.351538	3.126077	-3.423728

H	-0.587863	3.429744	-3.874921
C	-1.875664	5.325759	-2.240289
H	-1.000058	5.917710	-1.981919
C	4.829873	3.999664	-0.586874
H	4.751563	4.409656	-1.592193
C	4.445448	2.682023	-0.368792
C	0.654343	6.028993	1.304267
C	-0.415502	6.058339	2.194263
H	-0.383863	6.788736	2.996561
C	5.292694	4.803444	0.450946
C	5.036216	2.392582	3.452174
C	-2.951390	5.922047	-2.886478
C	5.365219	4.232904	1.723510
H	5.737139	4.858722	2.528610
C	6.576265	-0.617223	-2.941863
C	7.093303	-2.052664	-2.769933
C	4.973447	2.921630	2.011052
C	-4.061729	5.122490	-3.152803
H	-4.907862	5.588514	-3.647390
C	-1.515619	5.196546	2.106467
C	-4.134058	3.770774	-2.810299
C	5.831698	1.082218	3.550836
H	6.865793	1.218557	3.211783
H	5.874729	0.754827	4.596057
H	5.340419	0.289434	2.982601
C	-5.368674	2.950530	-3.183852
C	-2.705482	5.338723	3.059878
C	5.963879	-3.066327	-2.989764
H	5.577790	-2.996068	-4.010424
H	6.336616	-4.085861	-2.836288
H	5.142764	-2.887044	-2.295634
C	1.856882	6.911658	1.485604
H	2.125328	7.423285	0.554015
H	1.680880	7.675839	2.248432
H	2.732606	6.326467	1.794229
C	5.667848	6.240416	0.220191
H	4.791703	6.897155	0.285085
H	6.390500	6.589655	0.964151
H	6.108251	6.385953	-0.771287
C	-5.902496	2.188902	-1.960406
H	-6.078637	2.876642	-1.126057
H	-6.851995	1.693874	-2.196583
H	-5.163780	1.444102	-1.655642
C	-2.936928	7.382328	-3.240937
H	-3.146249	8.009182	-2.365466
H	-1.961154	7.690322	-3.630184
H	-3.690172	7.616612	-3.999246
C	7.456952	2.399047	-5.140957
H	7.434258	3.459760	-4.872145
H	8.503065	2.110600	-5.283835
H	6.959583	2.301977	-6.114092
C	7.652791	-2.242841	-1.353888
H	6.843445	-2.176363	-0.627628
H	8.100740	-3.237327	-1.247407
H	8.433172	-1.502411	-1.135037
C	8.218719	-2.390939	-3.752567
H	9.101047	-1.757670	-3.607610
H	8.527796	-3.429368	-3.595211
H	7.893210	-2.297910	-4.793542
C	3.612142	2.134733	3.953058
H	3.106118	1.414754	3.308899
H	3.629459	1.737501	4.975250
H	3.034575	3.062757	3.954234
C	-6.518371	3.816189	-3.707722
H	-6.253790	4.335246	-4.633723
H	-7.379466	3.175661	-3.929718
H	-6.833475	4.562858	-2.971256
C	-4.968688	1.969063	-4.293036
H	-4.162799	1.315480	-3.953014
H	-5.820977	1.351481	-4.600743
H	-4.617972	2.521833	-5.170432
C	5.700819	3.389675	4.406495
H	5.141660	4.327855	4.474053
H	5.734285	2.956467	5.411471
H	6.729747	3.620654	4.107369
C	-3.988620	5.509482	2.230107
H	-3.925896	6.414364	1.616637
H	-4.140586	4.657723	1.565339
H	-4.858557	5.602519	2.891274
C	-2.824240	4.106647	3.965134
H	-3.700772	4.193814	4.617848
H	-2.925436	3.201299	3.368677
H	-1.937057	4.004716	4.599357
C	-2.579461	6.566391	3.966389
H	-2.487167	7.491726	3.388207
H	-3.478154	6.647648	4.587231
H	-1.719875	6.493429	4.641209
N	0.581993	0.085103	0.506880
N	-0.522714	0.376083	1.072420
K	-0.637990	-0.371527	-1.895017
K	6.696357	0.083863	0.667731
K	-6.451873	-0.732899	-0.464413
O	-8.314573	-2.552137	0.160228
C	-8.634996	-3.437851	-0.890399
H	-9.593927	-3.941718	-0.701685
H	-7.850060	-4.194223	-1.020928
H	-8.716502	-2.837826	-1.799681
C	-8.224632	-3.209491	1.408062
H	-9.182793	-3.681333	1.669228
H	-7.969494	-2.460202	2.159514
H	-7.437176	-3.973869	1.392795
O	-8.650648	-0.285146	-2.111991
C	-8.786691	0.193154	-3.431226
H	-9.598760	-0.329693	-3.956329
H	-7.844935	0.006475	-3.949761
H	-8.995739	1.272248	-3.446104
C	-9.823600	-0.074838	-1.353439
H	-10.697248	-0.520040	-1.850430
H	-10.011690	0.997499	-1.202810
H	-9.678946	-0.568805	-0.390744
O	8.589741	1.918133	0.148749
C	8.376963	2.595789	-1.075573

H	9.266205	3.178437	-1.356584
H	7.509613	3.265209	-1.008462
H	8.181876	1.842457	-1.841188
C	8.841909	2.809770	1.213239
H	8.999169	2.203622	2.108891
H	7.989651	3.484232	1.373926
H	9.744051	3.408180	1.019546
O	8.796362	-0.509973	2.346985
C	10.022718	-0.651043	1.662241
H	10.226034	-1.704948	1.424596
H	10.855534	-0.258230	2.263032
H	9.946792	-0.068486	0.741777
C	8.823394	-1.119839	3.616961
H	9.018589	-2.199130	3.539833
H	7.844812	-0.967580	4.075736
H	9.595852	-0.666575	4.254606
Si	-0.367417	0.649657	2.853990
C	0.731519	-0.681612	3.578357
H	0.339263	-1.681052	3.374505
H	0.788898	-0.556246	4.665764
H	1.754865	-0.633759	3.193079
C	0.364064	2.340962	3.143024
H	-0.364309	3.135056	2.978575
H	1.199264	2.518821	2.460479
H	0.739186	2.420696	4.168823
C	-2.073357	0.495363	3.633120
H	-2.001917	0.918086	4.642289
H	-2.365063	-0.552909	3.732239
H	-2.898519	1.036690	3.158721

Complex 2 – Quintet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -8702.990597

Ce	2.743717	1.182734	-0.121572
Ce	-2.743709	-1.182725	0.121565
O	-2.610846	-2.048082	-2.053102
O	3.719316	-0.768653	0.877095
O	4.781261	0.977859	-1.327687
O	-1.777497	-2.822383	1.353133
C	2.752258	-2.333134	-2.473825
C	-0.078820	-4.137128	0.353135
C	4.181433	-1.990275	0.674398
C	5.396899	0.333918	-2.312641
C	4.998971	-0.994235	-2.652476
C	2.534056	-2.495681	-3.843165
H	3.258842	-2.125103	-4.560699
C	5.648817	-1.690586	-3.665621
H	5.335872	-2.707963	-3.893008
C	-1.745759	-4.208989	-1.552378
C	1.766200	-2.767494	-1.584464
H	1.904463	-2.597702	-0.520926
C	-2.740806	-3.382678	-2.130139
C	-0.782551	-3.685354	1.501568
C	0.585816	-3.368611	-2.006546
C	7.089081	0.168447	-4.038041
H	7.912559	0.608268	-4.591899
C	1.370242	-3.135271	-4.283631
H	1.215027	-3.284971	-5.349392
C	-0.510293	-3.563582	-0.974413
H	-0.764955	-2.524180	-0.730194
C	3.915832	-1.616837	-1.813255
H	3.435595	-0.771872	-1.327513
C	6.693947	-1.121882	-4.390286
C	0.962118	-5.048642	0.472532
H	1.500351	-5.354864	-0.422546
C	0.402892	-3.578009	-3.380410
H	-0.505010	-4.058950	-3.733184
C	-1.862336	-5.592490	-1.585370
H	-1.084767	-6.188794	-1.112136
C	4.995454	-3.698614	-0.876252
H	5.146509	-4.024674	-1.903880
C	4.422724	-2.450225	-0.647677
C	1.348838	-5.549969	1.714134
C	0.663704	-5.087457	2.836565
H	0.975360	-5.464484	3.806127
C	5.346982	-4.542866	0.169876
C	-2.946777	-6.214605	-2.197727
C	5.057038	-4.108168	1.467955
H	5.285720	-4.783127	2.287015
C	6.487479	0.914883	-3.020990
C	4.475959	-2.876083	1.756592
C	-3.911526	-5.394776	-2.781626
H	-4.755197	-5.877759	-3.265081
C	-0.383307	-4.164239	2.776597
C	-3.849979	-3.999779	-2.764631
O	2.610864	2.048081	2.053095
O	-3.719306	0.768662	-0.877100
O	-4.781265	-0.977854	1.327665
O	1.777505	2.822409	-1.353116
C	-2.752262	2.333126	2.473833
C	0.078806	4.137117	-0.353111
C	-4.181422	1.990284	-0.674399
C	-5.396902	-0.333921	2.312623
C	-4.998974	0.994229	2.652469
C	-2.534063	2.495664	3.843174
H	-3.258853	2.125083	4.560703
C	-5.648817	1.690570	3.665623
H	-5.335869	2.707944	3.893019
C	1.745755	4.208988	1.552399
C	-1.766202	2.767491	1.584477
H	-1.904463	2.597708	0.520937
C	2.740812	3.382678	2.130146
C	0.782548	3.685368	-1.501547
C	-0.585818	3.368601	2.006566
C	-7.089079	-0.168467	4.038031
H	-7.912554	-0.608296	4.591888
C	-1.370250	3.135249	4.283647
H	-1.215036	3.284941	5.349410
C	0.510290	3.563576	0.974434
H	0.764959	2.524176	0.730214
C	-3.915832	1.616834	1.813254
H	-3.435593	0.771872	1.327510

C	-6.693944	1.121859	4.390287
C	-0.962169	5.048590	-0.472506
H	-1.500417	5.354784	0.422574
C	-0.402896	3.577991	3.380431
H	0.505007	4.058926	3.733211
C	1.862321	5.592489	1.585407
H	1.084744	6.188792	1.112183
C	-4.995444	3.698617	0.876256
H	-5.146501	4.024673	1.903885
C	-4.422718	2.450228	0.647677
C	-1.348920	5.549895	-1.714107
C	-0.663766	5.087415	-2.836540
H	-0.975446	5.464422	-3.806102
C	-5.346958	4.542879	-0.169869
C	2.946760	6.214606	2.197765
C	-5.057010	4.108188	-1.467948
H	-5.285678	4.783155	-2.287005
C	-6.487481	-0.914891	3.020970
C	-4.475940	2.876100	-1.756590
C	3.911519	5.394778	2.781648
H	4.755190	5.877763	3.265102
C	0.383286	4.164245	-2.776574
C	3.849984	3.999780	2.764638
N	-0.585990	-0.187791	0.053364
N	0.585997	0.187793	-0.053368
K	0.428440	0.437205	2.717283
K	-0.428436	-0.437210	-2.717293
K	-6.462124	0.199695	-0.578861
K	6.462134	-0.199686	0.578835
O	8.505716	-1.740203	-0.186182
O	8.404700	0.054596	2.557308
O	-8.505714	1.740197	0.186165
O	-8.404689	-0.054589	-2.557336
C	4.155770	-2.473940	3.191164
C	6.980446	2.321152	-2.691771
C	5.042275	-1.282604	3.610611
H	6.103357	-1.549277	3.508003
H	4.846011	-1.018051	4.658178
H	4.808886	-0.413858	2.989929
C	-4.951176	-3.160169	-3.396698
C	-1.089046	-3.693611	4.043066
C	5.850284	3.344520	-2.928584
H	5.558073	3.347427	-3.984768
H	6.192559	4.351056	-2.654376
H	4.980026	3.083922	-2.323411
C	2.458004	-6.556099	1.834394
H	2.105983	-7.577567	1.624286
H	2.884313	-6.555850	2.846729
H	3.267297	-6.330061	1.128830
C	5.991298	-5.879125	-0.072773
H	6.037087	-6.102604	-1.146066
H	5.430593	-6.688769	0.415135
H	7.019237	-5.913512	0.319419
C	-5.613591	-2.292729	-2.307240
H	-6.003601	-2.929947	-1.503846
H	-6.439304	-1.713851	-2.737677
H	-4.858807	-1.609227	-1.908117
C	-3.074885	-7.711702	-2.217911
H	-3.234997	-8.112821	-1.206530
H	-2.167516	-8.187644	-2.615372
H	-3.921837	-8.027574	-2.840281
C	7.365829	-1.868958	-5.507922
H	7.509979	-2.928069	-5.253358
H	8.348990	-1.438248	-5.737427
H	6.769045	-1.835683	-6.431843
C	7.424482	2.418419	-1.214825
H	6.557534	2.266065	-0.568146
H	7.832006	3.417810	-1.015164
H	8.208617	1.677533	-0.999914
C	8.185021	2.744080	-3.553282
H	9.043715	2.078166	-3.397558
H	8.479902	3.760147	-3.264479
H	7.928195	2.755342	-4.619058
C	2.673287	-2.056529	3.302972
H	2.495924	-1.260851	2.575294
H	2.472142	-1.702449	4.325105
H	2.018114	-2.904431	3.078168
C	-6.062287	-4.010038	-4.039321
H	-5.666557	-4.639922	-4.844699
H	-6.813458	-3.335416	-4.470016
H	-6.557266	-4.647496	-3.296382
C	-4.368750	-2.240885	-4.492570
H	-3.598623	-1.597643	-4.060024
H	-5.164138	-1.615244	-4.919390
H	-3.930550	-2.848720	-5.293849
C	4.387120	-3.616652	4.195356
H	3.777541	-4.490352	3.936373
H	4.089110	-3.271032	5.193126
H	5.443453	-3.911330	4.238851
C	-2.568329	-4.128072	3.998644
H	-2.634667	-5.222509	3.982965
H	-3.041355	-3.728904	3.100451
H	-3.098522	-3.752685	4.884184
C	-1.021581	-2.152414	4.163370
H	-1.596532	-1.818351	5.037082
H	-1.447668	-1.709165	3.258154
H	0.027288	-1.851827	4.295364
C	-0.463217	-4.270208	5.326035
H	-0.535620	-5.363946	5.346803
H	-1.010624	-3.875483	6.191209
H	0.591251	-3.979764	5.419776
C	-4.155735	2.473977	-3.191164
C	-6.980449	-2.321157	2.691743
C	-5.042243	1.282656	-3.610647
H	-6.103325	1.549340	-3.508063
H	-4.845956	1.018113	-4.658212
H	-4.808881	0.413901	-2.989968
C	4.951190	3.160169	3.396687
C	1.089029	3.693636	-4.043046
C	-5.850290	-3.344529	2.928556
H	-5.558083	-3.347442	3.984742
H	-6.192567	-4.351064	2.654344

H	-4.980028	-3.083933	2.323388
C	-2.458147	6.555957	-1.834365
H	-2.106199	7.577439	-1.624201
H	-2.884419	6.555723	-2.846715
H	-3.267451	6.329840	-1.128839
C	-5.991255	5.879147	0.072785
H	-6.037048	6.102620	1.146079
H	-5.430532	6.688785	-0.415114
H	-7.019191	5.913553	-0.319415
C	5.613604	2.292747	2.307214
H	6.003598	2.929976	1.503822
H	6.439327	1.713874	2.737638
H	4.858822	1.609241	1.908093
C	3.074855	7.711704	2.217967
H	3.234941	8.112838	1.206587
H	2.167489	8.187632	2.615454
H	3.921817	8.027575	2.840322
C	-7.365821	1.868923	5.507933
H	-7.509963	2.928039	5.253385
H	-8.348985	1.438217	5.737431
H	-6.769038	1.835630	6.431854
C	-7.424484	-2.418415	1.214795
H	-6.557536	-2.266057	0.568118
H	-7.832010	-3.417804	1.015128
H	-8.208618	-1.677526	0.999888
C	-8.185026	-2.744078	3.553254
H	-9.043723	-2.078170	3.397517
H	-8.479902	-3.760150	3.264462
H	-7.928205	-2.755324	4.619031
C	-2.673252	2.056560	-3.302959
H	-2.495896	1.260874	-2.575288
H	-2.472098	1.702491	-4.325094
H	-2.018078	2.904457	-3.078140
C	6.062302	4.010031	4.039318
H	5.666575	4.639896	4.844714
H	6.813480	3.335405	4.469992
H	6.557270	4.647508	3.296389
C	4.368772	2.240864	4.492546
H	3.598648	1.597623	4.059991
H	5.164165	1.615222	4.919355
H	3.930570	2.848684	5.293835
C	-4.387062	3.616709	-4.195336
H	-3.777482	4.490400	-3.936327
H	-4.089040	3.271107	-5.193108
H	-5.443393	3.911394	-4.238841
C	2.568303	4.128129	-3.998636
H	2.634618	5.222567	-3.982962
H	3.041342	3.728975	-3.100445
H	3.098500	3.752749	-4.884178
C	1.021590	2.152438	-4.163351
H	1.596545	1.818382	-5.037063
H	1.447682	1.709193	-3.258135
H	-0.027274	1.851838	-4.295344
C	0.463177	4.270222	-5.326009
H	0.535568	5.363961	-5.346780
H	1.010577	3.875501	-6.191189
H	-0.591289	3.979766	-5.419734
C	8.626728	-2.821305	0.736600
H	9.521866	-3.421915	0.516255
H	7.736940	-3.465318	0.700063
H	8.716947	-2.377275	1.732686
C	8.369151	-2.224371	-1.522904
H	9.269887	-2.779294	-1.825041
H	8.231704	-1.357308	-2.173706
H	7.488391	-2.873282	-1.610221
C	8.381599	0.474586	3.915961
H	9.195610	-0.001443	4.482721
H	7.419755	0.168660	4.334863
H	8.481251	1.567273	3.996176
C	9.637124	0.418388	1.938217
H	10.489885	0.008250	2.499474
H	9.739128	1.512508	1.882795
H	9.627494	-0.013737	0.933731
C	-8.369150	2.224361	1.522889
H	-9.269888	2.779280	1.825028
H	-7.488391	2.873274	1.610208
H	-8.231700	1.357295	2.173686
C	-8.626730	2.821302	-0.736613
H	-8.716948	2.377276	-1.732701
H	-7.736943	3.465317	-0.700073
H	-9.521869	3.421909	-0.516266
C	-9.637107	-0.418395	-1.938243
H	-9.739100	-1.512516	-1.882826
H	-10.489874	-0.008263	-2.499497
H	-9.627480	0.013727	-0.933756
C	-8.381588	-0.474571	-3.915991
H	-8.481229	-1.567259	-3.996210
H	-7.419747	-0.168633	-4.334894
H	-9.195605	0.001452	-4.482746

Complex 7 – Quartet

SCF Energy (a.u.): -9122.292023

Ce	-2.858338	1.216697	0.208631
Ce	2.757685	-0.809601	-0.206650
O	3.437541	-2.404167	1.457536
O	-3.209259	-0.996173	-0.851436
O	-4.791548	0.481724	1.338721
O	1.854836	-2.497677	-1.491927
C	-2.229714	-2.604016	2.505096
C	0.458452	-4.132384	-0.498586
C	-3.643795	-2.230954	-0.657647
C	-5.273110	-0.258698	2.331523
C	-4.602322	-1.461942	2.705576
C	-2.062942	-3.027470	3.826450
H	-2.788327	-2.767110	4.587938
C	-5.133549	-2.274787	3.703834
H	-4.646002	-3.215748	3.941300
C	2.244579	-4.456702	1.224441
C	-1.206899	-2.877443	1.598902
H	-1.291629	-2.496086	0.586077
C	3.447776	-3.737799	1.456157
C	1.004807	-3.496306	-1.645863

C	-0.082963	-3.624977	1.922111
C	-6.943538	-0.760518	4.018446
H	-7.857585	-0.503305	4.543707
C	-0.957273	-3.810975	4.167423
H	-0.870521	-4.190741	5.183125
C	0.985553	-3.704590	0.853677
H	1.271463	-2.656174	0.736291
C	-3.411613	-1.880504	1.876157
H	-2.973330	-0.972682	1.462022
C	-6.293084	-1.934117	4.394589
C	-0.475131	-5.153303	-0.621459
H	-0.903522	-5.589116	0.279979
C	0.015892	-4.139152	3.219967
H	0.833259	-4.814241	3.471594
C	2.227641	-5.846183	1.300290
H	1.295658	-6.365365	1.086277
C	-4.360937	-3.977725	0.924347
H	-4.464901	-4.299708	1.958356
C	-3.843467	-2.712140	0.671360
C	-0.877205	-5.620926	-1.870419
C	-0.307742	-5.022366	-2.993687
H	-0.597159	-5.407430	-3.966730
C	-4.728515	-4.837724	-0.101223
C	3.370225	-6.578227	1.606002
C	-4.541649	-4.374294	-1.401903
H	-4.825433	-5.039642	-2.210602
C	-6.487315	0.080796	2.999875
C	-3.999744	-3.126288	-1.724163
C	4.552487	-5.867934	1.817362
H	5.448328	-6.440374	2.037331
C	0.616920	-3.975156	-2.929003
C	4.634797	-4.475586	1.743986
O	-2.824432	1.785853	-2.014051
O	4.374264	0.644932	0.969620
O	4.031649	-0.204137	-2.119729
O	-2.794629	3.393549	0.887651
C	2.646331	3.194605	-1.847685
C	-1.048391	4.732058	0.010173
C	4.346576	1.935894	1.285436
C	4.969100	0.672987	-2.396269
C	4.887729	1.995665	-1.876022
C	2.873377	3.846872	-3.057873
H	3.861269	3.827396	-3.508034
C	5.916878	2.913403	-2.066643
H	5.817341	3.901403	-1.619626
C	-2.222191	4.091193	-2.063200
C	1.365749	3.209681	-1.302538
H	1.187325	2.691650	-0.362795
C	-3.083686	3.038374	-2.438181
C	-2.078886	4.517908	0.959636
C	0.305124	3.853680	-1.927691
C	7.134064	1.296448	-3.323854
H	8.017275	1.040171	-3.902025
C	1.816188	4.493134	-3.698485
H	1.990926	4.994816	-4.646759
C	-1.016859	3.817829	-1.195408
H	-1.083734	2.790590	-0.822524
C	3.664137	2.375877	-1.088088
H	3.124293	1.445665	-0.930222
C	7.065795	2.586198	-2.784892
C	-0.176426	5.809261	0.121438
H	0.619340	5.920137	-0.611373
C	0.537133	4.496449	-3.146415
H	-0.281673	4.990735	-3.659410
C	-2.492187	5.402300	-2.443517
H	-1.832533	6.190253	-2.085690
C	3.881143	4.243821	0.605924
H	3.546980	4.933240	-0.166890
C	3.976920	2.894227	0.297326
C	-0.314129	6.744871	1.140677
C	-1.400760	6.595794	2.000011
H	-1.548382	7.359154	2.757318
C	4.156639	4.718591	1.887727
C	-3.595432	5.724096	-3.224441
C	4.567397	3.789366	2.840610
H	4.797517	4.162163	3.833654
C	6.129420	0.336497	-3.166573
C	4.686101	2.418994	2.582828
C	-4.442478	4.681131	-3.592165
H	-5.316707	4.929989	-4.184949
C	-2.310796	5.538204	1.925189
C	-4.229459	3.352875	-3.217953
N	0.753372	0.147403	0.217630
N	-0.444020	0.584828	0.653377
K	-0.572399	-0.116672	-2.101197
K	6.860041	0.549653	-0.096035
K	-6.266772	-1.035324	-0.523804
O	-8.039864	-2.891264	0.274317
O	-8.475713	-0.978166	-2.286651
O	8.322880	2.618093	0.788265
O	9.212347	-0.750649	0.393983
Si	-0.208793	1.051034	2.360595
C	0.674321	-0.336638	3.278418
H	0.026034	-1.214494	3.352100
H	0.975600	0.002888	4.276206
H	1.552572	-0.556829	2.665501
C	0.786326	2.628359	2.533470
H	0.268419	3.477458	2.075825
H	1.763827	2.528092	2.051472
H	0.957548	2.868375	3.589335
C	-1.870823	1.233375	3.244053
H	-1.666172	1.545645	4.275003
H	-2.440981	0.300248	3.307449
H	-2.499960	2.026022	2.830324
K	2.600461	-2.482264	3.944059
C	-3.905785	-2.773414	-3.217590
C	-7.268955	1.350851	2.645279
C	-5.188038	-2.037255	-3.626074
H	-6.072685	-2.636771	-3.380646
H	-5.197073	-1.840879	-4.704848
H	-5.256231	-1.067312	-3.127489
C	5.972340	-3.760103	1.961277

C	1.300955	-3.457737	-4.197788
C	-6.399716	2.573390	2.948403
H	-6.129761	2.599788	4.008229
H	-6.937242	3.497062	2.708368
H	-5.481961	2.549401	2.361231
C	-1.872403	-6.739304	-1.996718
H	-1.587136	-7.602960	-1.385006
H	-1.954808	-7.081162	-3.033123
H	-2.869355	-6.423463	-1.670025
C	-5.233228	-6.226854	0.172990
H	-4.404567	-6.930105	0.323299
H	-5.830620	-6.609770	-0.661002
H	-5.853096	-6.262690	1.075308
C	6.307983	-2.901867	0.733321
H	6.363109	-3.519798	-0.167208
H	7.275513	-2.402813	0.868238
H	5.533440	-2.146720	0.586574
C	3.346246	-8.080531	1.648450
H	3.418873	-8.509443	0.641537
H	2.417499	-8.455105	2.090352
H	4.181312	-8.477995	2.233310
C	-6.821600	-2.798020	5.505068
H	-6.586106	-3.854046	5.337049
H	-7.908138	-2.707400	5.600740
H	-6.388479	-2.521412	6.474527
C	-7.656326	1.371531	1.158670
H	-6.761453	1.405431	0.535267
H	-8.249942	2.264835	0.934566
H	-8.270521	0.498002	0.903971
C	-8.567127	1.482012	3.447720
H	-9.249032	0.642530	3.269646
H	-9.081625	2.400140	3.146289
H	-8.378401	1.551785	4.523522
C	-2.695402	-1.893571	-3.533928
H	-2.810093	-0.929525	-3.040964
H	-2.619712	-1.737160	-4.616222
H	-1.782729	-2.399594	-3.197333
C	7.132519	-4.736648	2.172269
H	6.999071	-5.349494	3.069962
H	8.062614	-4.170481	2.297090
H	7.261452	-5.405166	1.315233
C	5.895267	-2.855077	3.198857
H	5.166061	-2.060244	3.032804
H	6.861952	-2.377582	3.395996
H	5.632265	-3.441303	4.089727
C	-3.777748	-4.024272	-4.100410
H	-2.942017	-4.648215	-3.773092
H	-3.588215	-3.712674	-5.133113
H	-4.687204	-4.632530	-4.116192
C	2.783855	-3.852898	-4.121575
H	2.878486	-4.939462	-4.025045
H	3.259048	-3.382981	-3.257954
H	3.312847	-3.539312	-5.027879
C	1.186556	-1.931376	-4.338297
H	1.713628	-1.592967	-5.237487
H	1.636665	-1.433132	-3.477340
H	0.134394	-1.639513	-4.452584
C	0.708628	-4.069717	-5.470481
H	0.842279	-5.155566	-5.505359
H	1.217479	-3.647714	-6.343624
H	-0.361132	-3.850616	-5.566888
C	5.159943	1.466317	3.684418
C	6.239388	-1.030813	-3.841633
C	6.413972	0.706229	3.227241
H	7.191066	1.406237	2.900173
H	6.818259	0.098843	4.046255
H	6.152257	0.032798	2.409419
C	-5.214326	2.269655	-3.652263
C	-3.568582	5.556236	2.796615
C	5.066399	-1.173632	-4.822362
H	5.110291	-0.384960	-5.580996
H	5.111511	-2.142577	-5.331553
H	4.116293	-1.098308	-4.291766
C	0.620665	7.915710	1.265886
H	1.511708	7.776558	0.646557
H	0.144073	8.852163	0.949384
H	0.953180	8.061286	2.299948
C	3.957640	6.164775	2.240694
H	2.901290	6.373628	2.447074
H	4.529686	6.444141	3.130957
H	4.261029	6.826362	1.422635
C	-5.731102	1.511809	-2.419273
H	-6.102819	2.216358	-1.666455
H	-6.558513	0.848650	-2.697174
H	-4.914997	0.923944	-1.990800
C	-3.861656	7.138236	-3.657166
H	-3.580844	7.851733	-2.876090
H	-3.290102	7.401718	-4.556252
H	-4.920110	7.292495	-3.888598
C	8.165273	3.584980	-3.015553
H	8.146833	4.376961	-2.260357
H	9.153487	3.112819	-2.985256
H	8.071995	4.071794	-3.994251
C	6.190996	-2.155946	-2.798731
H	5.271953	-2.101132	-2.215243
H	6.232552	-3.136438	-3.286915
H	7.050542	-2.090392	-2.118599
C	7.538149	-1.194379	-4.635124
H	8.426334	-1.117019	-3.995800
H	7.552078	-2.186053	-5.098930
H	7.627511	-0.453197	-5.435985
C	4.046782	0.456401	3.990237
H	3.803467	-0.081844	3.069912
H	4.384150	-0.243859	4.770774
H	3.151032	0.974244	4.345313
C	-6.438028	2.835757	-4.378489
H	-6.163094	3.356596	-5.300651
H	-7.103582	2.010768	-4.656212
H	-7.003978	3.528446	-3.746429
C	-4.498813	1.312009	-4.614280
H	-3.638817	0.852227	-4.124643
H	-5.173837	0.520921	-4.959945

H	-4.144694	1.863026	-5.491494
C	5.509929	2.192068	4.985447
H	4.647885	2.721307	5.403327
H	5.844521	1.460639	5.729614
H	6.319949	2.914840	4.841784
C	-4.791265	5.509170	1.866390
H	-4.797141	6.385471	1.209755
H	-4.769268	4.615220	1.240738
H	-5.718622	5.512605	2.450990
C	-3.585425	4.373910	3.768837
H	-4.451872	4.437296	4.437609
H	-3.644248	3.433116	3.227860
H	-2.678150	4.366000	4.382346
C	-3.684531	6.833207	3.635623
H	-3.684972	7.734174	3.013610
H	-4.629563	6.809570	4.188958
H	-2.875935	6.919726	4.369650
C	-8.312016	-3.916984	-0.654746
H	-9.251505	-4.432683	-0.407505
H	-7.495432	-4.649866	-0.682247
H	-8.407073	-3.443012	-1.634312
C	-7.921808	-3.379159	1.595155
H	-8.856569	-3.860694	1.917429
H	-7.706881	-2.528876	2.244646
H	-7.097213	-4.098646	1.674627
C	-8.611589	-0.634773	-3.646928
H	-9.390985	-1.242248	-4.129095
H	-7.654677	-0.827328	-4.135127
H	-8.868337	0.427257	-3.767737
C	-9.672429	-0.757142	-1.570322
H	-10.512759	-1.292477	-2.035404
H	-9.917903	0.313490	-1.526960
H	-9.521565	-1.147085	-0.561953
C	7.694875	3.860688	1.032236
H	7.818850	4.536343	0.174758
H	8.115622	4.342245	1.926540
H	6.632842	3.672754	1.193502
C	9.697316	2.751723	0.523237
H	10.086760	1.751471	0.319514
H	10.230125	3.182362	1.384118
H	9.873600	3.392015	-0.352962
C	9.797031	-1.692339	-0.478457
H	9.518465	-2.718476	-0.200222
H	10.892652	-1.607148	-0.475061
H	9.425109	-1.483835	-1.483942
C	9.644603	-0.913155	1.725950
H	9.368141	-1.903500	2.116025
H	9.155164	-0.143028	2.325858
H	10.734426	-0.794509	1.805873

Complex 7 – Doublet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -9111.973926

Ce	-2.873249	1.198098	0.308311
Ce	2.722448	-0.818111	-0.067215
O	3.207089	-2.533889	1.501941
O	-3.314485	-0.885131	-0.900759
O	-4.762391	0.447700	1.475846
O	1.786035	-2.185888	-1.707853
C	-2.388894	-2.880507	2.214320
C	0.352059	-3.929217	-0.977223
C	-3.831685	-2.099045	-0.843870
C	-5.257198	-0.353542	2.412236
C	-4.693073	-1.649805	2.607307
C	-2.254479	-3.549927	3.433249
H	-2.990701	-3.426989	4.218134
C	-5.268331	-2.523326	3.525763
H	-4.877735	-3.532360	3.620581
C	2.091815	-4.514931	0.776089
C	-1.352554	-2.997358	1.288533
H	-1.420633	-2.430689	0.365933
C	3.224979	-3.855881	1.320289
C	0.907385	-3.124444	-2.013153
C	-0.244027	-3.809951	1.481413
C	-6.882162	-0.879712	4.128740
H	-7.732689	-0.592060	4.738477
C	-1.168554	-4.405256	3.636423
H	-1.111058	-4.978299	4.559760
C	0.852052	-3.716213	0.435286
H	1.119380	-2.657098	0.492100
C	-3.552464	-2.046895	1.701691
H	-3.082750	-1.118232	1.377704
C	-6.354959	-2.155636	4.316000
C	-0.615738	-4.885599	-1.255975
H	-1.048665	-5.451707	-0.432641
C	-0.180975	-4.563833	2.660653
H	0.622204	-5.287571	2.793812
C	2.092708	-5.897082	0.618456
H	1.220281	-6.365019	0.166713
C	-4.615743	-3.983190	0.527763
H	-4.720426	-4.427463	1.515645
C	-4.039061	-2.721786	0.422388
C	-1.061345	-5.115073	-2.555118
C	-0.495553	-4.343657	-3.568628
H	-0.828984	-4.531165	-4.584453
C	-5.036284	-4.691310	-0.589605
C	3.171750	-6.681433	1.015411
C	-4.851597	-4.076391	-1.827583
H	-5.183784	-4.621207	-2.705163
C	-6.379838	0.032326	3.197156
C	-4.262488	-2.822348	-2.004814
C	4.270974	-6.027543	1.573418
H	5.116170	-6.636394	1.879470
C	0.474795	-3.359297	-3.351897
C	4.342298	-4.641576	1.728632
O	-3.033763	1.941282	-1.838025
O	4.021880	0.786426	1.163325
O	4.808710	-0.591174	-1.435868
O	-2.495446	3.291091	1.070600
C	2.700033	2.618767	-2.105983
C	-0.661698	4.451020	0.117453
C	4.361952	2.065756	1.128469

C	5.421183	0.263166	-2.240777
C	5.051362	1.642111	-2.232308
C	2.614436	2.636833	-3.500413
H	3.465826	2.329172	-4.097475
C	5.703923	2.574267	-3.030760
H	5.378754	3.612523	-2.994606
C	-2.036481	4.097255	-1.877124
C	1.579535	2.979092	-1.357758
H	1.627034	2.936246	-0.272409
C	-3.110041	3.236196	-2.184832
C	-1.653775	4.324256	1.124472
C	0.385834	3.362905	-1.967991
C	7.117328	0.866141	-3.878421
H	7.933350	0.576805	-4.533153
C	1.431220	3.028302	-4.120129
H	1.373180	3.043845	-5.205495
C	-0.837561	3.586215	-1.107934
H	-1.062928	2.579468	-0.739222
C	3.892900	2.054388	-1.358555
H	3.544832	1.104855	-0.976906
C	6.743997	2.210816	-3.878494
C	0.331196	5.414025	0.210502
H	1.093910	5.463030	-0.563570
C	0.320757	3.390987	-3.364137
H	-0.604404	3.689652	-3.846964
C	-2.070156	5.438080	-2.242497
H	-1.227453	6.069773	-1.969411
C	4.616600	4.147118	-0.135529
H	4.501921	4.685323	-1.074980
C	4.290805	2.797485	-0.097041
C	0.369170	6.309336	1.278277
C	-0.674970	6.253447	2.196297
H	-0.681773	6.986865	2.996669
C	5.070351	4.824294	0.994608
C	-3.161350	5.986062	-2.905874
C	5.191237	4.090454	2.175091
H	5.554481	4.615919	3.053090
C	6.506413	-0.116658	-3.097045
C	4.855099	2.738333	2.286983
C	-4.231014	5.136808	-3.179669
H	-5.093956	5.562838	-3.681638
C	-1.704478	5.307764	2.142962
C	-4.246265	3.783558	-2.837472
N	0.677984	-0.003590	0.426736
N	-0.545651	0.409698	0.816127
K	-0.627619	-0.312043	-1.879996
K	6.634187	0.231664	0.443052
K	-6.404682	-0.726863	-0.444214
O	-8.315257	-2.471397	0.237700
O	-8.586660	-0.332793	-2.137331
O	8.542564	2.156726	0.229663
O	8.831916	-0.536802	1.937039
Si	-0.379062	0.763126	2.557921
C	0.594866	-0.624048	3.389929
H	0.108843	-1.563176	3.104874
H	0.564773	-0.488706	4.478730
H	1.623700	-0.583910	3.023825
C	0.493509	2.382628	2.892500
H	-0.123905	3.243331	2.628827
H	1.423227	2.439830	2.319022
H	0.744163	2.458064	3.956685
C	-2.038336	0.669207	3.481077
H	-1.885280	1.103386	4.476169
H	-2.331615	-0.376718	3.620199
H	-2.903060	1.198619	3.072395
K	2.171868	-3.025755	3.879265
C	-4.211260	-2.258045	-3.426999
C	-7.007925	1.415143	3.049045
C	-5.474195	-1.401885	-3.654676
H	-6.375986	-1.993069	-3.447274
H	-5.508482	-1.049764	-4.693466
H	-5.448182	-0.516189	-3.011419
C	5.618521	-3.977312	2.239680
C	1.127845	-2.642258	-4.533280
C	-5.970827	2.498866	3.409739
H	-5.632583	2.370797	4.444678
H	-6.417447	3.495234	3.305083
H	-5.106979	2.435090	2.746010
C	-2.101965	-6.160016	-2.841052
H	-1.791102	-7.148219	-2.472306
H	-2.287381	-6.249446	-3.919492
H	-3.054336	-5.907771	-2.354481
C	-5.612770	-6.075208	-0.484194
H	-4.844623	-6.840907	-0.670686
H	-6.415348	-6.236322	-1.217665
H	-6.024750	-6.259070	0.516839
C	6.202777	-3.125503	1.095230
H	6.472148	-3.771158	0.253132
H	7.102229	-2.591964	1.431710
H	5.449855	-2.410132	0.753337
C	3.170344	-8.170850	0.817125
H	3.509957	-8.437363	-0.194839
H	2.163236	-8.589290	0.942598
H	3.838961	-8.669635	1.530814
C	-6.934714	-3.102727	5.328675
H	-6.953151	-4.133721	4.948654
H	-7.961836	-2.820344	5.593540
H	-6.346577	-3.109451	6.258706
C	-7.495742	1.659731	1.602894
H	-6.641208	1.660163	0.922822
H	-7.985830	2.639595	1.539197
H	-8.226780	0.891718	1.310891
C	-8.226137	1.611493	3.971287
H	-9.023659	0.892835	3.741729
H	-8.619021	2.623483	3.816045
H	-7.947582	1.514347	5.027230
C	-2.973418	-1.384050	-3.702449
H	-3.004055	-0.486179	-3.082987
H	-2.967984	-1.089877	-4.760111
H	-2.068836	-1.974901	-3.508302
C	6.697410	-4.993578	2.657737
H	6.351921	-5.631554	3.481125

H	7.583894	-4.442544	2.996792
H	6.994456	-5.627847	1.814973
C	5.365966	-3.060110	3.457585
H	4.700266	-2.241234	3.171267
H	6.313994	-2.629638	3.799310
H	4.954064	-3.646077	4.294941
C	-4.199810	-3.371936	-4.497910
H	-3.371290	-4.064800	-4.316600
H	-4.058921	-2.905854	-5.480865
H	-5.141244	-3.931957	-4.531258
C	2.621407	-3.029090	-4.564888
H	2.726987	-4.112090	-4.701038
H	3.093483	-2.737230	-3.625124
H	3.124856	-2.514393	-5.393951
C	1.034684	-1.103059	-4.435801
H	1.566006	-0.648770	-5.281341
H	1.512391	-0.755343	-3.516744
H	-0.012915	-0.774630	-4.496545
C	0.503585	-3.036663	-5.885273
H	0.622801	-4.108150	-6.083836
H	1.018982	-2.483629	-6.680137
H	-0.563326	-2.779971	-5.922287
C	4.991074	2.010970	3.626245
C	7.013684	-1.555196	-3.156748
C	5.888663	0.758926	3.509412
H	6.895590	1.028924	3.165269
H	5.983467	0.286213	4.496895
H	5.422148	0.044037	2.826590
C	-5.443796	2.917665	-3.200796
C	-2.857332	5.359866	3.135648
C	5.857731	-2.526553	-3.467635
H	5.447157	-2.315243	-4.461134
H	6.224839	-3.561459	-3.451795
H	5.065907	-2.406679	-2.725863
C	1.493523	7.295083	1.421330
H	1.711078	7.800204	0.469488
H	1.255802	8.063845	2.167957
H	2.419260	6.792923	1.741454
C	5.403723	6.288976	0.946930
H	4.495349	6.907547	0.989259
H	6.038933	6.578461	1.794296
H	5.932340	6.550671	0.019974
C	-5.953779	2.148081	-1.963240
H	-6.219031	2.851790	-1.164042
H	-6.841963	1.558527	-2.223998
H	-5.152379	1.491054	-1.615392
C	-3.198691	7.442009	-3.275937
H	-3.276795	8.079812	-2.383146
H	-2.287644	7.743827	-3.811178
H	-4.058845	7.664275	-3.920659
C	7.421758	3.212852	-4.770282
H	7.419845	4.213706	-4.317852
H	8.464610	2.930758	-4.968171
H	6.915328	3.295385	-5.743944
C	7.631926	-1.948462	-1.799538
H	6.850214	-1.938285	-1.039274
H	8.038924	-2.967074	-1.851398
H	8.446545	-1.260374	-1.533081
C	8.100606	-1.767176	-4.227500
H	9.001732	-1.178142	-4.013813
H	8.379089	-2.828259	-4.231573
H	7.729283	-1.506614	-5.225635
C	3.604027	1.550929	4.119445
H	3.130071	0.936053	3.351288
H	3.713465	0.970766	5.048022
H	2.965864	2.417429	4.318164
C	-6.634675	3.732638	-3.740741
H	-6.383699	4.235721	-4.681487
H	-7.467722	3.045397	-3.937150
H	-6.965449	4.481031	-3.010367
C	-5.016069	1.925231	-4.301741
H	-4.197306	1.298218	-3.939673
H	-5.861101	1.289022	-4.593890
H	-4.676958	2.482824	-5.183232
C	5.606016	2.900751	4.722862
H	4.978963	3.776972	4.923129
H	5.679513	2.315791	5.648307
H	6.613863	3.236488	4.446191
C	-4.189438	5.439949	2.355311
H	-4.216379	6.360873	1.760011
H	-4.283203	4.582720	1.684476
H	-5.032151	5.446686	3.058675
C	-2.851615	4.107414	4.032524
H	-3.707224	4.131384	4.720543
H	-2.916470	3.215801	3.411823
H	-1.924052	4.066684	4.617889
C	-2.794629	6.590369	4.060329
H	-2.804903	7.522661	3.482723
H	-3.676586	6.577295	4.713213
H	-1.899743	6.570626	4.694736
C	-8.556839	-3.387486	-0.827346
H	-9.454608	-3.990801	-0.625116
H	-7.694036	-4.052960	-0.968515
H	-8.710688	-2.786835	-1.728460
C	-8.113295	-3.162756	1.469018
H	-9.009984	-3.741475	1.737299
H	-7.912643	-2.411757	2.236577
H	-7.247626	-3.834545	1.397238
C	-8.725838	0.184485	-3.455183
H	-9.555701	-0.311709	-3.980239
H	-7.789474	-0.012378	-3.981702
H	-8.908313	1.268716	-3.439641
C	-9.766617	-0.089667	-1.374062
H	-10.650974	-0.499376	-1.884605
H	-9.912974	0.988505	-1.213724
H	-9.636080	-0.602356	-0.417525
C	8.229486	3.115238	-0.782564
H	9.041423	3.852512	-0.875393
H	7.287455	3.631422	-0.551631
H	8.113125	2.570538	-1.722035
C	8.690613	2.797254	1.494290
H	8.933338	2.013904	2.218229

H	7.758444	3.301416	1.788476
H	9.506277	3.535709	1.462080
C	10.015682	-0.551106	1.141107
H	10.176988	-1.543825	0.696199
H	10.893048	-0.281747	1.747738
H	9.876284	0.200286	0.359609
C	8.977930	-1.360638	3.083399
H	9.131411	-2.414078	2.803968
H	8.055378	-1.270700	3.662203
H	9.827179	-1.027392	3.698709

Complex 7 – Quartet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -9111.985842

Ce	-2.871328	1.205271	0.208378
Ce	2.753109	-0.777630	-0.188705
O	3.421899	-2.391107	1.458532
O	-3.205137	-1.013035	-0.859312
O	-4.795741	0.456388	1.337967
O	1.851854	-2.464262	-1.481791
C	-2.228090	-2.617986	2.504734
C	0.460292	-4.115993	-0.509571
C	-3.638722	-2.247141	-0.660005
C	-5.280702	-0.288339	2.325729
C	-4.605707	-1.488413	2.701114
C	-2.059644	-3.044743	3.824762
H	-2.785823	-2.789040	4.587170
C	-5.136727	-2.306063	3.694549
H	-4.643423	-3.243687	3.933765
C	2.247635	-4.451652	1.211959
C	-1.205037	-2.886013	1.597928
H	-1.292364	-2.502584	0.586352
C	3.444724	-3.724506	1.448284
C	1.004872	-3.463484	-1.648640
C	-0.079480	-3.631902	1.917025
C	-6.956116	-0.804938	3.999448
H	-7.874849	-0.552325	4.518761
C	-0.951253	-3.825952	4.162657
H	-0.862607	-4.208185	5.177311
C	0.986879	-3.702096	0.846651
H	1.272724	-2.652780	0.737451
C	-3.410443	-1.897244	1.874773
H	-2.974903	-0.985365	1.466640
C	-6.302523	-1.974381	4.379649
C	-0.475205	-5.133162	-0.645128
H	-0.903766	-5.579703	0.250907
C	0.022009	-4.149537	3.213571
H	0.841477	-4.823076	3.462900
C	2.241333	-5.840592	1.279560
H	1.313046	-6.365018	1.061674
C	-4.346968	-3.997261	0.920629
H	-4.447289	-4.318746	1.955009
C	-3.835811	-2.727510	0.667107
C	-0.883284	-5.580166	-1.899661
C	-0.316601	-4.963487	-3.013574
H	-0.613034	-5.327808	-3.992339
C	-4.711517	-4.859699	-0.100974
C	3.390015	-6.566089	1.582471
C	-4.523792	-4.395352	-1.402924
H	-4.799431	-5.063889	-2.211398
C	-6.498553	0.042970	2.987187
C	-3.994916	-3.144601	-1.726354
C	4.565574	-5.846046	1.792134
H	5.468588	-6.410083	2.004986
C	0.613385	-3.922483	-2.936894
C	4.636969	-4.452756	1.726491
O	-2.816290	1.788724	-2.002985
O	4.366256	0.668145	0.984293
O	3.995571	-0.152672	-2.116493
O	-2.807320	3.369418	0.899570
C	2.658534	3.247738	-1.800257
C	-1.069675	4.733507	0.043693
C	4.379627	1.958196	1.305087
C	4.945012	0.710839	-2.392795
C	4.886899	2.031019	-1.864523
C	2.885222	3.917094	-3.001393
H	3.874525	3.909517	-3.448721
C	5.919998	2.940690	-2.069954
H	5.833065	3.928719	-1.620313
C	-2.218054	4.095682	-2.040784
C	1.375649	3.245519	-1.260392
H	1.196719	2.712342	-0.329143
C	-3.076855	3.042415	-2.422414
C	-2.109765	4.504727	0.981938
C	0.311165	3.883585	-1.885769
C	7.103876	1.315881	-3.343311
H	7.977018	1.049653	-3.931853
C	1.825544	4.560150	-3.640162
H	1.999844	5.073637	-4.582236
C	-1.016826	3.825110	-1.165740
H	-1.077321	2.794648	-0.800768
C	3.680026	2.420096	-1.055624
H	3.136502	1.494120	-0.887640
C	7.052458	2.608983	-2.811706
C	-0.217922	5.822955	0.163401
H	0.583542	5.945735	-0.561416
C	0.543435	4.541844	-3.095950
H	-0.278385	5.029788	-3.610022
C	-2.489095	5.406703	-2.417979
H	-1.832513	6.194321	-2.053853
C	4.013610	4.283412	0.622253
H	3.702761	4.984034	-0.150719
C	4.030763	2.930115	0.322153
C	-0.382071	6.757851	1.182223
C	-1.479640	6.595248	2.020449
H	-1.651806	7.357683	2.773303
C	4.349129	4.751178	1.893219
C	-3.588523	5.730175	-3.204251
C	4.708075	3.803448	2.847144
H	4.971017	4.165966	3.835835
C	6.096758	0.362448	-3.168846
C	4.745839	2.426255	2.598167

C	-4.431319	4.686483	-3.575273
H	-5.302899	4.934197	-4.172342
C	-2.372769	5.522463	1.936669
C	-4.219716	3.357246	-3.203333
N	0.748844	0.167256	0.249814
N	-0.457699	0.584579	0.681073
K	-0.585161	-0.180538	-2.043493
K	6.848580	0.525136	-0.105017
K	-6.265650	-1.047705	-0.531613
O	-8.121694	-2.808252	0.265866
O	-8.392352	-0.969770	-2.360061
O	8.458614	2.424143	0.881929
O	9.152442	-0.850832	0.285122
Si	-0.238319	1.050623	2.389582
C	0.676167	-0.320223	3.303034
H	0.066554	-1.228392	3.319622
H	0.917269	-0.000404	4.323613
H	1.590496	-0.476719	2.725548
C	0.734617	2.641222	2.572319
H	0.209892	3.488042	2.118950
H	1.713837	2.551056	2.090491
H	0.903177	2.876281	3.629758
C	-1.904033	1.168327	3.281567
H	-1.712290	1.548099	4.292180
H	-2.391768	0.194596	3.395648
H	-2.611703	1.881064	2.850693
K	2.591765	-2.479009	3.934170
C	-3.908730	-2.785273	-3.211612
C	-7.279244	1.305964	2.636503
C	-5.176994	-2.003131	-3.608955
H	-6.074748	-2.582802	-3.356087
H	-5.174131	-1.805271	-4.688846
H	-5.197447	-1.035766	-3.098261
C	5.962462	-3.727950	1.933877
C	1.287900	-3.389069	-4.196363
C	-6.421723	2.539953	2.967224
H	-6.183180	2.558501	4.036757
H	-6.966322	3.456470	2.710248
H	-5.490059	2.515774	2.400058
C	-1.874727	-6.700022	-2.039174
H	-1.517920	-7.618095	-1.549892
H	-2.059796	-6.934896	-3.095647
H	-2.835606	-6.432225	-1.580294
C	-5.242541	-6.239491	0.169306
H	-4.533686	-7.011250	-0.164287
H	-6.191917	-6.423799	-0.354783
H	-5.416251	-6.389349	1.242658
C	6.275359	-2.847740	0.705996
H	6.351324	-3.466481	-0.194722
H	7.224539	-2.316728	0.855291
H	5.467771	-2.124679	0.570882
C	3.367840	-8.067462	1.645291
H	3.104804	-8.502832	0.670654
H	2.628217	-8.430789	2.372887
H	4.348552	-8.465180	1.935502
C	-6.835571	-2.849005	5.479153
H	-6.690521	-3.913746	5.249669
H	-7.908435	-2.678567	5.637267
H	-6.328073	-2.650141	6.435104
C	-7.650849	1.355435	1.138036
H	-6.741254	1.400743	0.534797
H	-8.240972	2.258422	0.936312
H	-8.261608	0.482373	0.866730
C	-8.598205	1.427024	3.424025
H	-9.269036	0.582863	3.217087
H	-9.101199	2.351691	3.116227
H	-8.416152	1.485518	4.503450
C	-2.677965	-1.926430	-3.548154
H	-2.779590	-0.959611	-3.055455
H	-2.623443	-1.777475	-4.634242
H	-1.771672	-2.451704	-3.219583
C	7.149433	-4.691116	2.121278
H	7.034246	-5.304716	3.023239
H	8.066634	-4.096886	2.229233
H	7.265406	-5.350153	1.252746
C	5.899182	-2.826646	3.184967
H	5.161103	-2.037166	3.025268
H	6.871443	-2.348659	3.358979
H	5.651659	-3.428494	4.072237
C	-3.827322	-4.034729	-4.116799
H	-2.993321	-4.672853	-3.807248
H	-3.652267	-3.703226	-5.147898
H	-4.755853	-4.617080	-4.111859
C	2.778499	-3.794356	-4.143970
H	2.861302	-4.885532	-4.070727
H	3.255077	-3.336613	-3.272883
H	3.291307	-3.457767	-5.052530
C	1.193424	-1.851580	-4.319034
H	1.723078	-1.520403	-5.221292
H	1.662969	-1.381654	-3.451210
H	0.140886	-1.549402	-4.420690
C	0.683947	-3.976693	-5.485969
H	0.813645	-5.064345	-5.531027
H	1.202822	-3.536141	-6.346265
H	-0.384952	-3.739209	-5.566827
C	5.178783	1.460161	3.695763
C	6.197479	-1.006076	-3.827493
C	6.430688	0.670539	3.255961
H	7.232666	1.359854	2.963731
H	6.786597	0.039449	4.081076
H	6.164035	0.022570	2.417828
C	-5.205498	2.281501	-3.633454
C	-3.632117	5.518065	2.793376
C	5.038043	-1.145248	-4.838073
H	5.116201	-0.362880	-5.603147
H	5.085493	-2.125928	-5.326864
H	4.082523	-1.049992	-4.317101
C	0.569098	7.908740	1.344813
H	0.773981	8.402516	0.384436
H	0.167575	8.661106	2.035990
H	1.536757	7.573900	1.746373
C	4.309155	6.216835	2.218778

H	3.291420	6.618011	2.118137
H	4.639852	6.402608	3.248612
H	4.952837	6.800995	1.545239
C	-5.749253	1.536141	-2.394757
H	-6.165759	2.254954	-1.677279
H	-6.542107	0.839869	-2.694177
H	-4.924373	0.987861	-1.930174
C	-3.859847	7.147909	-3.621103
H	-3.789377	7.834241	-2.766024
H	-3.136869	7.492829	-4.375415
H	-4.863544	7.247606	-4.054108
C	8.143284	3.607793	-3.079521
H	8.180657	4.374783	-2.294200
H	9.128388	3.123380	-3.134355
H	7.984635	4.129999	-4.035065
C	6.103554	-2.135276	-2.780070
H	5.166490	-2.052811	-2.227680
H	6.139814	-3.112808	-3.278160
H	6.949950	-2.075135	-2.080951
C	7.517560	-1.206506	-4.594243
H	8.385530	-1.132944	-3.924003
H	7.512143	-2.209338	-5.038381
H	7.629329	-0.475349	-5.403817
C	4.042600	0.457445	3.983106
H	3.815429	-0.068835	3.050629
H	4.372449	-0.247109	4.765145
H	3.149770	0.991299	4.327005
C	-6.424918	2.849827	-4.384323
H	-6.125597	3.350441	-5.312267
H	-7.090128	2.017960	-4.648082
H	-6.983358	3.557165	-3.758927
C	-4.496779	1.291420	-4.580667
H	-3.661695	0.815984	-4.061457
H	-5.197085	0.520368	-4.924664
H	-4.114559	1.832900	-5.454631
C	5.523316	2.166607	5.019061
H	4.661730	2.719896	5.410830
H	5.811464	1.407443	5.757633
H	6.365236	2.858391	4.893700
C	-4.859350	5.433887	1.856857
H	-4.879370	6.311083	1.198741
H	-4.802441	4.533056	1.241355
H	-5.782104	5.413905	2.450141
C	-3.629348	4.336997	3.779504
H	-4.536605	4.358899	4.396840
H	-3.600491	3.398480	3.231007
H	-2.750618	4.394573	4.434092
C	-3.792723	6.802819	3.630014
H	-3.813396	7.694568	2.992091
H	-4.745127	6.743423	4.171860
H	-2.986968	6.906633	4.367423
C	-8.286677	-3.840809	-0.702099
H	-9.158285	-4.466890	-0.458726
H	-7.388149	-4.470506	-0.752678
H	-8.443114	-3.346366	-1.665158
C	-7.915773	-3.355852	1.567870
H	-8.785754	-3.955673	1.874843
H	-7.780965	-2.518574	2.256416
H	-7.011734	-3.978348	1.586471
C	-8.495650	-0.578442	-3.723727
H	-9.292059	-1.144500	-4.229741
H	-7.536391	-0.796886	-4.198842
H	-8.707735	0.496697	-3.813188
C	-9.614596	-0.714290	-1.671110
H	-10.455909	-1.213118	-2.175167
H	-9.817024	0.365590	-1.620336
H	-9.503111	-1.126733	-0.664990
C	7.844453	3.700293	1.061721
H	7.734276	4.215881	0.097666
H	8.443339	4.324189	1.741967
H	6.855761	3.532642	1.495329
C	9.746251	2.551480	0.293897
H	10.126416	1.537804	0.138343
H	10.426780	3.107780	0.956144
H	9.686758	3.070014	-0.673780
C	9.680882	-1.930778	-0.477116
H	9.368977	-2.898522	-0.058400
H	10.779080	-1.885542	-0.507275
H	9.283100	-1.834269	-1.491126
C	9.594630	-0.910409	1.637135
H	9.232618	-1.826712	2.127380
H	9.183879	-0.035107	2.148236
H	10.692831	-0.883995	1.692041

Complex 8 – Triplet

SCF Energy (a.u.): -9531.249240

Ce	-3.780024	-1.044738	-0.832493
Ce	3.586450	0.926125	-0.118536
O	3.968910	3.174013	-0.233468
O	-2.656895	0.356731	0.610613
O	-5.486588	0.433880	-1.178378
O	2.097751	1.510651	1.500951
C	-2.409316	3.289783	-1.521421
C	0.775576	3.488671	1.336989
C	-3.231185	1.400016	1.225132
C	-5.856098	1.585602	-1.750713
C	-4.954915	2.686018	-1.726528
C	-2.287600	3.867982	-2.786306
H	-3.108850	3.826078	-3.493958
C	-5.356158	3.917403	-2.232412
H	-4.671538	4.760134	-2.174655
C	2.205873	4.785481	-0.193320
C	-1.300648	3.325297	-0.670184
H	-1.397172	2.903929	0.324686
C	3.589571	4.433431	-0.160382
C	1.380893	2.462951	2.101368
C	-0.076517	3.896287	-1.027612
C	-7.459275	2.988211	-2.882561
H	-8.428173	3.125959	-3.351176
C	-1.097907	4.503081	-3.139565
H	-1.014734	4.985983	-4.109908
C	1.139721	3.700424	-0.128698

H	1.604774	2.782325	-0.514125
C	-3.608124	2.460217	-1.072138
H	-3.318059	1.443825	-1.356431
C	-6.606885	4.089663	-2.826427
C	-0.100078	4.390724	1.948774
H	-0.573416	5.155123	1.336938
C	-0.005659	4.517841	-2.277742
H	0.908191	5.015250	-2.584158
C	1.820733	6.124014	-0.133137
H	0.759219	6.362029	-0.165464
C	-4.342261	3.572198	1.040119
H	-4.719057	4.366613	0.400028
C	-3.742513	2.466990	0.441362
C	-0.394216	4.329808	3.300218
C	0.291046	3.379780	4.062449
H	0.123066	3.378005	5.134875
C	-4.472466	3.672021	2.420466
C	2.744371	7.159820	-0.008248
C	-3.974599	2.614474	3.185659
H	-4.065384	2.693521	4.263469
C	-7.131519	1.736404	-2.350122
C	-3.351904	1.482707	2.645760
C	4.097439	6.807659	0.031617
H	4.822671	7.608588	0.140726
C	1.194015	2.469615	3.520383
C	4.550308	5.487490	-0.052759
O	-4.406138	-2.433381	0.703099
O	3.986012	-1.303321	-1.085156
O	5.019912	-0.155281	1.455368
O	-2.849633	-2.710981	-1.892503
C	1.758498	-2.773477	2.035262
C	-1.339934	-4.172207	-0.794315
C	3.922069	-2.614498	-0.950167
C	5.188673	-1.104459	2.360278
C	4.273186	-2.201540	2.446192
C	1.482929	-2.890848	3.398725
H	2.251737	-2.665845	4.127251
C	4.512228	-3.234864	3.350267
H	3.827923	-4.079260	3.374843
C	-2.938484	-4.281308	1.084538
C	0.717900	-3.049445	1.133255
H	0.931620	-3.005809	0.069530
C	-4.226917	-3.704585	1.091988
C	-2.057190	-3.785590	-1.950574
C	-0.568152	-3.416659	1.551139
C	6.480112	-2.155816	4.137049
H	7.333250	-2.157692	4.807511
C	0.220211	-3.288470	3.830349
H	0.028462	-3.385428	4.895901
C	-1.711901	-3.549947	0.544236
H	-2.019584	-2.510929	0.354317
C	3.109468	-2.320388	1.464924
H	2.941565	-1.314789	1.065081
C	5.594283	-3.229624	4.222774
C	-0.390327	-5.185001	-0.883399
H	0.187192	-5.451749	-0.001320
C	-0.800662	-3.546067	2.923379
H	-1.784247	-3.840911	3.274040
C	-2.778280	-5.600074	1.509023
H	-1.781828	-6.035271	1.480897
C	3.502893	-4.577591	0.459041
H	3.157016	-4.979881	1.409051
C	3.511010	-3.195775	0.283913
C	-0.147012	-5.846559	-2.084809
C	-0.946320	-5.524533	-3.181631
H	-0.797317	-6.088544	-4.096891
C	3.921259	-5.450707	-0.536380
C	-3.846600	-6.367322	1.951462
C	4.302821	-4.885783	-1.754928
H	4.600241	-5.564319	-2.548486
C	6.329427	-1.103098	3.231757
C	4.304076	-3.512171	-2.005337
C	-5.116767	-5.786858	1.926698
H	-5.956637	-6.396135	2.245051
C	-1.923485	-4.527472	-3.147138
C	-5.343828	-4.480250	1.500449
N	2.069515	0.908545	-1.784437
N	1.628668	0.816397	-3.056778
K	0.040822	0.264644	0.369491
K	6.556802	-1.854634	-0.212728
K	-6.349054	1.068043	1.479829
O	-8.052937	3.121760	1.555702
O	-8.134205	0.406200	3.421730
O	7.767281	-4.197204	0.212688
O	7.964817	-0.024650	-1.649614
Si	0.345351	-0.369176	-3.388670
C	0.435523	-0.939171	-5.183734
H	-0.319824	-0.455758	-5.810055
H	0.266108	-2.019269	-5.223934
H	1.417763	-0.752947	-5.624190
C	0.575138	-1.783523	-2.183680
H	-0.241007	-1.825601	-1.455385
H	1.530716	-1.664645	-1.664884
H	0.561716	-2.757860	-2.679230
C	-1.364673	0.368465	-3.070077
H	-1.596623	1.216188	-3.719803
H	-1.445846	0.739071	-2.041279
H	-2.101721	-0.425811	-3.247086
Si	2.427555	1.851896	-4.274027
C	1.117114	2.477968	-5.468624
H	1.554129	3.220591	-6.145685
H	0.304285	2.962270	-4.919036
H	0.690678	1.680769	-6.083716
C	3.267593	3.292848	-3.429780
H	2.629079	3.763530	-2.681098
H	3.529633	4.020227	-4.210041
H	4.187552	2.994828	-2.922003
C	3.785435	0.957235	-5.227616
H	4.343339	1.691418	-5.820888
H	4.488472	0.475951	-4.540559
H	3.409673	0.192700	-5.912541
K	3.604821	6.875180	-3.184821

C	-2.865450	0.376138	3.590433
C	-8.118493	0.565084	-2.417105
C	-3.840134	-0.806937	3.533182
H	-4.840831	-0.505420	3.869799
H	-3.504070	-1.612079	4.196673
H	-3.916507	-1.227818	2.527464
C	6.050911	5.177142	-0.020915
C	2.076508	1.627336	4.444679
C	-7.513028	-0.584563	-3.237532
H	-7.314693	-0.260565	-4.263808
H	-8.203974	-1.434287	-3.273940
H	-6.574213	-0.926313	-2.798471
C	-1.373453	5.269849	3.942542
H	-1.749072	5.999968	3.219456
H	-0.918965	5.824044	4.771617
H	-2.236785	4.728875	4.347947
C	-5.082264	4.882084	3.068122
H	-4.312462	5.611897	3.343453
H	-5.622535	4.620037	3.983482
H	-5.780209	5.385085	2.392431
C	6.375413	4.244798	1.157227
H	6.130038	4.727876	2.108570
H	7.445634	4.003168	1.166657
H	5.803691	3.319484	1.094418
C	2.303594	8.591051	0.133694
H	2.078398	8.836426	1.178930
H	1.398805	8.792628	-0.449224
H	3.078687	9.286795	-0.203714
C	-7.007751	5.416283	-3.408512
H	-6.737191	6.244532	-2.745409
H	-8.085930	5.464663	-3.585257
H	-6.509993	5.599650	-4.368089
C	-8.457361	0.063569	-1.002527
H	-7.581606	-0.391055	-0.536046
H	-9.241591	-0.700397	-1.046332
H	-8.826365	0.890263	-0.382245
C	-9.439340	0.963095	-3.082447
H	-9.953643	1.756320	-2.528832
H	-10.104095	0.094012	-3.113359
H	-9.292086	1.301488	-4.112691
C	-1.463880	-0.114429	3.217863
H	-1.491016	-0.702797	2.302598
H	-1.082547	-0.771863	4.002703
H	-0.773075	0.729906	3.122802
C	6.909160	6.434725	0.144414
H	6.774424	7.140191	-0.683304
H	7.965911	6.147794	0.160510
H	6.693492	6.956319	1.082638
C	6.459777	4.515927	-1.345205
H	5.850187	3.630687	-1.532687
H	7.518462	4.230057	-1.321513
H	6.328223	5.209848	-2.184508
C	-2.782575	0.862608	5.043162
H	-2.125316	1.733618	5.135279
H	-2.367364	0.060537	5.660939
H	-3.762463	1.114008	5.463509
C	3.517921	2.108194	4.243399
H	3.610981	3.175834	4.467943
H	3.833068	1.940563	3.212721
H	4.192708	1.551951	4.901554
C	2.009157	0.128722	4.148649
H	2.750609	-0.400822	4.757770
H	2.228354	-0.075900	3.102698
H	1.024437	-0.279377	4.387019
C	1.720889	1.809707	5.923149
H	1.848313	2.844389	6.257466
H	2.386683	1.184137	6.526767
H	0.691409	1.499388	6.136523
C	4.649202	-2.997648	-3.407545
C	7.384702	0.016134	3.187333
C	5.818699	-2.005658	-3.371891
H	6.737210	-2.487732	-3.013309
H	6.030140	-1.624750	-4.377257
H	5.572001	-1.156650	-2.733690
C	-6.765660	-3.912546	1.417997
C	-2.886319	-4.313296	-4.320932
C	6.752156	1.369255	3.526331
H	6.367576	1.368415	4.549458
H	7.497701	2.168903	3.444289
H	5.929461	1.589774	2.847967
C	0.941973	-6.873843	-2.199166
H	1.051395	-7.446744	-1.273154
H	0.742695	-7.578904	-3.011909
H	1.909382	-6.397020	-2.396745
C	3.994981	-6.933276	-0.301038
H	3.208360	-7.268252	0.382131
H	3.887498	-7.494745	-1.233869
H	4.954883	-7.226209	0.145552
C	-7.111715	-3.596177	-0.046630
H	-7.036352	-4.497589	-0.662400
H	-8.135565	-3.210956	-0.124807
H	-6.434912	-2.847297	-0.461535
C	-3.648561	-7.772959	2.444594
H	-4.481258	-8.420971	2.153321
H	-2.728782	-8.207608	2.043059
H	-3.576848	-7.810028	3.538759
C	5.796792	-4.330803	5.225595
H	5.369647	-5.274894	4.872850
H	6.859307	-4.497988	5.429372
H	5.317741	-4.098944	6.185126
C	8.022746	0.120757	1.795202
H	7.269726	0.389534	1.053002
H	8.788050	0.905330	1.793810
H	8.521063	-0.817543	1.517415
C	8.527807	-0.220654	4.180037
H	9.068727	-1.151285	3.974873
H	9.243654	0.604264	4.102629
H	8.171663	-0.248597	5.214486
C	3.414795	-2.300809	-3.989348
H	3.138256	-1.438507	-3.379517
H	3.617949	-1.959918	-5.010009
H	2.569755	-2.994974	-4.023609

C	-7.816729	-4.903310	1.927232
H	-7.645823	-5.176791	2.973655
H	-8.808869	-4.443682	1.859870
H	-7.837845	-5.820445	1.330471
C	-6.892878	-2.640911	2.269416
H	-6.153924	-1.901946	1.959354
H	-7.899523	-2.217376	2.167744
H	-6.718168	-2.866047	3.326987
C	5.043526	-4.123702	-4.367633
H	4.230741	-4.842126	-4.513982
H	5.280760	-3.692049	-5.345454
H	5.929329	-4.669209	-4.022262
C	-4.319731	-4.571263	-3.824116
H	-4.421184	-5.600138	-3.464839
H	-4.576446	-3.900217	-3.001553
H	-5.038263	-4.418503	-4.638122
C	-2.790806	-2.894946	-4.897366
H	-3.506978	-2.773117	-5.718407
H	-3.008566	-2.147953	-4.134635
H	-1.790843	-2.700985	-5.294195
C	-2.615003	-5.287722	-5.470835
H	-2.709192	-6.331013	-5.153211
H	-3.344670	-5.116178	-6.269035
H	-1.617108	-5.145825	-5.899566
C	-8.670355	3.656485	2.703209
H	-9.729731	3.883319	2.514310
H	-8.167762	4.576979	3.030863
H	-8.593779	2.903875	3.489941
C	-8.049584	4.031459	0.475162
H	-9.075100	4.283061	0.169470
H	-7.536251	3.557482	-0.361830
H	-7.523719	4.958526	0.742132
C	-7.895688	-0.134966	4.703196
H	-8.551632	0.327971	5.453743
H	-6.855448	0.073884	4.961006
H	-8.054167	-1.221172	4.710982
C	-9.466051	0.202506	3.002270
H	-10.175670	0.663547	3.703729
H	-9.697198	-0.868208	2.917918
H	-9.578267	0.675154	2.024186
C	7.204243	-4.696384	1.412939
H	7.810705	-5.520783	1.814009
H	6.175577	-5.044020	1.249989
H	7.186918	-3.881841	2.140841
C	7.847568	-5.193206	-0.782652
H	8.283367	-4.734227	-1.673802
H	6.852160	-5.583568	-1.032413
H	8.492790	-6.022241	-0.458397
C	9.346849	0.193555	-1.477072
H	9.546611	0.824779	-0.600416
H	9.783533	0.670133	-2.365425
H	9.817620	-0.781027	-1.328837
C	7.261813	1.184654	-1.821923
H	7.273571	1.790598	-0.906055
H	6.230466	0.931223	-2.086452
H	7.681108	1.781856	-2.642702

Complex 8 – Triplet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -9520.944170

Ce	-3.799450	-1.024534	-0.813770
Ce	3.583411	0.898944	-0.129788
O	3.977273	3.143283	-0.257267
O	-2.668621	0.386292	0.603775
O	-5.485895	0.477806	-1.141065
O	2.087769	1.481702	1.476123
C	-2.399505	3.314653	-1.524036
C	0.793489	3.478931	1.325991
C	-3.215351	1.439201	1.227021
C	-5.855772	1.625509	-1.720760
C	-4.952505	2.724168	-1.709471
C	-2.276412	3.890119	-2.789853
H	-3.100639	3.855399	-3.494544
C	-5.354468	3.952009	-2.220949
H	-4.667351	4.793488	-2.173604
C	2.229678	4.769982	-0.202138
C	-1.287611	3.341823	-0.676376
H	-1.384104	2.922966	0.319402
C	3.610207	4.405049	-0.172838
C	1.386562	2.441114	2.083026
C	-0.059487	3.900329	-1.037603
C	-7.458514	3.019701	-2.857475
H	-8.428209	3.152258	-3.326072
C	-1.080916	4.512294	-3.147945
H	-0.995716	4.992220	-4.119628
C	1.155743	3.693063	-0.140130
H	1.614072	2.772731	-0.528208
C	-3.602024	2.495661	-1.065755
H	-3.321506	1.475333	-1.345220
C	-6.608200	4.122450	-2.809759
C	-0.066270	4.389443	1.947328
H	-0.532558	5.162889	1.341376
C	0.014282	4.518362	-2.289560
H	0.932136	5.005846	-2.600232
C	1.857573	6.111336	-0.136126
H	0.798236	6.358964	-0.168737
C	-4.287316	3.630745	1.050336
H	-4.656874	4.429513	0.411299
C	-3.721449	2.510847	0.447765
C	-0.353948	4.326125	3.299972
C	0.320939	3.360707	4.051513
H	0.158413	3.353687	5.124713
C	-4.384329	3.743608	2.432675
C	2.790717	7.138446	-0.005079
C	-3.896499	2.677422	3.191535
H	-3.963790	2.762449	4.270460
C	-7.129982	1.770743	-2.319092
C	-3.313439	1.526888	2.647161
C	4.138953	6.771047	0.034574
H	4.873197	7.562957	0.148515
C	1.207533	2.440857	3.501245
C	4.580111	5.447770	-0.059573

O	-4.384322	-2.383863	0.763259
O	3.967851	-1.334711	-1.075075
O	5.013153	-0.162335	1.449931
O	-2.863972	-2.704005	-1.841180
C	1.764207	-2.788447	2.069058
C	-1.344642	-4.162772	-0.756887
C	3.900011	-2.644630	-0.931094
C	5.193888	-1.105369	2.358427
C	4.282837	-2.204736	2.459987
C	1.498383	-2.934530	3.431459
H	2.271463	-2.722102	4.159114
C	4.537056	-3.233189	3.364934
H	3.858194	-4.081591	3.399064
C	-2.947081	-4.262011	1.108538
C	0.716773	-3.044636	1.169767
H	0.922515	-2.979159	0.105162
C	-4.228298	-3.671099	1.105495
C	-2.074802	-3.779989	-1.906187
C	-0.565412	-3.422809	1.588440
C	6.507314	-2.142871	4.123247
H	7.368526	-2.136970	4.783224
C	0.238431	-3.340890	3.863595
H	0.054516	-3.459839	4.928355
C	-1.710003	-3.538574	0.582952
H	-2.009711	-2.496468	0.396009
C	3.110725	-2.331973	1.490731
H	2.936763	-1.329019	1.087367
C	5.628726	-3.220449	4.225375
C	-0.394700	-5.173280	-0.855907
H	0.195358	-5.435830	0.019166
C	-0.788660	-3.581382	2.958810
H	-1.769990	-3.884483	3.309042
C	-2.810633	-5.591514	1.507709
H	-1.818272	-6.036718	1.490964
C	3.487279	-4.595455	0.496142
H	3.151133	-4.988882	1.453351
C	3.500964	-3.215622	0.312124
C	-0.164436	-5.837061	-2.059724
C	-0.980502	-5.519704	-3.144676
H	-0.843561	-6.084408	-4.061523
C	3.886028	-5.478432	-0.498965
C	-3.896652	-6.358128	1.905466
C	4.249858	-4.922013	-1.725505
H	4.531092	-5.606014	-2.520096
C	6.342367	-1.093801	3.216791
C	4.258796	-3.550057	-1.985027
C	-5.160883	-5.766399	1.848798
H	-6.016875	-6.376239	2.120144
C	-1.958237	-4.523817	-3.100629
C	-5.364351	-4.448984	1.448060
N	2.068562	0.889073	-1.799707
N	1.619716	0.798057	-3.069600
K	0.029872	0.258609	0.347192
K	6.552466	-1.854993	-0.225082
K	-6.321146	1.074685	1.506243
O	-8.092937	3.062780	1.548910
O	-8.084767	0.429074	3.447665
O	7.815800	-4.157351	0.193268
O	7.863023	-0.018518	-1.712367
Si	0.324942	-0.377332	-3.391650
C	0.409593	-0.957321	-5.183564
H	-0.312154	-0.440295	-5.822380
H	0.188028	-2.027529	-5.223729
H	1.406927	-0.819682	-5.607756
C	0.545040	-1.788766	-2.180849
H	-0.273699	-1.827547	-1.455363
H	1.500452	-1.672933	-1.660831
H	0.530495	-2.764112	-2.674056
C	-1.375910	0.383790	-3.077426
H	-1.586928	1.240908	-3.722137
H	-1.460423	0.749277	-2.047117
H	-2.128772	-0.392229	-3.266309
Si	2.429059	1.820089	-4.289773
C	1.127579	2.453003	-5.490809
H	1.573750	3.187192	-6.171076
H	0.319188	2.949385	-4.945181
H	0.693525	1.657213	-6.102249
C	3.275869	3.261248	-3.451557
H	2.642492	3.727220	-2.695466
H	3.527258	3.991403	-4.232821
H	4.201391	2.965003	-2.953346
C	3.782191	0.908912	-5.234848
H	4.346980	1.634826	-5.831801
H	4.479649	0.425195	-4.543921
H	3.400941	0.143004	-5.915146
K	3.674467	6.818194	-3.159238
C	-2.846554	0.414797	3.584310
C	-8.110524	0.602433	-2.378309
C	-3.868227	-0.741176	3.571647
H	-4.846553	-0.390819	3.932132
H	-3.530191	-1.543391	4.241078
H	-3.972493	-1.169003	2.569637
C	6.071300	5.124503	-0.042401
C	2.067659	1.570877	4.409886
C	-7.502507	-0.565476	-3.188285
H	-7.308825	-0.248785	-4.219671
H	-8.199180	-1.413208	-3.202100
H	-6.563124	-0.889283	-2.734246
C	-1.313979	5.276605	3.954639
H	-1.701072	6.002374	3.227774
H	-0.835964	5.836800	4.770921
H	-2.173338	4.739393	4.381393
C	-4.943038	4.976607	3.083227
H	-4.148446	5.710514	3.278287
H	-5.417578	4.744023	4.046001
H	-5.686946	5.463441	2.439212
C	6.405831	4.153799	1.112904
H	6.173417	4.621302	2.077307
H	7.476335	3.907249	1.092010
H	5.819316	3.239149	1.022281
C	2.363083	8.574136	0.128621
H	2.016955	8.792252	1.149990

H	1.537127	8.814532	-0.555425
H	3.192492	9.258907	-0.092226
C	-7.016472	5.450954	-3.381309
H	-6.909305	6.257238	-2.641993
H	-8.061820	5.433699	-3.713533
H	-6.395730	5.722508	-4.247027
C	-8.459408	0.099873	-0.957468
H	-7.577398	-0.349947	-0.495672
H	-9.240437	-0.668587	-1.018428
H	-8.833570	0.930093	-0.342603
C	-9.439641	0.988846	-3.054917
H	-9.953722	1.783347	-2.499367
H	-10.091192	0.107136	-3.075782
H	-9.280542	1.318809	-4.088092
C	-1.471761	-0.146687	3.181904
H	-1.552462	-0.721619	2.259890
H	-1.115242	-0.827917	3.960136
H	-0.745842	0.669478	3.084186
C	6.953150	6.373482	0.147586
H	6.819309	7.092447	-0.671036
H	8.004305	6.059395	0.152455
H	6.738781	6.870497	1.101406
C	6.473476	4.485779	-1.389655
H	5.836530	3.622002	-1.593242
H	7.526124	4.173637	-1.358509
H	6.360400	5.212928	-2.205927
C	-2.700441	0.907751	5.039786
H	-2.003619	1.753051	5.093244
H	-2.294518	0.085732	5.640967
H	-3.662760	1.196110	5.480735
C	3.536790	1.985497	4.194851
H	3.674926	3.052323	4.408899
H	3.825836	1.783606	3.161853
H	4.182489	1.396790	4.856582
C	1.951924	0.066584	4.116823
H	2.692285	-0.473542	4.720877
H	2.158563	-0.132618	3.065894
H	0.956385	-0.307981	4.369219
C	1.739902	1.763209	5.902708
H	1.905052	2.798664	6.223628
H	2.404665	1.114313	6.485961
H	0.702947	1.476801	6.122119
C	4.598677	-3.049473	-3.386275
C	7.387571	0.024888	3.157359
C	5.786029	-2.066249	-3.373481
H	6.698547	-2.560545	-3.011107
H	5.984124	-1.706683	-4.391231
H	5.543012	-1.208805	-2.743864
C	-6.771270	-3.869502	1.323501
C	-2.923595	-4.301039	-4.261643
C	6.759524	1.389508	3.499846
H	6.377040	1.384835	4.525483
H	7.518013	2.178319	3.410454
H	5.938232	1.605994	2.816777
C	0.923706	-6.864203	-2.181251
H	0.944496	-7.534416	-1.311115
H	0.792371	-7.477583	-3.081831
H	1.908762	-6.379625	-2.238949
C	3.940732	-6.960283	-0.256512
H	3.055628	-7.308881	0.292250
H	3.989986	-7.516146	-1.201575
H	4.824699	-7.238763	0.338481
C	-7.052530	-3.471661	-0.144546
H	-6.946193	-4.343134	-0.800924
H	-8.072279	-3.075665	-0.238149
H	-6.349860	-2.701412	-0.469084
C	-3.727105	-7.777153	2.369281
H	-4.523705	-8.424417	1.978459
H	-2.764583	-8.186786	2.038448
H	-3.756855	-7.848367	3.467014
C	5.850961	-4.320364	5.224925
H	5.449297	-5.275398	4.860555
H	6.919768	-4.458603	5.435879
H	5.354841	-4.102479	6.182835
C	8.017397	0.139812	1.753055
H	7.246059	0.403408	1.026181
H	8.773211	0.935778	1.759298
H	8.519609	-0.798347	1.475277
C	8.552854	-0.200935	4.141388
H	9.090584	-1.132626	3.923753
H	9.256737	0.634203	4.040343
H	8.200371	-0.222561	5.179129
C	3.370745	-2.330180	-3.977248
H	3.111798	-1.464473	-3.362648
H	3.596163	-1.994157	-4.996566
H	2.517577	-3.017190	-4.012954
C	-7.862477	-4.877993	1.731438
H	-7.744523	-5.190198	2.776115
H	-8.842813	-4.396666	1.623527
H	-7.844997	-5.765784	1.088620
C	-6.939926	-2.631578	2.230108
H	-6.171511	-1.893642	1.992700
H	-7.936734	-2.195085	2.079292
H	-6.832156	-2.919716	3.282952
C	4.972165	-4.188794	-4.353931
H	4.142017	-4.893380	-4.482254
H	5.200152	-3.749633	-5.332739
H	5.859305	-4.735882	-4.008904
C	-4.370462	-4.526150	-3.758595
H	-4.485336	-5.553377	-3.393423
H	-4.598685	-3.836646	-2.941379
H	-5.078239	-4.359100	-4.581065
C	-2.810415	-2.880583	-4.851658
H	-3.554979	-2.751553	-5.648304
H	-2.983913	-2.135357	-4.074326
H	-1.814586	-2.722518	-5.278015
C	-2.683982	-5.290132	-5.418277
H	-2.794350	-6.328302	-5.083183
H	-3.427869	-5.099992	-6.201660
H	-1.686248	-5.158326	-5.855059
C	-8.509377	3.645571	2.778638
H	-9.528493	4.050970	2.692428

H	-7.827728	4.453387	3.079444
H	-8.486804	2.850646	3.528302
C	-8.029514	4.042465	0.514755
H	-9.015933	4.503158	0.356223
H	-7.714107	3.538217	-0.400673
H	-7.300653	4.825817	0.766339
C	-7.888934	-0.260698	4.678220
H	-8.509062	0.178725	5.472935
H	-6.832604	-0.159202	4.940037
H	-8.131682	-1.326557	4.574470
C	-9.431557	0.299447	3.000614
H	-10.133939	0.673967	3.759743
H	-9.668494	-0.750699	2.778229
H	-9.527411	0.901922	2.093156
C	7.166027	-4.635099	1.374759
H	7.684090	-5.523139	1.766087
H	6.114404	-4.880933	1.171539
H	7.205906	-3.837751	2.122789
C	7.798277	-5.155241	-0.823311
H	8.308975	-4.737267	-1.696636
H	6.766388	-5.418419	-1.093757
H	8.332379	-6.057610	-0.490524
C	9.232040	0.324507	-1.528333
H	9.368599	0.936523	-0.625604
H	9.613981	0.874738	-2.399946
H	9.787499	-0.611482	-1.419753
C	7.069736	1.153126	-1.851180
H	7.059760	1.740181	-0.922012
H	6.054364	0.826266	-2.103122
H	7.436440	1.789917	-2.668535

Complex 8 – Quintet

SCF Energy (a.u.): -9531.242967

Ce	-3.799450	-1.024534	-0.813770
Ce	3.583411	0.898944	-0.129788
O	3.977273	3.143283	-0.257267
O	-2.668621	0.386292	0.603775
O	-5.485895	0.477806	-1.141065
O	2.087769	1.481702	1.476123
C	-2.399505	3.314653	-1.524036
C	0.793489	3.478931	1.325991
C	-3.215351	1.439201	1.227021
C	-5.855772	1.625509	-1.720760
C	-4.952505	2.724168	-1.709471
C	-2.276412	3.890119	-2.789853
H	-3.100639	3.855399	-3.494544
C	-5.354468	3.952009	-2.220949
H	-4.667351	4.793488	-2.173604
C	2.229678	4.769982	-0.202138
C	-1.287611	3.341823	-0.676376
H	-1.384104	2.922966	0.319402
C	3.610207	4.405049	-0.172838
C	1.386562	2.441114	2.083026
C	-0.059487	3.900329	-1.037603
C	-7.458514	3.019701	-2.857475
H	-8.428209	3.152258	-3.326072
C	-1.080916	4.512294	-3.147945
H	-0.995716	4.992220	-4.119628
C	1.155743	3.693063	-0.140130
H	1.614072	2.772731	-0.528208
C	-3.602024	2.495661	-1.065755
H	-3.321506	1.475333	-1.345220
C	-6.608200	4.122450	-2.809759
C	-0.066270	4.389443	1.947328
H	-0.532558	5.162889	1.341376
C	0.014282	4.518362	-2.289560
H	0.932136	5.005846	-2.600232
C	1.857573	6.111336	-0.136126
H	0.798236	6.358964	-0.168737
C	-4.287316	3.630745	1.050336
H	-4.656874	4.429513	0.411299
C	-3.721449	2.510847	0.447765
C	-0.353948	4.326125	3.299972
C	0.320939	3.360707	4.051513
H	0.158413	3.353687	5.124713
C	-4.384329	3.743608	2.432675
C	2.790717	7.138446	-0.005079
C	-3.896499	2.677422	3.191535
H	-3.963790	2.762449	4.270460
C	-7.129982	1.770743	-2.319092
C	-3.313439	1.526888	2.647161
C	4.138953	6.771047	0.034574
H	4.873197	7.562957	0.148515
C	1.207533	2.440857	3.501245
C	4.580111	5.447770	-0.059573
O	-4.384322	-2.383863	0.763259
O	3.967851	-1.334711	-1.075075
O	5.013153	-0.162335	1.449931
O	-2.863972	-2.704005	-1.841180
C	1.764207	-2.788447	2.069058
C	-1.344642	-4.162772	-0.756887
C	3.900011	-2.644630	-0.931094
C	5.193888	-1.105369	2.358427
C	4.282837	-2.204736	2.459987
C	1.498383	-2.934530	3.431459
H	2.271463	-2.722102	4.159114
C	4.537056	-3.233189	3.364934
H	3.858194	-4.081591	3.399064
C	-2.947081	-4.262011	1.108538
C	0.716773	-3.044636	1.169767
H	0.922515	-2.979159	0.105162
C	-4.228298	-3.671099	1.105495
C	-2.074802	-3.779989	-1.906187
C	-0.565412	-3.422809	1.588440
C	6.507314	-2.142871	4.123247
H	7.368526	-2.136970	4.783224
C	0.238431	-3.340890	3.863595
H	0.054516	-3.459839	4.928355
C	-1.710003	-3.538574	0.582952
H	-2.009711	-2.496468	0.396009
C	3.110725	-2.331973	1.490731
H	2.936763	-1.329019	1.087367

C	5.628726	-3.220449	4.225375
C	-0.394700	-5.173280	-0.855907
H	0.195358	-5.435830	0.019166
C	-0.788660	-3.581382	2.958810
H	-1.769990	-3.884483	3.309042
C	-2.810633	-5.591514	1.507709
H	-1.818272	-6.036718	1.490964
C	3.487279	-4.595455	0.496142
H	3.151133	-4.988882	1.453351
C	3.500964	-3.215622	0.312124
C	-0.164436	-5.837061	-2.059724
C	-0.980502	-5.519704	-3.144676
H	-0.843561	-6.084408	-4.061523
C	3.886028	-5.478432	-0.498965
C	-3.896652	-6.358128	1.905466
C	4.249858	-4.922013	-1.725505
H	4.531092	-5.606014	-2.520096
C	6.342367	-1.093801	3.216791
C	4.258796	-3.550057	-1.985027
C	-5.160883	-5.766399	1.848798
H	-6.016875	-6.376239	2.120144
C	-1.958237	-4.523817	-3.100629
C	-5.364351	-4.448984	1.448060
N	2.068562	0.889073	-1.799707
N	1.619716	0.798057	-3.069600
K	0.029872	0.258609	0.347192
K	6.552466	-1.854993	-0.225082
K	-6.321146	1.074685	1.506243
O	-8.092937	3.062780	1.548910
O	-8.084767	0.429074	3.447665
O	7.815800	-4.157351	0.193268
O	7.863023	-0.018518	-1.712367
Si	0.324942	-0.377332	-3.391650
C	0.409593	-0.957321	-5.183564
H	-0.312154	-0.440295	-5.822380
H	0.188028	-2.027529	-5.223729
H	1.406927	-0.819682	-5.607756
C	0.545040	-1.788766	-2.180849
H	-0.273699	-1.827547	-1.455363
H	1.500452	-1.672933	-1.660831
H	0.530495	-2.764112	-2.674056
C	-1.375910	0.383790	-3.077426
H	-1.586928	1.240908	-3.722137
H	-1.460423	0.749277	-2.047117
H	-2.128772	-0.392229	-3.266309
Si	2.429059	1.820089	-4.289773
C	1.127579	2.453003	-5.490809
H	1.573750	3.187192	-6.171076
H	0.319188	2.949385	-4.945181
H	0.693525	1.657213	-6.102249
C	3.275869	3.261248	-3.451557
H	2.642492	3.727220	-2.695466
H	3.527258	3.991403	-4.232821
H	4.201391	2.965003	-2.953346
C	3.782191	0.908912	-5.234848
H	4.346980	1.634826	-5.831801
H	4.479649	0.425195	-4.543921
H	3.400941	0.143004	-5.915146
K	3.674467	6.818194	-3.159238
C	-2.846554	0.414797	3.584310
C	-8.110524	0.602433	-2.378309
C	-3.868227	-0.741176	3.571647
H	-4.846553	-0.390819	3.932132
H	-3.530191	-1.543391	4.241078
H	-3.972493	-1.169003	2.569637
C	6.071300	5.124503	-0.042401
C	2.067659	1.570877	4.409886
C	-7.502507	-0.565476	-3.188285
H	-7.308825	-0.248785	-4.219671
H	-8.199180	-1.413208	-3.202100
H	-6.563124	-0.889283	-2.734246
C	-1.313979	5.276605	3.954639
H	-1.701072	6.002374	3.227774
H	-0.835964	5.836800	4.770921
H	-2.173338	4.739393	4.381393
C	-4.943038	4.976607	3.083227
H	-4.148446	5.710514	3.278287
H	-5.417578	4.744023	4.046001
H	-5.686946	5.463441	2.439212
C	6.405831	4.153799	1.112904
H	6.173417	4.621302	2.077307
H	7.476335	3.907249	1.092010
H	5.819316	3.239149	1.022281
C	2.363083	8.574136	0.128621
H	2.016955	8.792252	1.149990
H	1.537127	8.814532	-0.555425
H	3.192492	9.258907	-0.092226
C	-7.016472	5.450954	-3.381309
H	-6.909305	6.257238	-2.641993
H	-8.061820	5.433699	-3.713533
H	-6.395730	5.722508	-4.247027
C	-8.459408	0.099873	-0.957468
H	-7.577398	-0.349947	-0.495672
H	-9.240437	-0.668587	-1.018428
H	-8.833570	0.930093	-0.342603
C	-9.439641	0.988846	-3.054917
H	-9.953722	1.783347	-2.499367
H	-10.091192	0.107136	-3.075782
H	-9.280542	1.318809	-4.088092
C	-1.471761	-0.146687	3.181904
H	-1.552462	-0.721619	2.259890
H	-1.115242	-0.827917	3.960136
H	-0.745842	0.669478	3.084186
C	6.953150	6.373482	0.147586
H	6.819309	7.092447	-0.671036
H	8.004305	6.059395	0.152455
H	6.738781	6.870497	1.101406
C	6.473476	4.485779	-1.389655
H	5.836530	3.622002	-1.593242
H	7.526124	4.173637	-1.358509
H	6.360400	5.212928	-2.205927
C	-2.700441	0.907751	5.039786

H	-2.003619	1.753051	5.093244
H	-2.294518	0.085732	5.640967
H	-3.662760	1.196110	5.480735
C	3.536790	1.985497	4.194851
H	3.674926	3.052323	4.408899
H	3.825836	1.783606	3.161853
H	4.182489	1.396790	4.856582
C	1.951924	0.066584	4.116823
H	2.692285	-0.473542	4.720877
H	2.158563	-0.132618	3.065894
H	0.956385	-0.307981	4.369219
C	1.739902	1.763209	5.902708
H	1.905052	2.798664	6.223628
H	2.404665	1.114313	6.485961
H	0.702947	1.476801	6.122119
C	4.598677	-3.049473	-3.386275
C	7.387571	0.024888	3.157359
C	5.786029	-2.066249	-3.373481
H	6.698547	-2.560545	-3.011107
H	5.984124	-1.706683	-4.391231
H	5.543012	-1.208805	-2.743864
C	-6.771270	-3.869502	1.323501
C	-2.923595	-4.301039	-4.261643
C	6.759524	1.389508	3.499846
H	6.377040	1.384835	4.525483
H	7.518013	2.178319	3.410454
H	5.938232	1.605994	2.816777
C	0.923706	-6.864203	-2.181251
H	0.944496	-7.534416	-1.311115
H	0.792371	-7.477583	-3.081831
H	1.908762	-6.379625	-2.238949
C	3.940732	-6.960283	-0.256512
H	3.055628	-7.308881	0.292250
H	3.989986	-7.516146	-1.201575
H	4.824699	-7.238763	0.338481
C	-7.052530	-3.471661	-0.144546
H	-6.946193	-4.343134	-0.800924
H	-8.072279	-3.075665	-0.238149
H	-6.349860	-2.701412	-0.469084
C	-3.727105	-7.777153	2.369281
H	-4.523705	-8.424417	1.978459
H	-2.764583	-8.186786	2.038448
H	-3.756855	-7.848367	3.467014
C	5.850961	-4.320364	5.224925
H	5.449297	-5.275398	4.860555
H	6.919768	-4.458603	5.435879
H	5.354841	-4.102479	6.182835
C	8.017397	0.139812	1.753055
H	7.246059	0.403408	1.026181
H	8.773211	0.935778	1.759298
H	8.519609	-0.798347	1.475277
C	8.552854	-0.200935	4.141388
H	9.090584	-1.132626	3.923753
H	9.256737	0.634203	4.040343
H	8.200371	-0.222561	5.179129
C	3.370745	-2.330180	-3.977248
H	3.111798	-1.464473	-3.362648
H	3.596163	-1.994157	-4.996566
H	2.517577	-3.017190	-4.012954
C	-7.862477	-4.877993	1.731438
H	-7.744523	-5.190198	2.776115
H	-8.842813	-4.396666	1.623527
H	-7.844997	-5.765784	1.088620
C	-6.939926	-2.631578	2.230108
H	-6.171511	-1.893642	1.992700
H	-7.936734	-2.195085	2.079292
H	-6.832156	-2.919716	3.282952
C	4.972165	-4.188794	-4.353931
H	4.142017	-4.893380	-4.482254
H	5.200152	-3.749633	-5.332739
H	5.859305	-4.735882	-4.008904
C	-4.370462	-4.526150	-3.758595
H	-4.485336	-5.553377	-3.393423
H	-4.598685	-3.836646	-2.941379
H	-5.078239	-4.359100	-4.581065
C	-2.810415	-2.880583	-4.851658
H	-3.554979	-2.751553	-5.648304
H	-2.983913	-2.135357	-4.074326
H	-1.814586	-2.722518	-5.278015
C	-2.683982	-5.290132	-5.418277
H	-2.794350	-6.328302	-5.083183
H	-3.427869	-5.099992	-6.201660
H	-1.686248	-5.158326	-5.855059
C	-8.509377	3.645571	2.778638
H	-9.528493	4.050970	2.692428
H	-7.827728	4.453387	3.079444
H	-8.486804	2.850646	3.528302
C	-8.029514	4.042465	0.514755
H	-9.015933	4.503158	0.356223
H	-7.714107	3.538217	-0.400673
H	-7.300653	4.825817	0.766339
C	-7.888934	-0.260698	4.678220
H	-8.509062	0.178725	5.472935
H	-6.832604	-0.159202	4.940037
H	-8.131682	-1.326557	4.574470
C	-9.431557	0.299447	3.000614
H	-10.133939	0.673967	3.759743
H	-9.668494	-0.750699	2.778229
H	-9.527411	0.901922	2.093156
C	7.166027	-4.635099	1.374759
H	7.684090	-5.523139	1.766087
H	6.114404	-4.880933	1.171539
H	7.205906	-3.837751	2.122789
C	7.798277	-5.155241	-0.823311
H	8.308975	-4.737267	-1.696636
H	6.766388	-5.418419	-1.093757
H	8.332379	-6.057610	-0.490524
C	9.232040	0.324507	-1.528333
H	9.368599	0.936523	-0.625604
H	9.613981	0.874738	-2.399946
H	9.787499	-0.611482	-1.419753
C	7.069736	1.153126	-1.851180

H	7.059760	1.740181	-0.922012
H	6.054364	0.826266	-2.103122
H	7.436440	1.789917	-2.668535

Complex 8 – Quintet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): 0.000000

Ce	-3.799450	-1.024534	-0.813770
Ce	3.583411	0.898944	-0.129788
O	3.977273	3.143283	-0.257267
O	-2.668621	0.386292	0.603775
O	-5.485895	0.477806	-1.141065
O	2.087769	1.481702	1.476123
C	-2.399505	3.314653	-1.524036
C	0.793489	3.478931	1.325991
C	-3.215351	1.439201	1.227021
C	-5.855772	1.625509	-1.720760
C	-4.952505	2.724168	-1.709471
C	-2.276412	3.890119	-2.789853
H	-3.100639	3.855399	-3.494544
C	-5.354468	3.952009	-2.220949
H	-4.667351	4.793488	-2.173604
C	2.229678	4.769982	-0.202138
C	-1.287611	3.341823	-0.676376
H	-1.384104	2.922966	0.319402
C	3.610207	4.405049	-0.172838
C	1.386562	2.441114	2.083026
C	-0.059487	3.900329	-1.037603
C	-7.458514	3.019701	-2.857475
H	-8.428209	3.152258	-3.326072
C	-1.080916	4.512294	-3.147945
H	-0.995716	4.992220	-4.119628
C	1.155743	3.693063	-0.140130
H	1.614072	2.772731	-0.528208
C	-3.602024	2.495661	-1.065755
H	-3.321506	1.475333	-1.345220
C	-6.608200	4.122450	-2.809759
C	-0.066270	4.389443	1.947328
H	-0.532558	5.162889	1.341376
C	0.014282	4.518362	-2.289560
H	0.932136	5.005846	-2.600232
C	1.857573	6.111336	-0.136126
H	0.798236	6.358964	-0.168737
C	-4.287316	3.630745	1.050336
H	-4.656874	4.429513	0.411299
C	-3.721449	2.510847	0.447765
C	-0.353948	4.326125	3.299972
C	0.320939	3.360707	4.051513
H	0.158413	3.353687	5.124713
C	-4.384329	3.743608	2.432675
C	2.790717	7.138446	-0.005079
C	-3.896499	2.677422	3.191535
H	-3.963790	2.762449	4.270460
C	-7.129982	1.770743	-2.319092
C	-3.313439	1.526888	2.647161
C	4.138953	6.771047	0.034574
H	4.873197	7.562957	0.148515
C	1.207533	2.440857	3.501245
C	4.580111	5.447770	-0.059573
O	-4.384322	-2.383863	0.763259
O	3.967851	-1.334711	-1.075075
O	5.013153	-0.162335	1.449931
O	-2.863972	-2.704005	-1.841180
C	1.764207	-2.788447	2.069058
C	-1.344642	-4.162772	-0.756887
C	3.900011	-2.644630	-0.931094
C	5.193888	-1.105369	2.358427
C	4.282837	-2.204736	2.459987
C	1.498383	-2.934530	3.431459
H	2.271463	-2.722102	4.159114
C	4.537056	-3.233189	3.364934
H	3.858194	-4.081591	3.399064
C	-2.947081	-4.262011	1.108538
C	0.716773	-3.044636	1.169767
H	0.922515	-2.979159	0.105162
C	-4.228298	-3.671099	1.105495
C	-2.074802	-3.779989	-1.906187
C	-0.565412	-3.422809	1.588440
C	6.507314	-2.142871	4.123247
H	7.368526	-2.136970	4.783224
C	0.238431	-3.340890	3.863595
H	0.054516	-3.459839	4.928355
C	-1.710003	-3.538574	0.582952
H	-2.009711	-2.496468	0.396009
C	3.110725	-2.331973	1.490731
H	2.936763	-1.329019	1.087367
C	5.628726	-3.220449	4.225375
C	-0.394700	-5.173280	-0.855907
H	0.195358	-5.435830	0.019166
C	-0.788660	-3.581382	2.958810
H	-1.769990	-3.884483	3.309042
C	-2.810633	-5.591514	1.507709
H	-1.818272	-6.036718	1.490964
C	3.487279	-4.595455	0.496142
H	3.151133	-4.988882	1.453351
C	3.500964	-3.215622	0.312124
C	-0.164436	-5.837061	-2.059724
C	-0.980502	-5.519704	-3.144676
H	-0.843561	-6.084408	-4.061523
C	3.886028	-5.478432	-0.498965
C	-3.896652	-6.358128	1.905466
C	4.249858	-4.922013	-1.725505
H	4.531092	-5.606014	-2.520096
C	6.342367	-1.093801	3.216791
C	4.258796	-3.550057	-1.985027
C	-5.160883	-5.766399	1.848798
H	-6.016875	-6.376239	2.120144
C	-1.958237	-4.523817	-3.100629
C	-5.364351	-4.448984	1.448060
N	2.068562	0.889073	-1.799707
N	1.619716	0.798057	-3.069600
K	0.029872	0.258609	0.347192

K	6.552466	-1.854993	-0.225082
K	-6.321146	1.074685	1.506243
O	-8.092937	3.062780	1.548910
O	-8.084767	0.429074	3.447665
O	7.815800	-4.157351	0.193268
O	7.863023	-0.018518	-1.712367
Si	0.324942	-0.377332	-3.391650
C	0.409593	-0.957321	-5.183564
H	-0.312154	-0.440295	-5.822380
H	0.188028	-2.027529	-5.223729
H	1.406927	-0.819682	-5.607756
C	0.545040	-1.788766	-2.180849
H	-0.273699	-1.827547	-1.455363
H	1.500452	-1.672933	-1.660831
H	0.530495	-2.764112	-2.674056
C	-1.375910	0.383790	-3.077426
H	-1.586928	1.240908	-3.722137
H	-1.460423	0.749277	-2.047117
H	-2.128772	-0.392229	-3.266309
Si	2.429059	1.820089	-4.289773
C	1.127579	2.453003	-5.490809
H	1.573750	3.187192	-6.171076
H	0.319188	2.949385	-4.945181
H	0.693525	1.657213	-6.102249
C	3.275869	3.261248	-3.451557
H	2.642492	3.727220	-2.695466
H	3.527258	3.991403	-4.232821
H	4.201391	2.965003	-2.953346
C	3.782191	0.908912	-5.234848
H	4.346980	1.634826	-5.831801
H	4.479649	0.425195	-4.543921
H	3.400941	0.143004	-5.915146
K	3.674467	6.818194	-3.159238
C	-2.846554	0.414797	3.584310
C	-8.110524	0.602433	-2.378309
C	-3.868227	-0.741176	3.571647
H	-4.846553	-0.390819	3.932132
H	-3.530191	-1.543391	4.241078
H	-3.972493	-1.169003	2.569637
C	6.071300	5.124503	-0.042401
C	2.067659	1.570877	4.409886
C	-7.502507	-0.565476	-3.188285
H	-7.308825	-0.248785	-4.219671
H	-8.199180	-1.413208	-3.202100
H	-6.563124	-0.889283	-2.734246
C	-1.313979	5.276605	3.954639
H	-1.701072	6.002374	3.227774
H	-0.835964	5.836800	4.770921
H	-2.173338	4.739393	4.381393
C	-4.943038	4.976607	3.083227
H	-4.148446	5.710514	3.278287
H	-5.417578	4.744023	4.046001
H	-5.686946	5.463441	2.439212
C	6.405831	4.153799	1.112904
H	6.173417	4.621302	2.077307
H	7.476335	3.907249	1.092010
H	5.819316	3.239149	1.022281
C	2.363083	8.574136	0.128621
H	2.016955	8.792252	1.149990
H	1.537127	8.814532	-0.555425
H	3.192492	9.258907	-0.092226
C	-7.016472	5.450954	-3.381309
H	-6.909305	6.257238	-2.641993
H	-8.061820	5.433699	-3.713533
H	-6.395730	5.722508	-4.247027
C	-8.459408	0.099873	-0.957468
H	-7.577398	-0.349947	-0.495672
H	-9.240437	-0.668587	-1.018428
H	-8.833570	0.930093	-0.342603
C	-9.439641	0.988846	-3.054917
H	-9.953722	1.783347	-2.499367
H	-10.091192	0.107136	-3.075782
H	-9.280542	1.318809	-4.088092
C	-1.471761	-0.146687	3.181904
H	-1.552462	-0.721619	2.259890
H	-1.115242	-0.827917	3.960136
H	-0.745842	0.669478	3.084186
C	6.953150	6.373482	0.147586
H	6.819309	7.092447	-0.671036
H	8.004305	6.059395	0.152455
H	6.738781	6.870497	1.101406
C	6.473476	4.485779	-1.389655
H	5.836530	3.622002	-1.593242
H	7.526124	4.173637	-1.358509
H	6.360400	5.212928	-2.205927
C	-2.700441	0.907751	5.039786
H	-2.003619	1.753051	5.093244
H	-2.294518	0.085732	5.640967
H	-3.662760	1.196110	5.480735
C	3.536790	1.985497	4.194851
H	3.674926	3.052323	4.408899
H	3.825836	1.783606	3.161853
H	4.182489	1.396790	4.856582
C	1.951924	0.066584	4.116823
H	2.692285	-0.473542	4.720877
H	2.158563	-0.132618	3.065894
H	0.956385	-0.307981	4.369219
C	1.739902	1.763209	5.902708
H	1.905052	2.798664	6.223628
H	2.404665	1.114313	6.485961
H	0.702947	1.476801	6.122119
C	4.598677	-3.049473	-3.386275
C	7.387571	0.024888	3.157359
C	5.786029	-2.066249	-3.373481
H	6.698547	-2.560545	-3.011107
H	5.984124	-1.706683	-4.391231
H	5.543012	-1.208805	-2.743864
C	-6.771270	-3.869502	1.323501
C	-2.923595	-4.301039	-4.261643
C	6.759524	1.389508	3.499846
H	6.377040	1.384835	4.525483
H	7.518013	2.178319	3.410454

H	5.938232	1.605994	2.816777
C	0.923706	-6.864203	-2.181251
H	0.944496	-7.534416	-1.311115
H	0.792371	-7.477583	-3.081831
H	1.908762	-6.379625	-2.238949
C	3.940732	-6.960283	-0.256512
H	3.055628	-7.308881	0.292250
H	3.989986	-7.516146	-1.201575
H	4.824699	-7.238763	0.338481
C	-7.052530	-3.471661	-0.144546
H	-6.946193	-4.343134	-0.800924
H	-8.072279	-3.075665	-0.238149
H	-6.349860	-2.701412	-0.469084
C	-3.727105	-7.777153	2.369281
H	-4.523705	-8.424417	1.978459
H	-2.764583	-8.186786	2.038448
H	-3.756855	-7.848367	3.467014
C	5.850961	-4.320364	5.224925
H	5.449297	-5.275398	4.860555
H	6.919768	-4.458603	5.435879
H	5.354841	-4.102479	6.182835
C	8.017397	0.139812	1.753055
H	7.246059	0.403408	1.026181
H	8.773211	0.935778	1.759298
H	8.519609	-0.798347	1.475277
C	8.552854	-0.200935	4.141388
H	9.090584	-1.132626	3.923753
H	9.256737	0.634203	4.040343
H	8.200371	-0.222561	5.179129
C	3.370745	-2.330180	-3.977248
H	3.111798	-1.464473	-3.362648
H	3.596163	-1.994157	-4.996566
H	2.517577	-3.017190	-4.012954
C	-7.862477	-4.877993	1.731438
H	-7.744523	-5.190198	2.776115
H	-8.842813	-4.396666	1.623527
H	-7.844997	-5.765784	1.088620
C	-6.939926	-2.631578	2.230108
H	-6.171511	-1.893642	1.992700
H	-7.936734	-2.195085	2.079292
H	-6.832156	-2.919716	3.282952
C	4.972165	-4.188794	-4.353931
H	4.142017	-4.893380	-4.482254
H	5.200152	-3.749633	-5.332739
H	5.859305	-4.735882	-4.008904
C	-4.370462	-4.526150	-3.758595
H	-4.485336	-5.553377	-3.393423
H	-4.598685	-3.836646	-2.941379
H	-5.078239	-4.359100	-4.581065
C	-2.810415	-2.880583	-4.851658
H	-3.554979	-2.751553	-5.648304
H	-2.983913	-2.135357	-4.074326
H	-1.814586	-2.722518	-5.278015
C	-2.683982	-5.290132	-5.418277
H	-2.794350	-6.328302	-5.083183
H	-3.427869	-5.099992	-6.201660
H	-1.686248	-5.158326	-5.855059
C	-8.509377	3.645571	2.778638
H	-9.528493	4.050970	2.692428
H	-7.827728	4.453387	3.079444
H	-8.486804	2.850646	3.528302
C	-8.029514	4.042465	0.514755
H	-9.015933	4.503158	0.356223
H	-7.714107	3.538217	-0.400673
H	-7.300653	4.825817	0.766339
C	-7.888934	-0.260698	4.678220
H	-8.509062	0.178725	5.472935
H	-6.832604	-0.159202	4.940037
H	-8.131682	-1.326557	4.574470
C	-9.431557	0.299447	3.000614
H	-10.133939	0.673967	3.759743
H	-9.668494	-0.750699	2.778229
H	-9.527411	0.901922	2.093156
C	7.166027	-4.635099	1.374759
H	7.684090	-5.523139	1.766087
H	6.114404	-4.880933	1.171539
H	7.205906	-3.837751	2.122789
C	7.798277	-5.155241	-0.823311
H	8.308975	-4.737267	-1.696636
H	6.766388	-5.418419	-1.093757
H	8.332379	-6.057610	-0.490524
C	9.232040	0.324507	-1.528333
H	9.368599	0.936523	-0.625604
H	9.613981	0.874738	-2.399946
H	9.787499	-0.611482	-1.419753
C	7.069736	1.153126	-1.851180
H	7.059760	1.740181	-0.922012
H	6.054364	0.826266	-2.103122
H	7.436440	1.789917	-2.668535

Complex 9 – Doublet

SCF Energy (a.u.): -8658.561932

Ce	-3.355838	-1.365521	-0.900015
Ce	3.477915	1.203284	0.223054
O	3.414293	3.013391	-1.421831
O	-2.959375	0.197456	0.683298
O	-5.049230	-0.098399	-1.712412
O	2.398998	2.393561	1.911276
C	-2.189013	2.980393	-1.805884
C	0.611545	3.853648	1.385298
C	-3.536877	1.349492	1.024125
C	-5.402744	0.986238	-2.411236
C	-4.608419	2.157259	-2.317488
C	-1.942920	3.450858	-3.101138
H	-2.647584	3.252534	-3.901763
C	-5.017391	3.318423	-2.969763
H	-4.419006	4.220397	-2.867690
C	2.245262	4.787701	-0.343764
C	-1.220359	3.204537	-0.826521
H	-1.397520	2.839404	0.179894
C	3.370860	4.289255	-1.058532
C	1.318209	3.020695	2.300910

C	-0.027218	3.892185	-1.077322
C	-6.907736	2.172890	-3.874758
H	-7.794270	2.197551	-4.500418
C	-0.793549	4.201420	-3.356342
H	-0.633664	4.609645	-4.351813
C	1.089573	3.853396	-0.048960
H	1.486561	2.834976	-0.193504
C	-3.386444	2.114483	-1.421301
H	-2.991575	1.095907	-1.483947
C	-6.162994	3.346881	-3.762118
C	-0.489123	4.595433	1.806523
H	-1.000547	5.234691	1.087863
C	0.152491	4.434355	-2.356502
H	1.049904	5.013798	-2.560541
C	2.195191	6.117324	0.059106
H	1.331429	6.455395	0.629451
C	-4.424637	3.525008	0.373532
H	-4.599902	4.262264	-0.407025
C	-3.796830	2.328304	0.031412
C	-0.975466	4.509658	3.107864
C	-0.326195	3.633548	3.981617
H	-0.716294	3.551130	4.992600
C	-4.826148	3.793890	1.676967
C	3.224956	7.007227	-0.231055
C	-4.547296	2.829816	2.649933
H	-4.829410	3.055156	3.672533
C	-6.570430	0.987633	-3.216970
C	-3.913074	1.615939	2.374121
C	4.314454	6.520280	-0.956470
H	5.112319	7.218789	-1.192016
C	0.798795	2.886273	3.628107
C	4.422950	5.195075	-1.379709
O	-4.319612	-2.847030	0.402842
O	4.708682	-0.588082	-0.943346
O	4.422598	-0.031321	2.090874
O	-1.083323	-1.407657	-1.107130
C	2.102906	-2.837348	1.516810
C	-1.456011	-3.707068	-0.661866
C	4.233592	-1.694498	-1.481902
C	5.069673	-1.153645	2.200047
C	4.584911	-2.337467	1.562260
C	2.122759	-2.917506	2.913407
H	3.052496	-2.734636	3.442540
C	5.291388	-3.532738	1.631323
H	4.883238	-4.403768	1.119448
C	-2.718769	-4.278230	1.422497
C	0.884885	-3.070713	0.864823
H	0.859264	-2.990594	-0.214812
C	-4.062154	-3.935711	1.138439
C	-1.110308	-2.663584	-1.561099
C	-0.295821	-3.341793	1.565309
C	6.977945	-2.481326	2.947724
H	7.915659	-2.555954	3.492052
C	0.955044	-3.177300	3.624436
H	0.984895	-3.209438	4.710287
C	-1.631524	-3.408526	0.823820
H	-2.005813	-2.375517	0.929680
C	3.297472	-2.264363	0.775037
H	3.020056	-1.205369	0.722722
C	6.507112	-3.634732	2.309891
C	-1.566932	-5.018350	-1.128086
H	-1.827167	-5.801868	-0.421591
C	-0.254680	-3.369657	2.963950
H	-1.164884	-3.545002	3.529513
C	-2.439639	-5.432717	2.147056
H	-1.401756	-5.692007	2.342247
C	3.075340	-3.838142	-1.220661
H	2.540927	-4.541035	-0.584139
C	3.513609	-2.639268	-0.675609
C	-1.362619	-5.331409	-2.464441
C	-1.057035	-4.288442	-3.346941
H	-0.911275	-4.539560	-4.392756
C	3.278038	-4.157135	-2.566564
C	-3.458291	-6.253363	2.626075
C	3.967869	-3.233766	-3.348682
H	4.125947	-3.482731	-4.394126
C	6.307844	-1.253965	2.919721
C	4.457939	-2.018834	-2.853169
C	-4.776289	-5.894110	2.342528
H	-5.565808	-6.542367	2.709800
C	-0.934907	-2.961735	-2.943683
C	-5.114926	-4.758038	1.605184
N	1.964643	0.514435	-0.458613
K	-0.098002	0.120339	1.020346
K	7.025894	-1.566888	-0.066319
K	-6.453420	0.544274	0.675328
O	-8.313474	2.362288	0.125739
O	-7.999928	0.741320	2.920110
O	7.779663	-3.787836	-1.342257
O	9.267086	-0.065229	-0.151923
K	1.553260	1.691974	-2.767062
C	-3.659037	0.599657	3.496720
C	-7.416321	-0.280395	-3.387061
C	-4.537431	-0.641363	3.280503
H	-5.600542	-0.377845	3.339633
H	-4.343953	-1.389780	4.057361
H	-4.331051	-1.119721	2.319092
C	5.628027	4.719843	-2.197046
C	1.516113	2.004178	4.653677
C	-6.570437	-1.372410	-4.061007
H	-6.248774	-1.049394	-5.055969
H	-7.151349	-2.295244	-4.170601
H	-5.681276	-1.594345	-3.467482
C	-2.132977	5.349030	3.569593
H	-2.714991	5.717521	2.719619
H	-1.799742	6.223236	4.144149
H	-2.812770	4.779853	4.214141
C	-5.545764	5.065879	2.028745
H	-5.345997	5.362976	3.062157
H	-6.633630	4.959624	1.919919
H	-5.236576	5.889714	1.378926
C	6.366625	3.586458	-1.466177

H	6.676703	3.906057	-0.465144
H	7.263533	3.299737	-2.030189
H	5.721426	2.710626	-1.374393
C	3.187122	8.431358	0.249095
H	3.632787	8.535304	1.246847
H	2.159572	8.802938	0.316642
H	3.740201	9.096230	-0.422581
C	-6.565386	4.593884	-4.498984
H	-6.232481	5.493640	-3.972976
H	-7.651283	4.655971	-4.620379
H	-6.125877	4.626178	-5.503460
C	-7.927973	-0.795622	-2.030406
H	-7.100503	-1.161862	-1.420097
H	-8.622307	-1.629923	-2.178870
H	-8.465534	-0.001740	-1.497043
C	-8.646513	-0.036313	-4.266433
H	-9.315276	0.715234	-3.832258
H	-9.211942	-0.968521	-4.363636
H	-8.371778	0.288363	-5.274736
C	-2.185594	0.169752	3.537071
H	-1.969298	-0.507728	2.711752
H	-1.976394	-0.372174	4.465475
H	-1.523502	1.042208	3.501077
C	6.642380	5.839345	-2.445288
H	6.200037	6.674543	-2.998183
H	7.474417	5.450031	-3.042537
H	7.056767	6.229083	-1.509345
C	5.150540	4.207635	-3.565615
H	4.439592	3.391431	-3.426060
H	5.998374	3.841593	-4.158729
H	4.664032	5.013488	-4.126266
C	-3.990842	1.180419	4.875080
H	-3.384061	2.064917	5.095554
H	-3.776272	0.428408	5.640534
H	-5.048772	1.449050	4.972002
C	2.911288	2.595853	4.907141
H	2.824370	3.616256	5.296067
H	3.483471	2.623457	3.978150
H	3.456564	1.992649	5.642217
C	1.653575	0.556789	4.153621
H	2.176183	-0.052131	4.901073
H	2.231911	0.502945	3.230432
H	0.666880	0.099588	4.007031
C	0.775181	1.950942	5.993200
H	0.703568	2.936713	6.464859
H	1.322307	1.295775	6.679547
H	-0.238407	1.546807	5.883775
C	5.191352	-1.039148	-3.778557
C	6.867159	-0.028816	3.645002
C	6.586283	-0.692774	-3.231630
H	7.168497	-1.604184	-3.049703
H	7.137239	-0.075065	-3.950839
H	6.478237	-0.127454	-2.304384
C	-6.573238	-4.430279	1.267281
C	-0.533476	-1.860627	-3.925165
C	5.848513	0.430927	4.697229
H	5.708087	-0.346560	5.456332
H	6.196937	1.341338	5.199587
H	4.889258	0.637051	4.222448
C	-1.439164	-6.749116	-2.955835
H	-1.957977	-7.389980	-2.238099
H	-1.965981	-6.815603	-3.913194
H	-0.436795	-7.167746	-3.108022
C	2.725166	-5.427727	-3.150233
H	1.633250	-5.375062	-3.251795
H	3.141252	-5.624451	-4.143411
H	2.944816	-6.295395	-2.517712
C	-6.776011	-4.476525	-0.255951
H	-6.552774	-5.476859	-0.640046
H	-7.816179	-4.237928	-0.510128
H	-6.121771	-3.762502	-0.758785
C	-3.147993	-7.475607	3.444117
H	-3.914319	-8.246660	3.318752
H	-2.184021	-7.909596	3.162222
H	-3.095388	-7.240469	4.514478
C	7.288586	-4.919769	2.326419
H	7.758747	-5.119850	1.354228
H	8.085211	-4.889332	3.076236
H	6.648614	-5.778300	2.556761
C	7.119287	1.111586	2.644576
H	6.188671	1.393596	2.150414
H	7.519311	1.992053	3.161154
H	7.849066	0.807743	1.884161
C	8.190530	-0.319528	4.356588
H	8.978027	-0.624867	3.656928
H	8.533026	0.588284	4.864495
H	8.084218	-1.102374	5.114909
C	4.381628	0.261030	-3.896735
H	4.219394	0.687117	-2.904070
H	4.913065	1.000082	-4.508252
H	3.417959	0.049036	-4.375355
C	-7.553668	-5.422765	1.897262
H	-7.475813	-5.435795	2.989522
H	-8.578128	-5.134379	1.638049
H	-7.395343	-6.441189	1.528826
C	-6.934435	-3.031863	1.792299
H	-6.253624	-2.293634	1.365949
H	-7.968871	-2.781964	1.520944
H	-6.838959	-2.992702	2.882672
C	5.382599	-1.599260	-5.190621
H	4.426239	-1.815298	-5.678388
H	5.908511	-0.861337	-5.805856
H	5.979317	-2.518107	-5.186240
C	-1.543619	-0.697804	-3.917964
H	-2.567161	-1.053305	-4.103472
H	-1.506692	-0.152330	-2.972185
H	-1.312466	0.013395	-4.720022
C	0.854959	-1.347738	-3.520221
H	1.173829	-0.578491	-4.238860
H	0.871636	-0.952479	-2.498171
H	1.598654	-2.148116	-3.563322
C	-0.445173	-2.379952	-5.362832

H	-1.402868	-2.775820	-5.718681
H	-0.158004	-1.557248	-6.026123
H	0.314488	-3.160996	-5.464027
C	-9.690473	2.271976	0.405509
H	-10.264557	2.029129	-0.500180
H	-10.073455	3.215706	0.820039
H	-9.819159	1.478446	1.144523
C	-8.016859	3.391217	-0.797183
H	-8.544129	3.234432	-1.746231
H	-6.943740	3.362685	-0.991317
H	-8.290635	4.373480	-0.386530
C	-7.992216	2.052806	3.444317
H	-8.995869	2.343485	3.786164
H	-7.676825	2.723282	2.643324
H	-7.292122	2.138382	4.286122
C	-8.410346	-0.205712	3.882246
H	-9.426144	0.012791	4.240694
H	-7.726795	-0.218471	4.742747
H	-8.398991	-1.187084	3.405691
C	6.689636	-4.623357	-1.681784
H	6.812555	-5.621818	-1.238223
H	6.592463	-4.719556	-2.770880
H	5.778741	-4.163496	-1.295504
C	9.003026	-4.280914	-1.824304
H	9.783768	-3.574416	-1.531735
H	8.994585	-4.369760	-2.920579
H	9.233542	-5.267542	-1.395925
C	10.342458	-0.144710	0.754631
H	10.233818	0.586977	1.567347
H	11.302162	0.027468	0.246704
H	10.338938	-1.149994	1.182638
C	9.166280	1.210331	-0.749029
H	8.974387	1.987434	0.003341
H	8.328873	1.182070	-1.448534
H	10.083415	1.462236	-1.299763

Complex 9 – Doublet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -8648.255331

Ce	-3.326322	-1.344187	-0.895718
Ce	3.484742	1.212157	0.217185
O	3.388241	3.035689	-1.408279
O	-2.936659	0.237385	0.668578
O	-5.010023	-0.082730	-1.723326
O	2.375683	2.377796	1.902972
C	-2.183140	3.024112	-1.814585
C	0.597254	3.856624	1.405578
C	-3.534681	1.380798	1.000992
C	-5.373616	0.990911	-2.432063
C	-4.592218	2.172366	-2.344300
C	-1.931609	3.514377	-3.101348
H	-2.628904	3.321835	-3.909794
C	-5.012904	3.322050	-3.005464
H	-4.426527	4.232475	-2.907290
C	2.246803	4.807558	-0.302119
C	-1.221676	3.240875	-0.826395
H	-1.403395	2.860364	0.173387
C	3.369164	4.302347	-1.014039
C	1.297715	3.000530	2.304027
C	-0.030238	3.936999	-1.059483
C	-6.880907	2.145417	-3.913482
H	-7.761518	2.150581	-4.547821
C	-0.784770	4.275670	-3.337963
H	-0.620625	4.698534	-4.326645
C	1.081074	3.880622	-0.026527
H	1.478072	2.863734	-0.182795
C	-3.374233	2.144539	-1.442856
H	-2.968213	1.130036	-1.502306
C	-6.157563	3.330794	-3.802495
C	-0.506644	4.586461	1.838890
H	-1.015967	5.240703	1.132285
C	0.154333	4.499092	-2.329388
H	1.051372	5.083508	-2.519999
C	2.216636	6.131355	0.123631
H	1.352908	6.475274	0.690596
C	-4.443961	3.543816	0.340944
H	-4.619995	4.277249	-0.442909
C	-3.797502	2.354149	0.006229
C	-0.999452	4.469215	3.135289
C	-0.351890	3.572831	3.989347
H	-0.747277	3.462789	4.995680
C	-4.866323	3.807684	1.636998
C	3.266513	7.005544	-0.136497
C	-4.583395	2.846252	2.612287
H	-4.884142	3.064964	3.630833
C	-6.531878	0.968346	-3.245257
C	-3.932321	1.641361	2.346008
C	4.359751	6.505774	-0.849547
H	5.178653	7.189172	-1.056624
C	0.774110	2.834505	3.624968
C	4.449873	5.187770	-1.293550
O	-4.305565	-2.815672	0.403418
O	4.734394	-0.602904	-0.851922
O	4.461760	0.019294	2.078966
O	-1.051969	-1.391550	-1.059944
C	2.098402	-2.834534	1.596127
C	-1.432766	-3.690295	-0.622775
C	4.254828	-1.705860	-1.389211
C	5.096407	-1.103119	2.222712
C	4.576875	-2.313037	1.668113
C	2.108838	-2.944719	2.990492
H	3.035517	-2.775581	3.529212
C	5.236320	-3.524844	1.845018
H	4.780679	-4.421862	1.425789
C	-2.727661	-4.262449	1.437028
C	0.884292	-3.051800	0.931764
H	0.867760	-2.949151	-0.146130
C	-4.064910	-3.913183	1.130857
C	-1.078017	-2.645854	-1.516026
C	-0.301447	-3.336052	1.617846
C	6.983082	-2.422379	3.031754
H	7.931590	-2.479297	3.559366

C	0.935741	-3.217416	3.687816
H	0.958171	-3.273312	4.772961
C	-1.628343	-3.393104	0.860706
H	-1.999827	-2.358838	0.963300
C	3.297808	-2.256749	0.865927
H	3.020049	-1.198318	0.800202
C	6.448658	-3.616524	2.531625
C	-1.532955	-5.001506	-1.091684
H	-1.797245	-5.786646	-0.388560
C	-0.269826	-3.393332	3.015767
H	-1.184013	-3.578607	3.571505
C	-2.466613	-5.424432	2.154724
H	-1.433321	-5.689029	2.366755
C	3.083021	-3.837840	-1.130394
H	2.535792	-4.535354	-0.498817
C	3.529491	-2.645168	-0.581965
C	-1.311280	-5.313055	-2.425292
C	-1.006431	-4.265891	-3.302640
H	-0.848685	-4.513296	-4.347539
C	3.286250	-4.157174	-2.476731
C	-3.497006	-6.247543	2.606088
C	3.984541	-3.237710	-3.257000
H	4.135878	-3.481703	-4.305031
C	6.361117	-1.179113	2.897792
C	4.474743	-2.022810	-2.761425
C	-4.806266	-5.880933	2.297564
H	-5.605985	-6.529589	2.641383
C	-0.893068	-2.940230	-2.897039
C	-5.127917	-4.736561	1.565326
N	1.980935	0.510987	-0.476857
K	-0.079285	0.174126	1.028942
K	7.028724	-1.770277	-0.089934
K	-6.446853	0.547897	0.646209
O	-8.258900	2.399524	0.137635
O	-8.008513	0.701614	2.867134
O	7.663260	-3.963685	-1.553659
O	9.251012	-0.271728	-0.354176
K	1.508242	1.740871	-2.742650
C	-3.684824	0.630970	3.465740
C	-7.352583	-0.308356	-3.411645
C	-4.540045	-0.634518	3.239940
H	-5.609180	-0.385112	3.276935
H	-4.337233	-1.369947	4.029336
H	-4.296779	-1.104365	2.282193
C	5.665294	4.694057	-2.071688
C	1.476135	1.919888	4.622426
C	-6.482873	-1.410334	-4.059887
H	-6.151706	-1.092778	-5.055408
H	-7.063557	-2.336510	-4.156799
H	-5.605783	-1.605559	-3.437559
C	-2.170308	5.282238	3.609615
H	-2.720925	5.703987	2.758959
H	-1.852581	6.118701	4.251162
H	-2.873630	4.669945	4.192549
C	-5.599764	5.070814	1.988485
H	-5.174419	5.541959	2.884277
H	-6.664096	4.874398	2.191559
H	-5.548239	5.796610	1.167497
C	6.364525	3.539338	-1.317574
H	6.682709	3.869711	-0.320812
H	7.246083	3.210561	-1.885185
H	5.674561	2.698421	-1.217610
C	3.246701	8.427445	0.351408
H	3.902565	8.564899	1.224646
H	2.233895	8.724625	0.652714
H	3.587955	9.126519	-0.425262
C	-6.590557	4.581952	-4.513914
H	-6.803087	5.395608	-3.805134
H	-7.498234	4.406010	-5.104438
H	-5.810994	4.945996	-5.197735
C	-7.879848	-0.827654	-2.053078
H	-7.045409	-1.166415	-1.434535
H	-8.549112	-1.681212	-2.218003
H	-8.445065	-0.037282	-1.539492
C	-8.581754	-0.097878	-4.316546
H	-9.265169	0.648542	-3.891887
H	-9.121310	-1.048566	-4.402275
H	-8.287553	0.218433	-5.323986
C	-2.200477	0.212870	3.535677
H	-1.967179	-0.447896	2.699853
H	-2.017360	-0.342734	4.463688
H	-1.551070	1.097216	3.526259
C	6.717928	5.796745	-2.289871
H	6.300692	6.635827	-2.859776
H	7.555677	5.376216	-2.860773
H	7.104718	6.172272	-1.334561
C	5.232459	4.182180	-3.465190
H	4.507062	3.375083	-3.339068
H	6.106872	3.806409	-4.014566
H	4.778483	4.999702	-4.039599
C	-4.050949	1.203544	4.849152
H	-3.458207	2.099024	5.073121
H	-3.829771	0.444694	5.608805
H	-5.118746	1.447672	4.919439
C	2.889218	2.479966	4.900058
H	2.813724	3.484965	5.333626
H	3.449166	2.530595	3.963334
H	3.419112	1.826126	5.604586
C	1.609309	0.477094	4.083953
H	2.129970	-0.145577	4.823508
H	2.197614	0.462155	3.164268
H	0.617519	0.032110	3.921073
C	0.732324	1.832748	5.968887
H	0.671458	2.812318	6.458436
H	1.287553	1.154332	6.628520
H	-0.282040	1.432858	5.838367
C	5.161242	-1.018828	-3.687767
C	6.998655	0.088738	3.451153
C	6.547537	-0.584681	-3.160312
H	7.200012	-1.456433	-3.030294
H	7.020282	0.096090	-3.880764
H	6.413359	-0.064342	-2.209343

C	-6.572404	-4.398935	1.208295
C	-0.494872	-1.840020	-3.870001
C	6.064602	0.717091	4.507436
H	5.941384	0.029832	5.354204
H	6.494445	1.658158	4.875607
H	5.090411	0.914812	4.058019
C	-1.377949	-6.728728	-2.922830
H	-1.809593	-7.392944	-2.164610
H	-1.986597	-6.808044	-3.833864
H	-0.373543	-7.106339	-3.165702
C	2.735270	-5.429881	-3.057978
H	1.634866	-5.429810	-3.033012
H	3.047422	-5.553668	-4.103568
H	3.072050	-6.315117	-2.498535
C	-6.758381	-4.400794	-0.326648
H	-6.537312	-5.396183	-0.729541
H	-7.796660	-4.142333	-0.575532
H	-6.087256	-3.673315	-0.788378
C	-3.202079	-7.483258	3.409050
H	-4.064985	-8.161034	3.425400
H	-2.345610	-8.033301	2.996694
H	-2.955969	-7.234911	4.452231
C	7.127686	-4.937836	2.765380
H	7.087065	-5.579050	1.873455
H	8.184335	-4.797584	3.030370
H	6.653608	-5.495419	3.586926
C	7.227381	1.108907	2.311432
H	6.274216	1.330699	1.826845
H	7.647568	2.037861	2.719142
H	7.926805	0.701422	1.569425
C	8.361531	-0.169279	4.118698
H	9.085395	-0.589791	3.407804
H	8.756079	0.785998	4.486641
H	8.264529	-0.850595	4.972826
C	4.290272	0.252902	-3.799682
H	4.106995	0.643397	-2.795151
H	4.804906	1.019526	-4.394170
H	3.340264	-0.003510	-4.285645
C	-7.577828	-5.406342	1.795745
H	-7.518789	-5.435873	2.890621
H	-8.591752	-5.097269	1.512097
H	-7.405905	-6.414825	1.401556
C	-6.946647	-3.005665	1.760754
H	-6.249160	-2.266242	1.361147
H	-7.975533	-2.754002	1.465308
H	-6.872548	-3.002559	2.855048
C	5.367070	-1.567027	-5.112102
H	4.410021	-1.811404	-5.588725
H	5.865539	-0.799854	-5.717555
H	5.997884	-2.465004	-5.103727
C	-1.498146	-0.660688	-3.863304
H	-2.522050	-1.011107	-4.068984
H	-1.458641	-0.131011	-2.906854
H	-1.236540	0.051273	-4.658405
C	0.903752	-1.325183	-3.474255
H	1.210056	-0.555427	-4.200045
H	0.924687	-0.929019	-2.450499
H	1.641735	-2.132793	-3.524354
C	-0.408856	-2.351328	-5.320570
H	-1.372523	-2.743673	-5.669325
H	-0.122216	-1.514562	-5.969663
H	0.356360	-3.129893	-5.418483
C	-9.657140	2.258621	0.349664
H	-10.164828	1.944388	-0.574495
H	-10.098551	3.205888	0.693392
H	-9.784917	1.495050	1.122002
C	-7.980395	3.402370	-0.837626
H	-8.441961	3.150897	-1.800829
H	-6.896886	3.434037	-0.969815
H	-8.342020	4.383017	-0.495079
C	-7.986954	2.024092	3.400522
H	-8.962961	2.281342	3.838332
H	-7.766761	2.700386	2.571017
H	-7.209011	2.119500	4.170400
C	-8.323128	-0.243199	3.885352
H	-9.320195	-0.043976	4.304550
H	-7.579683	-0.210691	4.695028
H	-8.309846	-1.233079	3.424276
C	6.621236	-4.901068	-1.273272
H	6.959447	-5.926297	-1.488853
H	5.720381	-4.673641	-1.857587
H	6.387161	-4.812245	-0.209851
C	8.025775	-4.036375	-2.924618
H	8.816186	-3.299197	-3.094404
H	7.164859	-3.808316	-3.569746
H	8.405238	-5.038905	-3.174831
C	10.368113	-0.387866	0.518017
H	10.305280	0.342387	1.337546
H	11.309616	-0.237948	-0.030352
H	10.350162	-1.399042	0.935740
C	9.198152	1.025525	-0.941083
H	9.087622	1.801671	-0.170926
H	8.325631	1.047959	-1.597649
H	10.105093	1.222272	-1.531377

Complex 9 – Quartet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -8648.220134

Ce	-3.278317	-1.343387	-0.855429
Ce	3.468876	1.211198	0.157255
O	3.306218	3.054376	-1.450851
O	-2.940642	0.276556	0.680128
O	-4.998331	-0.149070	-1.717026
O	2.189536	2.263872	1.839517
C	-2.265640	3.029458	-1.843407
C	0.504316	3.856569	1.373081
C	-3.575915	1.404858	0.993218
C	-5.393220	0.900757	-2.443994
C	-4.652754	2.109425	-2.368919
C	-2.023147	3.530776	-3.127327
H	-2.721193	3.338414	-3.935079
C	-5.106776	3.234846	-3.049456

H	-4.552502	4.166055	-2.959943
C	2.164012	4.809326	-0.317462
C	-1.302629	3.248154	-0.858271
H	-1.477709	2.859940	0.139569
C	3.291640	4.310273	-1.024866
C	1.173515	2.968509	2.263443
C	-0.115569	3.948543	-1.091766
C	-6.928262	1.982985	-3.951474
H	-7.804607	1.949388	-4.590865
C	-0.881459	4.300794	-3.363122
H	-0.725462	4.733270	-4.349045
C	0.993306	3.882346	-0.058024
H	1.389626	2.867097	-0.221739
C	-3.439361	2.131222	-1.463250
H	-3.008568	1.126494	-1.504607
C	-6.245420	3.193375	-3.854156
C	-0.574444	4.619574	1.814059
H	-1.071937	5.285015	1.109389
C	0.062745	4.519961	-2.357920
H	0.956409	5.110026	-2.547870
C	2.138574	6.126173	0.131937
H	1.270835	6.466752	0.694453
C	-4.544854	3.531557	0.299333
H	-4.742552	4.246710	-0.496178
C	-3.868056	2.353661	-0.017266
C	-1.057019	4.522183	3.115573
C	-0.413545	3.627251	3.975675
H	-0.791838	3.546607	4.991424
C	-4.965508	3.808567	1.593181
C	3.198354	6.996369	-0.096153
C	-4.664879	2.865761	2.581726
H	-4.974578	3.090473	3.596429
C	-6.544924	0.828071	-3.263658
C	-3.986885	1.672184	2.333087
C	4.304058	6.497890	-0.791561
H	5.135566	7.175633	-0.964004
C	0.683632	2.851824	3.602782
C	4.390421	5.188089	-1.258245
O	-4.231333	-2.820968	0.456507
O	4.778221	-0.600666	-0.873889
O	4.526096	0.118740	2.040359
O	-1.000148	-1.365214	-1.008647
C	2.180230	-2.789912	1.647220
C	-1.353420	-3.664429	-0.553308
C	4.301345	-1.718464	-1.379395
C	5.171503	-0.993575	2.208428
C	4.654129	-2.225456	1.698876
C	2.200580	-2.900363	3.040607
H	3.130870	-2.732178	3.573396
C	5.321882	-3.426615	1.914851
H	4.868191	-4.340321	1.531157
C	-2.637782	-4.235086	1.510616
C	0.962571	-3.005563	0.989091
H	0.940711	-2.900806	-0.088647
C	-3.977614	-3.908589	1.193866
C	-1.021632	-2.621584	-1.458133
C	-0.218721	-3.288981	1.681699
C	7.076048	-2.273514	3.040767
H	8.030863	-2.306638	3.559020
C	1.030688	-3.171450	3.744815
H	1.059054	-3.227671	4.829796
C	-1.546980	-3.358100	0.928761
H	-1.927142	-2.326132	1.022620
C	3.371002	-2.213966	0.899626
H	3.070120	-1.165658	0.801321
C	6.541114	-3.487832	2.592627
C	-1.445691	-4.979718	-1.010759
H	-1.690505	-5.762653	-0.298198
C	-0.178787	-3.345239	3.079848
H	-1.089680	-3.529897	3.641193
C	-2.364427	-5.388587	2.238898
H	-1.328825	-5.637909	2.457434
C	3.146521	-3.849884	-1.052981
H	2.610142	-4.534427	-0.398267
C	3.596396	-2.643406	-0.539084
C	-1.244868	-5.298169	-2.346178
C	-0.975493	-4.252832	-3.236407
H	-0.841350	-4.505550	-4.283180
C	3.329796	-4.197552	-2.395407
C	-3.384568	-6.222808	2.690709
C	4.009009	-3.291606	-3.207991
H	4.143390	-3.557889	-4.253102
C	6.446104	-1.039236	2.867863
C	4.500073	-2.063469	-2.747870
C	-4.697751	-5.879744	2.368907
H	-5.489700	-6.539300	2.710189
C	-0.870224	-2.922224	-2.842667
C	-5.031247	-4.746983	1.625488
N	1.847696	0.358368	-0.699936
K	-0.062974	0.280911	1.077558
K	7.076843	-1.752836	-0.112532
K	-6.471052	0.497038	0.622113
O	-8.344903	2.268144	0.072097
O	-8.042884	0.643345	2.836716
O	7.679228	-4.002887	-1.514225
O	9.291781	-0.258757	-0.447510
K	1.492218	1.810164	-2.880390
C	-3.729574	0.677607	3.464814
C	-7.322335	-0.477158	-3.414355
C	-4.560860	-0.604506	3.243989
H	-5.634320	-0.372947	3.266259
H	-4.354409	-1.327702	4.043678
H	-4.298352	-1.081092	2.294636
C	5.624233	4.692291	-2.006258
C	1.397962	1.950578	4.605177
C	-6.412298	-1.561289	-4.036935
H	-6.084167	-1.250500	-5.035621
H	-6.961921	-2.507404	-4.121468
H	-5.534101	-1.717101	-3.405187
C	-2.217138	5.350337	3.591090
H	-2.699135	5.862421	2.747996
H	-1.902465	6.118020	4.314364

H	-2.979729	4.728214	4.082294
C	-5.697506	5.075204	1.934529
H	-5.113132	5.694536	2.628865
H	-6.664537	4.866135	2.415710
H	-5.891273	5.671427	1.034294
C	6.287764	3.517903	-1.249460
H	6.561437	3.821325	-0.231202
H	7.193213	3.199219	-1.783788
H	5.594471	2.674934	-1.205632
C	3.173034	8.416768	0.396065
H	3.991867	8.614711	1.103403
H	2.229134	8.633135	0.912459
H	3.275992	9.136151	-0.429920
C	-6.714864	4.418392	-4.587652
H	-6.948382	5.239081	-3.893764
H	-7.618536	4.206012	-5.172326
H	-5.947460	4.791106	-5.280587
C	-7.842207	-0.989042	-2.050248
H	-7.001454	-1.287951	-1.419815
H	-8.480867	-1.867809	-2.203645
H	-8.437599	-0.208837	-1.555469
C	-8.550651	-0.322479	-4.331450
H	-9.261687	0.407729	-3.924319
H	-9.057819	-1.291838	-4.404970
H	-8.259208	-0.013300	-5.341928
C	-2.239492	0.284947	3.551659
H	-1.985762	-0.373698	2.720028
H	-2.057887	-0.264233	4.483872
H	-1.604712	1.179511	3.545649
C	6.695601	5.786571	-2.171090
H	6.305972	6.639998	-2.739136
H	7.546528	5.366482	-2.722424
H	7.055697	6.141020	-1.197486
C	5.234527	4.207190	-3.421998
H	4.500806	3.402498	-3.334588
H	6.124743	3.835647	-3.948282
H	4.805155	5.037489	-3.996909
C	-4.117365	1.256565	4.839623
H	-3.542659	2.164604	5.060059
H	-3.889074	0.508915	5.608240
H	-5.189917	1.482178	4.898857
C	2.828887	2.493270	4.821330
H	2.787442	3.514202	5.220545
H	3.360670	2.496963	3.866698
H	3.368497	1.852776	5.530911
C	1.503440	0.488312	4.113594
H	2.013878	-0.116937	4.874164
H	2.092813	0.436725	3.195678
H	0.506031	0.052136	3.964379
C	0.691481	1.918349	5.973781
H	0.657460	2.914415	6.431476
H	1.255274	1.254449	6.640717
H	-0.331566	1.529274	5.884081
C	5.160086	-1.071205	-3.705737
C	7.085777	0.251755	3.363533
C	6.549523	-0.611055	-3.208999
H	7.216302	-1.471798	-3.077257
H	7.000779	0.064150	-3.948440
H	6.423743	-0.078566	-2.263519
C	-6.477366	-4.439101	1.248440
C	-0.516282	-1.827345	-3.839873
C	6.166232	0.919588	4.408904
H	6.058581	0.266176	5.284037
H	6.600320	1.874891	4.732906
H	5.183758	1.096536	3.968656
C	-1.301214	-6.718588	-2.831325
H	-1.749436	-7.375643	-2.076412
H	-1.888986	-6.806285	-3.755036
H	-0.291601	-7.098680	-3.047721
C	2.775664	-5.485284	-2.939591
H	1.675400	-5.484076	-2.909575
H	3.082413	-5.636981	-3.983098
H	3.115010	-6.355452	-2.358498
C	-6.643921	-4.460957	-0.288579
H	-6.399446	-5.456419	-0.677548
H	-7.683424	-4.224234	-0.553369
H	-5.980391	-3.726383	-0.750019
C	-3.080377	-7.444874	3.510824
H	-3.841264	-8.222769	3.365850
H	-2.103663	-7.869213	3.244771
H	-3.051422	-7.209767	4.585550
C	7.226945	-4.796749	2.872090
H	7.175589	-5.475484	2.008957
H	8.286870	-4.643487	3.116084
H	6.765859	-5.320246	3.722957
C	7.295210	1.226988	2.181602
H	6.333875	1.427284	1.704431
H	7.719837	2.171835	2.545990
H	7.983117	0.791802	1.444657
C	8.459108	0.024359	4.020988
H	9.174064	-0.422130	3.317057
H	8.855671	0.994585	4.345085
H	8.376476	-0.622874	4.902666
C	4.272004	0.188473	-3.829136
H	4.075712	0.580455	-2.827871
H	4.778961	0.957096	-4.428682
H	3.326367	-0.084896	-4.313419
C	-7.471374	-5.458729	1.834325
H	-7.424972	-5.476044	2.930074
H	-8.487214	-5.171057	1.535390
H	-7.276535	-6.467867	1.452710
C	-6.884515	-3.047389	1.781051
H	-6.195931	-2.299275	1.382500
H	-7.914121	-2.818407	1.469962
H	-6.824607	-3.031319	2.876127
C	5.349268	-1.646001	-5.121881
H	4.387311	-1.911308	-5.576879
H	5.828174	-0.885553	-5.751302
H	5.990946	-2.536122	-5.106327
C	-1.502188	-0.634479	-3.784143
H	-2.541342	-0.970360	-3.933967
H	-1.402580	-0.100558	-2.834548

H	-1.276648	0.068206	-4.598392
C	0.907540	-1.326158	-3.525994
H	1.185631	-0.569492	-4.277008
H	0.990454	-0.911024	-2.512517
H	1.631798	-2.144853	-3.599941
C	-0.519880	-2.343341	-5.291947
H	-1.503480	-2.736899	-5.578236
H	-0.274499	-1.508315	-5.959919
H	0.237636	-3.121922	-5.436902
C	-9.738534	2.107978	0.299059
H	-10.250712	1.780687	-0.618012
H	-10.190442	3.050680	0.641799
H	-9.847056	1.347492	1.077294
C	-8.090129	3.270036	-0.910180
H	-8.558961	3.008404	-1.867264
H	-7.008600	3.315723	-1.054696
H	-8.461040	4.247354	-0.567872
C	-8.057141	1.975099	3.346405
H	-9.042455	2.216704	3.772122
H	-7.846372	2.641905	2.506644
H	-7.287895	2.102673	4.120418
C	-8.340509	-0.290872	3.869665
H	-9.345456	-0.110039	4.278302
H	-7.604102	-0.224738	4.683695
H	-8.298294	-1.288118	3.426533
C	6.664644	-4.943007	-1.154269
H	6.995123	-5.968653	-1.379976
H	5.725618	-4.729353	-1.681020
H	6.501839	-4.843062	-0.078664
C	7.946255	-4.089839	-2.906682
H	8.721928	-3.353900	-3.138497
H	7.041678	-3.869546	-3.491515
H	8.309926	-5.094573	-3.171325
C	10.413178	-0.357864	0.421328
H	10.367822	0.405629	1.211161
H	11.353002	-0.245682	-0.138787
H	10.382071	-1.350905	0.879846
C	9.254648	1.014854	-1.084548
H	9.160609	1.821839	-0.344348
H	8.378300	1.023953	-1.736608
H	10.160820	1.174685	-1.687051

Complex 10 – Triplet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -9057.321766

Ce	3.554087	1.271672	-0.307304
Ce	-3.558209	-1.197540	-0.051712
O	-3.776625	-3.190386	-1.259179
O	2.728130	-0.538467	0.948672
O	5.256851	-0.011666	-1.095979
O	-2.221493	-2.290824	1.515537
C	2.351998	-2.954924	-1.876869
C	-0.680454	-4.012696	0.973228
C	3.350577	-1.677562	1.221400
C	5.647811	-0.989380	-1.913759
C	4.836191	-2.148631	-2.046795
C	2.229505	-3.324520	-3.219506
H	3.010922	-3.082214	-3.931412
C	5.304686	-3.226817	-2.793303
H	4.694175	-4.123646	-2.866115
C	-2.158080	-4.912870	-0.876460
C	1.282316	-3.221461	-1.020452
H	1.370145	-2.937974	0.022710
C	-3.471607	-4.484189	-1.211451
C	-1.316855	-3.163143	1.917272
C	0.114212	-3.866010	-1.431552
C	7.273876	-2.003968	-3.373259
H	8.205897	-1.955223	-3.928094
C	1.099909	-4.025233	-3.640729
H	1.034990	-4.357838	-4.674013
C	-1.081140	-3.912061	-0.489274
H	-1.514786	-2.906826	-0.600926
C	3.521579	-2.170201	-1.290555
H	3.164798	-1.136062	-1.288255
C	6.527468	-3.180230	-3.461121
C	0.308726	-4.903680	1.387652
H	0.802821	-5.524494	0.642480
C	0.057736	-4.311703	-2.758178
H	-0.795653	-4.903017	-3.085699
C	-1.848624	-6.272100	-0.888778
H	-0.836773	-6.575243	-0.627059
C	4.354601	-3.771089	0.446487
H	4.624965	-4.411438	-0.390541
C	3.755452	-2.541028	0.168797
C	0.714018	-4.986997	2.713093
C	0.083037	-4.146750	3.633142
H	0.394844	-4.215266	4.671174
C	4.612503	-4.187831	1.746331
C	-2.786035	-7.243936	-1.213056
C	4.251186	-3.311269	2.776587
H	4.450783	-3.628677	3.794633
C	6.873737	-0.897039	-2.621365
C	3.640197	-2.074822	2.566187
C	-4.076600	-6.810425	-1.523943
H	-4.816830	-7.567424	-1.764935
C	-0.925614	-3.248515	3.289806
C	-4.452037	-5.469588	-1.525318
O	3.945443	2.655774	1.358068
O	-4.767034	0.669600	-0.970641
O	-4.876989	-0.340033	1.789147
O	3.028293	3.005418	-1.526509
C	-2.140876	2.591442	1.734398
C	1.130873	4.228889	-0.803919
C	-4.502786	1.942872	-1.181997
C	-5.233791	0.757687	2.408535
C	-4.581631	1.994490	2.139406
C	-1.930842	2.516564	3.115485
H	-2.730389	2.163488	3.757709
C	-4.981347	3.165214	2.782809
H	-4.444924	4.086284	2.562153
C	2.457115	4.520472	1.286130
C	-1.077716	3.021526	0.923895

H	-1.215335	3.052793	-0.151325
C	3.718885	3.956919	1.583681
C	2.046810	3.859630	-1.819175
C	0.155527	3.408393	1.468776
C	-6.692027	1.982318	3.932613
H	-7.518627	1.993495	4.636803
C	-0.708429	2.889818	3.666995
H	-0.564103	2.827956	4.742492
C	1.374224	3.704182	0.599279
H	1.803138	2.705182	0.482847
C	-3.445288	2.066765	1.131972
H	-3.203151	1.040946	0.852809
C	-6.030344	3.191301	3.692290
C	0.100570	5.114716	-1.097012
H	-0.605024	5.387399	-0.315164
C	0.325258	3.342492	2.856298
H	1.275907	3.640826	3.287993
C	2.203698	5.859070	1.571473
H	1.225673	6.266243	1.323225
C	-3.852611	4.121369	-0.287234
H	-3.418248	4.710085	0.519124
C	-3.906237	2.738780	-0.153781
C	-0.067157	5.630446	-2.380400
C	0.849511	5.258306	-3.361035
H	0.713755	5.666491	-4.357522
C	-4.350409	4.771878	-1.416838
C	3.169182	6.680673	2.137308
C	-4.788683	3.970778	-2.471985
H	-5.102327	4.472940	-3.383155
C	-6.341082	0.777866	3.326651
C	-4.840536	2.574570	-2.414450
C	4.426005	6.122748	2.380004
H	5.193405	6.771848	2.790144
C	1.911642	4.385202	-3.123455
C	4.737964	4.791199	2.113674
N	-1.832169	-0.493363	-1.208637
K	-0.158354	-0.500469	1.103823
K	-7.049639	1.174346	0.184434
K	6.509626	-1.403168	0.976261
O	8.388465	-3.245578	0.339552
O	8.731755	-0.597824	2.210153
O	-8.273988	3.559007	-0.088178
O	-8.630112	-0.292315	-1.355677
Si	-0.862502	0.439631	-2.213361
C	0.909107	0.702920	-1.501057
H	1.327623	-0.273069	-1.233029
H	0.833188	1.367452	-0.630197
H	1.518451	1.201046	-2.260456
C	-1.380230	2.178493	-2.772618
H	-0.501508	2.771190	-3.052201
H	-1.938698	2.735438	-2.018155
H	-2.029720	2.119311	-3.653047
C	-0.353456	-0.326617	-3.919056
H	0.380214	0.351625	-4.369921
H	-1.175753	-0.379769	-4.649005
H	0.138701	-1.305883	-3.843428
K	-2.361380	-2.316044	-3.259522
C	3.329573	-1.164418	3.751011
C	7.686472	0.396176	-2.609250
C	4.247938	0.073847	3.698890
H	5.305298	-0.224644	3.763062
H	4.034474	0.738196	4.546204
H	4.074426	0.646193	2.783556
C	-5.890129	-5.057265	-1.820030
C	-1.681341	-2.480284	4.371983
C	6.841086	1.537954	-3.221766
H	6.573033	1.298790	-4.257449
H	7.413979	2.473827	-3.211510
H	5.923331	1.685551	-2.648725
C	1.771332	-5.956766	3.155926
H	2.299279	-6.378993	2.291663
H	1.340517	-6.792438	3.727876
H	2.516449	-5.466413	3.798213
C	5.247547	-5.516301	2.050786
H	5.300607	-6.142251	1.150524
H	4.666556	-6.066724	2.802042
H	6.268553	-5.404580	2.447056
C	-6.486846	-4.354266	-0.578395
H	-6.465855	-5.034642	0.281053
H	-7.528317	-4.065993	-0.771452
H	-5.902432	-3.464305	-0.333781
C	-2.441694	-8.706759	-1.191602
H	-3.009516	-9.263212	-1.949305
H	-2.669226	-9.158632	-0.214153
H	-1.372523	-8.865236	-1.383748
C	7.028700	-4.359915	-4.246862
H	6.196900	-4.956949	-4.641424
H	7.644016	-5.028868	-3.624391
H	7.650401	-4.040567	-5.093099
C	8.109942	0.806409	-1.179303
H	7.228043	1.012684	-0.569516
H	8.714408	1.721217	-1.227581
H	8.716470	0.020749	-0.711437
C	8.978096	0.278026	-3.440798
H	9.641832	-0.499220	-3.039744
H	9.509340	1.236330	-3.400536
H	8.758586	0.054430	-4.491257
C	1.860603	-0.689621	3.743743
H	1.713817	0.043024	2.948920
H	1.625364	-0.208446	4.701064
H	1.189771	-1.546853	3.609963
C	-6.798226	-6.260144	-2.139843
H	-6.845838	-6.958011	-1.295635
H	-6.448421	-6.798301	-3.029478
H	-7.812870	-5.891993	-2.337464
C	-5.953958	-4.107518	-3.039282
H	-5.377731	-3.203012	-2.830048
H	-6.997363	-3.836201	-3.250263
H	-5.544122	-4.611038	-3.925172
C	3.559404	-1.867969	5.103232
H	2.918668	-2.753742	5.197584
H	3.300176	-1.167875	5.905971

H	4.607876	-2.161173	5.240662
C	-3.093096	-3.100979	4.461769
H	-3.017331	-4.162228	4.728057
H	-3.593310	-3.007442	3.494296
H	-3.687884	-2.581248	5.222410
C	-1.826617	-0.966844	4.087528
H	-2.350063	-0.491632	4.927653
H	-2.414396	-0.799960	3.184354
H	-0.843535	-0.485542	4.001297
C	-1.019926	-2.611943	5.758792
H	-1.000622	-3.653706	6.099521
H	-1.608477	-2.031868	6.480031
H	0.004061	-2.216784	5.751024
C	-5.273979	1.781393	-3.651032
C	-7.112095	-0.500478	3.643743
C	-4.603794	0.388185	-3.743814
H	-5.031192	-0.300288	-3.014915
H	-4.753757	-0.004568	-4.760511
H	-3.532930	0.478554	-3.535061
C	6.144078	4.251759	2.358366
C	2.900830	4.013875	-4.223693
C	-6.148185	-1.565362	4.200179
H	-5.702493	-1.211133	5.137619
H	-6.690593	-2.499422	4.398153
H	-5.353197	-1.748637	3.477535
C	-1.235271	6.509290	-2.716632
H	-1.454914	7.218023	-1.907052
H	-1.050901	7.084280	-3.633282
H	-2.138455	5.902103	-2.873288
C	-4.452135	6.270424	-1.472536
H	-3.644345	6.747779	-0.903964
H	-4.403429	6.642421	-2.504103
H	-5.404829	6.619648	-1.042472
C	6.745104	3.721493	1.036046
H	6.791550	4.523802	0.290157
H	7.762651	3.345924	1.211618
H	6.128305	2.912215	0.640568
C	2.880525	8.116758	2.472453
H	3.749102	8.757650	2.269600
H	2.034746	8.495892	1.884907
H	2.624389	8.239513	3.535810
C	-6.450507	4.459112	4.383326
H	-5.702079	5.248737	4.239363
H	-7.410688	4.839007	3.999596
H	-6.573669	4.305287	5.464201
C	-7.786584	-1.059397	2.371072
H	-7.029292	-1.249428	1.604747
H	-8.291458	-2.006756	2.600032
H	-8.552754	-0.364865	1.994731
C	-8.226466	-0.285974	4.684544
H	-8.982100	0.426238	4.328108
H	-8.721045	-1.248031	4.866837
H	-7.816133	0.073070	5.635798
C	-4.884576	2.530207	-4.947925
H	-3.809163	2.741231	-4.958846
H	-5.132762	1.901011	-5.811904
H	-5.430663	3.473067	-5.057851
C	7.107819	5.330952	2.887668
H	6.770101	5.726759	3.852931
H	8.096888	4.877166	3.031208
H	7.209441	6.159357	2.176426
C	6.108933	3.116175	3.403636
H	5.456598	2.313003	3.059917
H	7.123198	2.726055	3.565370
H	5.727663	3.498454	4.358524
C	-6.805346	1.588934	-3.670653
H	-7.305856	2.563032	-3.719518
H	-7.099284	1.001342	-4.552193
H	-7.147503	1.060400	-2.775873
C	4.327715	4.456122	-3.823503
H	4.365575	5.547368	-3.721033
H	4.608956	4.000186	-2.871540
H	5.041511	4.148459	-4.599413
C	2.893225	2.489167	-4.479418
H	3.579088	2.248754	-5.302509
H	3.218266	1.954835	-3.584484
H	1.884187	2.154482	-4.751671
C	2.566044	4.695800	-5.563863
H	2.591982	5.788221	-5.471133
H	3.316666	4.396510	-6.305795
H	1.578202	4.390191	-5.930549
C	7.929535	-4.422225	-0.325137
H	7.070652	-4.793217	0.236945
H	8.718457	-5.188988	-0.340718
H	7.616725	-4.188956	-1.350727
C	9.525386	-2.710821	-0.332412
H	10.348242	-3.441158	-0.344722
H	9.831877	-1.820375	0.222812
H	9.269704	-2.432525	-1.364542
C	9.361194	-1.561025	3.050188
H	9.046049	-1.436388	4.096478
H	10.456001	-1.469979	2.994249
H	9.063792	-2.546965	2.681376
C	9.136434	0.723861	2.550081
H	10.225516	0.835335	2.444609
H	8.844814	0.973896	3.580051
H	8.633247	1.405930	1.860809
C	-7.520040	4.492708	0.688077
H	-8.056151	5.450699	0.761465
H	-6.527616	4.655487	0.245026
H	-7.393790	4.062436	1.684362
C	-8.447427	4.054975	-1.411145
H	-9.014861	3.303862	-1.968939
H	-7.474173	4.212962	-1.897409
H	-9.008289	5.001748	-1.400683
C	-8.073382	-1.363463	-2.106486
H	-8.280535	-1.240551	-3.179468
H	-8.468867	-2.328062	-1.762868
H	-6.992105	-1.345382	-1.948927
C	-10.041126	-0.237794	-1.503417
H	-10.319650	-0.100897	-2.558820
H	-10.395901	0.618313	-0.921820

H -10.512354 -1.156249 -1.124038

Complex 10 – Quintet
(Optimised at the PBE0-D3BJ/BS1′ level of theory)
SCF Energy (a.u.): -9057.235194

Ce 3.653233 1.249851 -0.342326
Ce -3.573643 -1.090819 -0.141900
O -3.765654 -3.010125 -1.353036
O 2.844806 -0.552563 0.911353
O 5.328336 -0.053989 -1.134924
O -2.213618 -2.024488 1.432390
C 2.414969 -2.976517 -1.919472
C -0.683051 -3.768486 0.927971
C 3.446952 -1.708455 1.179789
C 5.730462 -1.036316 -1.943169
C 4.918037 -2.197188 -2.076621
C 2.312335 -3.454274 -3.228197
H 3.117889 -3.300511 -3.937606
C 5.402775 -3.285661 -2.795422
H 4.798015 -4.186603 -2.863137
C -2.175523 -4.719260 -0.828317
C 1.309156 -3.126090 -1.079970
H 1.377592 -2.750212 -0.064483
C -3.503844 -4.296409 -1.089345
C -1.332420 -2.920565 1.859933
C 0.132412 -3.763676 -1.471892
C 7.385484 -2.072489 -3.352425
H 8.330574 -2.034455 -3.885234
C 1.164247 -4.138850 -3.625287
H 1.098955 -4.533651 -4.635614
C -1.071703 -3.712816 -0.543012
H -1.493726 -2.715249 -0.722719
C 3.594823 -2.206322 -1.336472
H 3.259074 -1.166580 -1.333160
C 6.637806 -3.246260 -3.443390
C 0.287418 -4.668394 1.368939
H 0.795814 -5.291244 0.636485
C 0.089376 -4.312542 -2.755883
H -0.785627 -4.873145 -3.075320
C -1.894790 -6.080872 -0.725174
H -0.868077 -6.389074 -0.541130
C 4.371396 -3.834384 0.397881
H 4.605905 -4.487529 -0.439845
C 3.812647 -2.584728 0.124353
C 0.647750 -4.766857 2.705663
C -0.007124 -3.932595 3.613338
H 0.264619 -4.016091 4.661111
C 4.632410 -4.256710 1.695033
C -2.884139 -7.048742 -0.833476
C 4.325291 -3.361871 2.726050
H 4.537627 -3.678978 3.741398
C 6.971121 -0.954399 -2.622720
C 3.753505 -2.105402 2.520091
C -4.200688 -6.607095 -0.975879
H -4.983335 -7.358130 -0.998244
C -0.994358 -3.020880 3.243421
C -4.549215 -5.261950 -1.082635
O 3.956831 2.596486 1.370780
O -4.343358 0.885148 -1.147615
O -5.140915 -0.296087 1.418053
O 2.984158 2.986562 -1.490811
C -2.170151 2.559963 1.903529
C 1.056552 4.133858 -0.732191
C -4.309405 2.205289 -1.122205
C -5.411144 0.690661 2.259120
C -4.634209 1.883396 2.259990
C -1.933462 2.513119 3.278959
H -2.721715 2.187177 3.947911
C -4.965129 2.931499 3.119093
H -4.361841 3.836391 3.094245
C 2.429116 4.427076 1.309275
C -1.116364 2.949421 1.058390
H -1.285428 2.954786 -0.014350
C 3.711140 3.898239 1.574118
C 1.981547 3.822646 -1.759904
C 0.137134 3.320792 1.561940
C -6.776215 1.677216 4.010846
H -7.606509 1.611779 4.706728
C -0.689111 2.873680 3.793160
H -0.520624 2.833920 4.866070
C 1.336410 3.590701 0.657861
H 1.763481 2.587418 0.526328
C -3.478723 2.067358 1.285343
H -3.220934 1.081261 0.897904
C -6.025856 2.855694 4.011118
C -0.001924 4.997183 -0.994420
H -0.710828 5.229440 -0.202974
C 0.335905 3.281825 2.948723
H 1.301692 3.571143 3.352105
C 2.153439 5.765204 1.582532
H 1.158364 6.145635 1.361412
C -3.976679 4.262089 0.163059
H -3.656760 4.743036 1.085598
C -3.909978 2.879152 0.072254
C -0.191280 5.546373 -2.261133
C 0.738537 5.237590 -3.252155
H 0.588963 5.672458 -4.235076
C -4.450412 5.045326 -0.889291
C 3.117323 6.619256 2.097503
C -4.785528 4.383321 -2.066834
H -5.129941 4.989154 -2.901806
C -6.515428 0.598501 3.167654
C -4.695480 2.996079 -2.242476
C 4.396025 6.095294 2.302573
H 5.162143 6.770326 2.670742
C 1.831286 4.394289 -3.043758
C 4.729703 4.767161 2.050188
N -1.601234 -0.125812 -0.975919
K -0.023980 -0.253208 1.303511
K -6.916462 0.908269 -0.456847
K 6.606874 -1.538790 0.894288
O 8.489094 -3.391305 0.368266

O	8.713269	-0.690790	2.257431
O	-8.270500	3.170315	-0.073396
O	-8.260002	-0.735706	-2.084469
Si	-0.701960	0.363856	-2.364724
C	1.113783	0.479045	-1.812023
H	1.393794	-0.442830	-1.294734
H	1.128016	1.351470	-1.145258
H	1.788107	0.663024	-2.654052
C	-1.213120	2.088376	-2.925126
H	-0.429699	2.814255	-2.693780
H	-2.134756	2.424802	-2.444593
H	-1.370946	2.095894	-4.008379
C	-0.760901	-0.819015	-3.829877
H	-0.056486	-0.514338	-4.612959
H	-1.759832	-0.810910	-4.282713
H	-0.500534	-1.840744	-3.536744
K	-3.388366	-3.345158	-4.106743
C	3.520464	-1.177334	3.709824
C	7.795249	0.331322	-2.593471
C	4.512169	0.002005	3.634621
H	5.550730	-0.359548	3.674280
H	4.358411	0.679248	4.484614
H	4.349580	0.582951	2.722374
C	-6.016590	-4.836196	-1.113531
C	-1.765735	-2.240139	4.304957
C	6.971814	1.484520	-3.214712
H	6.720637	1.252640	-4.256120
H	7.554041	2.414259	-3.189323
H	6.045022	1.637090	-2.657244
C	1.679238	-5.752476	3.173385
H	2.191063	-6.213696	2.319912
H	1.224497	-6.556953	3.770127
H	2.441136	-5.265626	3.798013
C	5.213890	-5.610094	1.995151
H	5.290207	-6.216246	1.083282
H	4.583242	-6.160742	2.705816
H	6.217447	-5.537040	2.440986
C	-6.324079	-3.951945	0.117108
H	-6.129430	-4.501850	1.045477
H	-7.376091	-3.637894	0.102241
H	-5.697562	-3.057476	0.109490
C	-2.557866	-8.514331	-0.784406
H	-3.342879	-9.082202	-0.267579
H	-1.609128	-8.690917	-0.261733
H	-2.461236	-8.935581	-1.796488
C	7.127806	-4.424737	-4.238104
H	6.521466	-4.577581	-5.142196
H	7.076987	-5.355265	-3.654553
H	8.167994	-4.281862	-4.556425
C	8.200260	0.728891	-1.154672
H	7.310659	0.928427	-0.553244
H	8.804941	1.644261	-1.185624
H	8.802708	-0.060767	-0.687286
C	9.098734	0.204430	-3.405189
H	9.751297	-0.576703	-2.993708
H	9.635835	1.159091	-3.357186
H	8.893535	-0.018583	-4.458608
C	2.086540	-0.604905	3.733577
H	1.982831	0.141593	2.945582
H	1.904415	-0.113429	4.697403
H	1.356116	-1.414587	3.610763
C	-6.976058	-6.041828	-1.050221
H	-6.823855	-6.626694	-0.135538
H	-6.849945	-6.694987	-1.922138
H	-8.007382	-5.667357	-1.049900
C	-6.373325	-4.053174	-2.393795
H	-5.825647	-3.107938	-2.431359
H	-7.449091	-3.834520	-2.399486
H	-6.148203	-4.650272	-3.287995
C	3.734544	-1.890395	5.059632
H	3.050918	-2.742031	5.166124
H	3.525689	-1.176814	5.865148
H	4.768104	-2.237472	5.181323
C	-3.224059	-2.744791	4.298996
H	-3.254567	-3.815870	4.531777
H	-3.665708	-2.577795	3.314225
H	-3.811801	-2.198039	5.046767
C	-1.780545	-0.718346	4.050847
H	-2.358959	-0.221644	4.840148
H	-2.260101	-0.498271	3.095648
H	-0.764382	-0.302285	4.080853
C	-1.197147	-2.449480	5.721467
H	-1.255858	-3.500346	6.027612
H	-1.793845	-1.857032	6.425710
H	-0.154058	-2.112807	5.785634
C	-5.048369	2.440082	-3.628490
C	-7.385625	-0.656900	3.236634
C	-4.641630	0.970939	-3.874231
H	-5.217386	0.276295	-3.259099
H	-4.814106	0.734991	-4.932869
H	-3.584208	0.813640	-3.648411
C	6.154381	4.265959	2.267864
C	2.836390	4.103745	-4.153846
C	-6.528388	-1.883989	3.606871
H	-6.087462	-1.749714	4.600635
H	-7.154038	-2.786189	3.617266
H	-5.726228	-2.007502	2.878043
C	-1.384544	6.407513	-2.557854
H	-1.508418	7.197695	-1.803880
H	-1.291115	6.889135	-3.539303
H	-2.307499	5.809156	-2.560383
C	-4.576451	6.536375	-0.754751
H	-3.591580	7.023371	-0.729335
H	-5.132001	6.962482	-1.600043
H	-5.101544	6.811957	0.170456
C	6.731246	3.686108	0.955674
H	6.730899	4.448409	0.167481
H	7.764250	3.349046	1.118602
H	6.129760	2.838153	0.622659
C	2.811792	8.056798	2.410092
H	3.576816	8.728984	1.997517
H	1.842072	8.351747	1.990230

H	2.771961	8.234276	3.495199
C	-6.368599	3.992765	4.931928
H	-5.661040	4.822370	4.809594
H	-7.378597	4.382354	4.735943
H	-6.340688	3.681189	5.985822
C	-8.068104	-0.942901	1.880380
H	-7.303901	-1.174338	1.134505
H	-8.725140	-1.816791	1.978788
H	-8.683810	-0.083869	1.574411
C	-8.510104	-0.542016	4.283617
H	-9.197498	0.280704	4.048698
H	-9.081422	-1.478212	4.283292
H	-8.102679	-0.393555	5.290401
C	-4.330995	3.270051	-4.724360
H	-3.247925	3.239377	-4.569243
H	-4.559132	2.840698	-5.707781
H	-4.654836	4.315596	-4.727287
C	7.112602	5.386239	2.716996
H	6.803733	5.813056	3.678566
H	8.116189	4.959535	2.840298
H	7.168052	6.187264	1.970239
C	6.171991	3.180118	3.364927
H	5.533049	2.345852	3.074195
H	7.198763	2.822366	3.520673
H	5.802971	3.598418	4.309390
C	-6.570800	2.561783	-3.871289
H	-6.894317	3.605393	-3.786063
H	-6.818051	2.196752	-4.876952
H	-7.137021	1.964549	-3.144716
C	4.247971	4.564625	-3.720945
H	4.255195	5.649745	-3.563022
H	4.537791	4.069463	-2.791137
H	4.973642	4.316483	-4.506832
C	2.872801	2.593937	-4.481965
H	3.569217	2.412488	-5.310871
H	3.209139	2.031084	-3.609278
H	1.875236	2.242693	-4.774771
C	2.492311	4.841545	-5.461592
H	2.482944	5.928250	-5.314325
H	3.258571	4.603269	-6.209383
H	1.518874	4.523875	-5.855241
C	8.029083	-4.562548	-0.307238
H	7.174053	-4.941595	0.256533
H	8.819248	-5.327189	-0.335115
H	7.711452	-4.319441	-1.329362
C	9.617561	-2.840654	-0.306373
H	10.446248	-3.563609	-0.331431
H	9.921594	-1.953230	0.255793
H	9.353243	-2.553961	-1.334185
C	9.368156	-1.629548	3.105718
H	9.023391	-1.527458	4.145048
H	10.458269	-1.486675	3.075578
H	9.124706	-2.625766	2.724900
C	9.039788	0.646737	2.618747
H	10.124527	0.814168	2.549718
H	8.702458	0.873082	3.640132
H	8.525664	1.308950	1.917800
C	-7.637383	3.720273	1.084889
H	-8.236293	4.548346	1.492696
H	-6.626922	4.079193	0.847086
H	-7.567650	2.927722	1.835004
C	-8.399331	4.164886	-1.084041
H	-8.886194	3.695086	-1.943403
H	-7.412691	4.544824	-1.383639
H	-9.019705	5.000478	-0.726926
C	-8.130409	-0.930494	-3.492884
H	-9.025094	-0.565916	-4.018710
H	-7.975929	-1.991545	-3.727558
H	-7.257267	-0.364502	-3.822662
C	-9.345017	-1.502587	-1.572872
H	-10.295837	-1.188913	-2.028662
H	-9.386028	-1.336039	-0.492926
H	-9.187777	-2.572537	-1.765245

Complex 11 – Doublet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -9466.328107

Ce	4.133016	1.304870	-0.795614
Ce	-3.419271	-0.828486	-0.163851
O	-3.827178	-3.047365	0.034855
O	3.279531	-0.072390	0.813996
O	5.637548	-0.350190	-1.267141
O	-1.698174	-1.347019	1.289366
C	2.471872	-3.103970	-1.559372
C	-0.852705	-3.570637	1.022204
C	3.637907	-1.239180	1.345519
C	5.955544	-1.564718	-1.706315
C	5.010106	-2.617308	-1.583827
C	2.460329	-3.603640	-2.863237
H	3.338081	-3.510597	-3.494421
C	5.383141	-3.916167	-1.923599
H	4.650388	-4.713973	-1.827486
C	-2.237348	-4.668359	-0.660061
C	1.309758	-3.216900	-0.796687
H	1.321455	-2.867052	0.230653
C	-3.554818	-4.305992	-0.248917
C	-1.223431	-2.474135	1.837429
C	0.124542	-3.766571	-1.293496
C	7.560198	-3.159630	-2.547419
H	8.544356	-3.388796	-2.944510
C	1.311687	-4.216433	-3.354776
H	1.308367	-4.613881	-4.365970
C	-1.146544	-3.626704	-0.470735
H	-1.558575	-2.665253	-0.801014
C	3.642093	-2.313348	-0.989216
H	3.417117	-1.269516	-1.234328
C	6.654281	-4.213026	-2.409586
C	-0.227706	-4.686420	1.576240
H	0.034828	-5.508363	0.913186
C	0.150960	-4.288156	-2.589664
H	-0.743746	-4.725312	-3.014380
C	-1.958743	-5.979387	-1.027070

H	-0.946131	-6.241220	-1.325219
C	3.972852	-3.642124	1.112363
H	3.995780	-4.516762	0.466810
C	3.731168	-2.395653	0.530189
C	0.061958	-4.777740	2.927774
C	-0.355886	-3.720620	3.734407
H	-0.180585	-3.806227	4.801447
C	4.172543	-3.792515	2.478617
C	-2.935535	-6.977047	-1.004669
C	4.177922	-2.628901	3.256363
H	4.376358	-2.737271	4.317177
C	7.253722	-1.838138	-2.215559
C	3.942747	-1.352707	2.739716
C	-4.190074	-6.630335	-0.503059
H	-4.927170	-7.421581	-0.399558
C	-1.021829	-2.593221	3.250959
C	-4.525386	-5.333035	-0.090117
O	4.564996	2.962882	0.535660
O	-3.952984	1.409113	-0.891237
O	-4.813341	0.075698	1.540851
O	2.744649	2.396886	-2.042800
C	-1.593367	2.749192	2.075929
C	1.207412	3.927443	-1.081625
C	-3.968025	2.711955	-0.709148
C	-4.952497	0.957131	2.518721
C	-4.062531	2.070262	2.635072
C	-1.213114	2.902041	3.408713
H	-1.921309	2.691244	4.200133
C	-4.269785	3.026439	3.628265
H	-3.624601	3.900898	3.656891
C	2.820838	4.585587	0.690977
C	-0.631287	3.001907	1.082798
H	-0.921792	2.904798	0.040007
C	4.186246	4.232685	0.739102
C	1.845738	3.376390	-2.215328
C	0.667171	3.417514	1.387329
C	-6.131151	1.815516	4.467091
H	-6.932397	1.732496	5.193741
C	0.080727	3.311862	3.730821
H	0.358736	3.429783	4.774974
C	1.729465	3.589300	0.305858
H	2.202325	2.599841	0.243134
C	-2.973450	2.300974	1.595828
H	-2.809118	1.337523	1.106118
C	-5.279005	2.914031	4.575728
C	0.195292	4.867281	-1.258622
H	-0.326378	5.259469	-0.388436
C	1.012827	3.576506	2.736171
H	2.012111	3.915182	2.991752
C	2.444931	5.902573	0.957808
H	1.388725	6.158288	0.923972
C	-3.455000	4.616296	0.756429
H	-3.025507	4.980414	1.687962
C	-3.469278	3.249222	0.514393
C	-0.179460	5.304734	-2.525620
C	0.530953	4.813729	-3.619396
H	0.263758	5.186202	-4.602753
C	-3.970288	5.527540	-0.161083
C	3.373879	6.888529	1.252324
C	-4.496455	4.999813	-1.336308
H	-4.900420	5.701773	-2.063337
C	-6.024504	0.849195	3.466326
C	-4.512854	3.636798	-1.656245
C	4.723751	6.526000	1.252582
H	5.454266	7.302056	1.457957
C	1.548321	3.864908	-3.507268
C	5.163387	5.230718	0.998228
N	-2.532296	-0.985672	-2.411860
K	0.684253	-0.219376	1.558077
K	-6.574497	1.625047	-0.126187
K	6.674936	-1.754153	1.091362
O	8.275117	-3.854793	1.421316
O	8.651313	-0.677099	2.496884
O	-7.796560	3.862170	0.720960
O	-8.086549	0.084740	-1.780597
Si	-1.147007	-0.091051	-2.895600
C	-0.031447	0.178342	-1.383303
H	0.331477	-0.794688	-1.035666
H	-0.590547	0.694021	-0.592656
H	0.816160	0.817088	-1.657172
C	-1.515565	1.642897	-3.528341
H	-0.593444	2.204428	-3.706666
H	-2.097440	2.191268	-2.781194
H	-2.089823	1.618182	-4.460072
C	-0.076569	-0.976607	-4.173233
H	0.874203	-0.454567	-4.317631
H	-0.570966	-1.036063	-5.148640
H	0.145229	-1.994384	-3.845313
Si	-3.530968	-1.755679	-3.571020
C	-5.274951	-1.950580	-2.842221
H	-5.725049	-0.989551	-2.563164
H	-5.948897	-2.409600	-3.577987
H	-5.264312	-2.599097	-1.957869
C	-3.707702	-0.889112	-5.246935
H	-2.756621	-0.886099	-5.789784
H	-4.046841	0.144983	-5.165225
H	-4.430732	-1.436554	-5.863906
C	-2.977009	-3.504320	-4.045207
H	-1.979493	-3.472244	-4.495341
H	-3.651461	-3.934829	-4.798108
H	-2.920383	-4.159824	-3.168520
K	-5.407996	-5.768012	-3.349041
C	4.111279	-0.122648	3.634323
C	8.268562	-0.713933	-2.411237
C	5.304448	0.716509	3.125946
H	6.237306	0.138096	3.170496
H	5.427765	1.606530	3.755218
H	5.119775	1.067862	2.107673
C	-5.815407	-5.077004	0.686293
C	-1.639164	-1.614241	4.247317
C	7.705633	0.322972	-3.410464
H	7.527369	-0.149693	-4.383083

H	8.424119	1.141904	-3.541270
H	6.762915	0.731606	-3.039004
C	0.720108	-5.994795	3.512641
H	1.427462	-6.444040	2.803311
H	-0.021468	-6.766428	3.768393
H	1.265243	-5.748513	4.434237
C	4.376886	-5.140570	3.109131
H	4.487176	-5.920834	2.345188
H	3.515494	-5.414865	3.732259
H	5.267742	-5.158246	3.753289
C	-5.406405	-4.727450	2.137545
H	-4.861869	-5.569195	2.581790
H	-6.299564	-4.522391	2.740469
H	-4.760716	-3.845237	2.141664
C	-2.629416	-8.376570	-1.459828
H	-3.441185	-9.064145	-1.190792
H	-1.701747	-8.751591	-1.005168
H	-2.501014	-8.430495	-2.552002
C	7.021867	-5.612997	-2.816440
H	6.703345	-5.823851	-3.847751
H	6.538781	-6.358802	-2.170971
H	8.107365	-5.770787	-2.770880
C	8.593878	-0.001088	-1.077630
H	7.685302	0.430114	-0.648800
H	9.310663	0.809565	-1.260930
H	9.052835	-0.700572	-0.365644
C	9.605463	-1.225009	-2.980942
H	10.083678	-1.940311	-2.299134
H	10.281541	-0.371246	-3.108355
H	9.467683	-1.699700	-3.959321
C	2.871370	0.792687	3.654750
H	2.699169	1.230649	2.670399
H	3.039912	1.617988	4.356851
H	1.986856	0.244628	4.003726
C	-6.730013	-6.315486	0.747041
H	-6.234193	-7.158635	1.242102
H	-7.056893	-6.628250	-0.254475
H	-7.623711	-6.058247	1.328761
C	-6.660709	-3.920911	0.113198
H	-6.081307	-2.997552	0.116088
H	-7.557340	-3.787680	0.733827
H	-6.986016	-4.145657	-0.912656
C	4.411671	-0.500918	5.097956
H	3.591374	-1.081590	5.537732
H	4.525199	0.422894	5.677046
H	5.344627	-1.071935	5.186918
C	-3.169183	-1.668723	4.078572
H	-3.535819	-2.687367	4.249776
H	-3.446682	-1.354018	3.071241
H	-3.650164	-0.986773	4.791114
C	-1.204910	-0.156372	4.043046
H	-1.713179	0.475995	4.779529
H	-1.502346	0.192329	3.053518
H	-0.123572	-0.032354	4.199427
C	-1.319918	-1.967464	5.713357
H	-1.703095	-2.958620	5.981069
H	-1.811563	-1.228197	6.357421
H	-0.240191	-1.931478	5.911378
C	-5.101248	3.282145	-3.027415
C	-7.054065	-0.282421	3.405430
C	-5.153121	1.780734	-3.354141
H	-5.846687	1.239894	-2.704134
H	-5.513848	1.668584	-4.385552
H	-4.178170	1.307272	-3.253624
C	6.652747	4.895057	0.976359
C	2.341455	3.403145	-4.726144
C	-6.385515	-1.653487	3.612826
H	-5.916580	-1.706339	4.600784
H	-7.142328	-2.445021	3.539852
H	-5.627177	-1.819583	2.847337
C	-1.309771	6.277588	-2.700515
H	-1.165061	7.178027	-2.086042
H	-1.402061	6.592824	-3.747445
H	-2.263141	5.823695	-2.397174
C	-3.928108	7.008734	0.084540
H	-3.055284	7.468790	-0.402925
H	-4.823050	7.507748	-0.311912
H	-3.861748	7.231129	1.157421
C	7.061947	4.343604	-0.409969
H	6.855873	5.086353	-1.189599
H	8.135385	4.111094	-0.416244
H	6.500559	3.433393	-0.632171
C	2.956052	8.301744	1.545783
H	3.438009	9.013503	0.860656
H	1.870405	8.418810	1.441241
H	3.228049	8.598691	2.569122
C	-5.455061	3.933425	5.665559
H	-4.917421	4.860426	5.427573
H	-6.514316	4.184395	5.815082
H	-5.069368	3.566940	6.628872
C	-7.768312	-0.322239	2.038629
H	-7.032035	-0.554390	1.265421
H	-8.525293	-1.116600	2.043586
H	-8.279852	0.629895	1.836691
C	-8.156218	-0.141462	4.474006
H	-8.714763	0.795841	4.356514
H	-8.857255	-0.976892	4.357887
H	-7.739875	-0.188779	5.487005
C	-4.259916	3.963574	-4.135596
H	-3.227220	3.606042	-4.098367
H	-4.683228	3.719993	-5.119077
H	-4.258178	5.052632	-4.017435
C	7.536900	6.128269	1.245271
H	7.339007	6.551226	2.237489
H	8.589220	5.820031	1.208004
H	7.379884	6.904725	0.487196
C	6.991268	3.848094	2.060663
H	6.413921	2.937434	1.894594
H	8.065614	3.618925	2.024132
H	6.752643	4.246808	3.054599
C	-6.549773	3.817016	-3.144650
H	-6.595234	4.903059	-3.014746

H	-6.947251	3.570795	-4.138307
H	-7.202530	3.357861	-2.390139
C	3.838241	3.740553	-4.527027
H	3.968951	4.823233	-4.413349
H	4.220686	3.244473	-3.631273
H	4.412372	3.401762	-5.399129
C	2.181210	1.886123	-4.957992
H	2.803939	1.574272	-5.806961
H	2.479354	1.328747	-4.067260
H	1.136621	1.648382	-5.186512
C	1.886933	4.105747	-6.019780
H	2.010257	5.193212	-5.949037
H	2.504553	3.742270	-6.850237
H	0.838935	3.876190	-6.247502
C	7.712551	-5.114228	1.052897
H	6.778797	-5.222509	1.610752
H	8.394823	-5.935148	1.316430
H	7.498038	-5.142448	-0.023716
C	9.505753	-3.632131	0.736607
H	10.238683	-4.412366	0.988491
H	9.881078	-2.658505	1.066197
H	9.349122	-3.617706	-0.351874
C	9.009927	-1.368043	3.690753
H	8.456034	-0.971585	4.554572
H	10.088238	-1.276854	3.884913
H	8.757254	-2.421525	3.536701
C	9.005292	0.701621	2.570599
H	10.089972	0.816041	2.707408
H	8.479322	1.201219	3.395779
H	8.706961	1.163376	1.626294
C	-7.018638	4.148086	1.887461
H	-7.528979	4.893401	2.515666
H	-6.021826	4.517641	1.612598
H	-6.914848	3.220626	2.456454
C	-8.001313	5.050840	-0.033363
H	-8.611478	4.786943	-0.901672
H	-7.041645	5.465813	-0.372233
H	-8.532822	5.803293	0.568346
C	-8.459173	0.376337	-3.125427
H	-9.545857	0.269575	-3.256051
H	-7.941916	-0.295271	-3.824728
H	-8.166009	1.407388	-3.334203
C	-8.482934	-1.245355	-1.445697
H	-9.574845	-1.352630	-1.521908
H	-8.171263	-1.433774	-0.416980
H	-7.997483	-1.974504	-2.107154

Complex 11 – Quartet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -9466.328107

Ce	4.133016	1.304870	-0.795614
Ce	-3.419271	-0.828486	-0.163851
O	-3.827178	-3.047365	0.034855
O	3.279531	-0.072390	0.813996
O	5.637548	-0.350190	-1.267141
O	-1.698174	-1.347019	1.289366
C	2.471872	-3.103970	-1.559372
C	-0.852705	-3.570637	1.022204
C	3.637907	-1.239180	1.345519
C	5.955544	-1.564718	-1.706315
C	5.010106	-2.617308	-1.583827
C	2.460329	-3.603640	-2.863237
H	3.338081	-3.510597	-3.494421
C	5.383141	-3.916167	-1.923599
H	4.650388	-4.713973	-1.827486
C	-2.237348	-4.668359	-0.660061
C	1.309758	-3.216900	-0.796687
H	1.321455	-2.867052	0.230653
C	-3.554818	-4.305992	-0.248917
C	-1.223431	-2.474135	1.837429
C	0.124542	-3.766571	-1.293496
C	7.560198	-3.159630	-2.547419
H	8.544356	-3.388796	-2.944510
C	1.311687	-4.216433	-3.354776
H	1.308367	-4.613881	-4.365970
C	-1.146544	-3.626704	-0.470735
H	-1.558575	-2.665253	-0.801014
C	3.642093	-2.313348	-0.989216
H	3.417117	-1.269516	-1.234328
C	6.654281	-4.213026	-2.409586
C	-0.227706	-4.686420	1.576240
H	0.034828	-5.508363	0.913186
C	0.150960	-4.288156	-2.589664
H	-0.743746	-4.725312	-3.014380
C	-1.958743	-5.979387	-1.027070
H	-0.946131	-6.241220	-1.325219
C	3.972852	-3.642124	1.112363
H	3.995780	-4.516762	0.466810
C	3.731168	-2.395653	0.530189
C	0.061958	-4.777740	2.927774
C	-0.355886	-3.720620	3.734407
H	-0.180585	-3.806227	4.801447
C	4.172543	-3.792515	2.478617
C	-2.935535	-6.977047	-1.004669
C	4.177922	-2.628901	3.256363
H	4.376358	-2.737271	4.317177
C	7.253722	-1.838138	-2.215559
C	3.942747	-1.352707	2.739716
C	-4.190074	-6.630335	-0.503059
H	-4.927170	-7.421581	-0.399558
C	-1.021829	-2.593221	3.250959
C	-4.525386	-5.333035	-0.090117
O	4.564996	2.962882	0.535660
O	-3.952984	1.409113	-0.891237
O	-4.813341	0.075698	1.540851
O	2.744649	2.396886	-2.042800
C	-1.593367	2.749192	2.075929
C	1.207412	3.927443	-1.081625
C	-3.968025	2.711955	-0.709148
C	-4.952497	0.957131	2.518721
C	-4.062531	2.070262	2.635072
C	-1.213114	2.902041	3.408713

H	-1.921309	2.691244	4.200133
C	-4.269785	3.026439	3.628265
H	-3.624601	3.900898	3.656891
C	2.820838	4.585587	0.690977
C	-0.631287	3.001907	1.082798
H	-0.921792	2.904798	0.040007
C	4.186246	4.232685	0.739102
C	1.845738	3.376390	-2.215328
C	0.667171	3.417514	1.387329
C	-6.131151	1.815516	4.467091
H	-6.932397	1.732496	5.193741
C	0.080727	3.311862	3.730821
H	0.358736	3.429783	4.774974
C	1.729465	3.589300	0.305858
H	2.202325	2.599841	0.243134
C	-2.973450	2.300974	1.595828
H	-2.809118	1.337523	1.106118
C	-5.279005	2.914031	4.575728
C	0.195292	4.867281	-1.258622
H	-0.326378	5.259469	-0.388436
C	1.012827	3.576506	2.736171
H	2.012111	3.915182	2.991752
C	2.444931	5.902573	0.957808
H	1.388725	6.158288	0.923972
C	-3.455000	4.616296	0.756429
H	-3.025507	4.980414	1.687962
C	-3.469278	3.249222	0.514393
C	-0.179460	5.304734	-2.525620
C	0.530953	4.813729	-3.619396
H	0.263758	5.186202	-4.602753
C	-3.970288	5.527540	-0.161083
C	3.373879	6.888529	1.252324
C	-4.496455	4.999813	-1.336308
H	-4.900420	5.701773	-2.063337
C	-6.024504	0.849195	3.466326
C	-4.512854	3.636798	-1.656245
C	4.723751	6.526000	1.252582
H	5.454266	7.302056	1.457957
C	1.548321	3.864908	-3.507268
C	5.163387	5.230718	0.998228
N	-2.532296	-0.985672	-2.411860
K	0.684253	-0.219376	1.558077
K	-6.574497	1.625047	-0.126187
K	6.674936	-1.754153	1.091362
O	8.275117	-3.854793	1.421316
O	8.651313	-0.677099	2.496884
O	-7.796560	3.862170	0.720960
O	-8.086549	0.084740	-1.780597
Si	-1.147007	-0.091051	-2.895600
C	-0.031447	0.178342	-1.383303
H	0.331477	-0.794688	-1.035666
H	-0.590547	0.694021	-0.592656
H	0.816160	0.817088	-1.657172
C	-1.515565	1.642897	-3.528341
H	-0.593444	2.204428	-3.706666
H	-2.097440	2.191268	-2.781194
H	-2.089823	1.618182	-4.460072
C	-0.076569	-0.976607	-4.173233
H	0.874203	-0.454567	-4.317631
H	-0.570966	-1.036063	-5.148640
H	0.145229	-1.994384	-3.845313
Si	-3.530968	-1.755679	-3.571020
C	-5.274951	-1.950580	-2.842221
H	-5.725049	-0.989551	-2.563164
H	-5.948897	-2.409600	-3.577987
H	-5.264312	-2.599097	-1.957869
C	-3.707702	-0.889112	-5.246935
H	-2.756621	-0.886099	-5.789784
H	-4.046841	0.144983	-5.165225
H	-4.430732	-1.436554	-5.863906
C	-2.977009	-3.504320	-4.045207
H	-1.979493	-3.472244	-4.495341
H	-3.651461	-3.934829	-4.798108
H	-2.920383	-4.159824	-3.168520
K	-5.407996	-5.768012	-3.349041
C	4.111279	-0.122648	3.634323
C	8.268562	-0.713933	-2.411237
C	5.304448	0.716509	3.125946
H	6.237306	0.138096	3.170496
H	5.427765	1.606530	3.755218
H	5.119775	1.067862	2.107673
C	-5.815407	-5.077004	0.686293
C	-1.639164	-1.614241	4.247317
C	7.705633	0.322972	-3.410464
H	7.527369	-0.149693	-4.383083
H	8.424119	1.141904	-3.541270
H	6.762915	0.731606	-3.039004
C	0.720108	-5.994795	3.512641
H	1.427462	-6.444040	2.803311
H	-0.021468	-6.766428	3.768393
H	1.265243	-5.748513	4.434237
C	4.376886	-5.140570	3.109131
H	4.487176	-5.920834	2.345188
H	3.515494	-5.414865	3.732259
H	5.267742	-5.158246	3.753289
C	-5.406405	-4.727450	2.137545
H	-4.861869	-5.569195	2.581790
H	-6.299564	-4.522391	2.740469
H	-4.760716	-3.845237	2.141664
C	-2.629416	-8.376570	-1.459828
H	-3.441185	-9.064145	-1.190792
H	-1.701747	-8.751591	-1.005168
H	-2.501014	-8.430495	-2.552002
C	7.021867	-5.612997	-2.816440
H	6.703345	-5.823851	-3.847751
H	6.538781	-6.358802	-2.170971
H	8.107365	-5.770787	-2.770880
C	8.593878	-0.001088	-1.077630
H	7.685302	0.430114	-0.648800
H	9.310663	0.809565	-1.260930
H	9.052835	-0.700572	-0.365644
C	9.605463	-1.225009	-2.980942

H	10.083678	-1.940311	-2.299134
H	10.281541	-0.371246	-3.108355
H	9.467683	-1.699700	-3.959321
C	2.871370	0.792687	3.654750
H	2.699169	1.230649	2.670399
H	3.039912	1.617988	4.356851
H	1.986856	0.244628	4.003726
C	-6.730013	-6.315486	0.747041
H	-6.234193	-7.158635	1.242102
H	-7.056893	-6.628250	-0.254475
H	-7.623711	-6.058247	1.328761
C	-6.660709	-3.920911	0.113198
H	-6.081307	-2.997552	0.116088
H	-7.557340	-3.787680	0.733827
H	-6.986016	-4.145657	-0.912656
C	4.411671	-0.500918	5.097956
H	3.591374	-1.081590	5.537732
H	4.525199	0.422894	5.677046
H	5.344627	-1.071935	5.186918
C	-3.169183	-1.668723	4.078572
H	-3.535819	-2.687367	4.249776
H	-3.446682	-1.354018	3.071241
H	-3.650164	-0.986773	4.791114
C	-1.204910	-0.156372	4.043046
H	-1.713179	0.475995	4.779529
H	-1.502346	0.192329	3.053518
H	-0.123572	-0.032354	4.199427
C	-1.319918	-1.967464	5.713357
H	-1.703095	-2.958620	5.981069
H	-1.811563	-1.228197	6.357421
H	-0.240191	-1.931478	5.911378
C	-5.101248	3.282145	-3.027415
C	-7.054065	-0.282421	3.405430
C	-5.153121	1.780734	-3.354141
H	-5.846687	1.239894	-2.704134
H	-5.513848	1.668584	-4.385552
H	-4.178170	1.307272	-3.253624
C	6.652747	4.895057	0.976359
C	2.341455	3.403145	-4.726144
C	-6.385515	-1.653487	3.612826
H	-5.916580	-1.706339	4.600784
H	-7.142328	-2.445021	3.539852
H	-5.627177	-1.819583	2.847337
C	-1.309771	6.277588	-2.700515
H	-1.165061	7.178027	-2.086042
H	-1.402061	6.592824	-3.747445
H	-2.263141	5.823695	-2.397174
C	-3.928108	7.008734	0.084540
H	-3.055284	7.468790	-0.402925
H	-4.823050	7.507748	-0.311912
H	-3.861748	7.231129	1.157421
C	7.061947	4.343604	-0.409969
H	6.855873	5.086353	-1.189599
H	8.135385	4.111094	-0.416244
H	6.500559	3.433393	-0.632171
C	2.956052	8.301744	1.545783
H	3.438009	9.013503	0.860656
H	1.870405	8.418810	1.441241
H	3.228049	8.598691	2.569122
C	-5.455061	3.933425	5.665559
H	-4.917421	4.860426	5.427573
H	-6.514316	4.184395	5.815082
H	-5.069368	3.566940	6.628872
C	-7.768312	-0.322239	2.038629
H	-7.032035	-0.554390	1.265421
H	-8.525293	-1.116600	2.043586
H	-8.279852	0.629895	1.836691
C	-8.156218	-0.141462	4.474006
H	-8.714763	0.795841	4.356514
H	-8.857255	-0.976892	4.357887
H	-7.739875	-0.188779	5.487005
C	-4.259916	3.963574	-4.135596
H	-3.227220	3.606042	-4.098367
H	-4.683228	3.719993	-5.119077
H	-4.258178	5.052632	-4.017435
C	7.536900	6.128269	1.245271
H	7.339007	6.551226	2.237489
H	8.589220	5.820031	1.208004
H	7.379884	6.904725	0.487196
C	6.991268	3.848094	2.060663
H	6.413921	2.937434	1.894594
H	8.065614	3.618925	2.024132
H	6.752643	4.246808	3.054599
C	-6.549773	3.817016	-3.144650
H	-6.595234	4.903059	-3.014746
H	-6.947251	3.570795	-4.138307
H	-7.202530	3.357861	-2.390139
C	3.838241	3.740553	-4.527027
H	3.968951	4.823233	-4.413349
H	4.220686	3.244473	-3.631273
H	4.412372	3.401762	-5.399129
C	2.181210	1.886123	-4.957992
H	2.803939	1.574272	-5.806961
H	2.479354	1.328747	-4.067260
H	1.136621	1.648382	-5.186512
C	1.886933	4.105747	-6.019780
H	2.010257	5.193212	-5.949037
H	2.504553	3.742270	-6.850237
H	0.838935	3.876190	-6.247502
C	7.712551	-5.114228	1.052897
H	6.778797	-5.222509	1.610752
H	8.394823	-5.935148	1.316430
H	7.498038	-5.142448	-0.023716
C	9.505753	-3.632131	0.736607
H	10.238683	-4.412366	0.988491
H	9.881078	-2.658505	1.066197
H	9.349122	-3.617706	-0.351874
C	9.009927	-1.368043	3.690753
H	8.456034	-0.971585	4.554572
H	10.088238	-1.276854	3.884913
H	8.757254	-2.421525	3.536701
C	9.005292	0.701621	2.570599

H	10.089972	0.816041	2.707408
H	8.479322	1.201219	3.395779
H	8.706961	1.163376	1.626294
C	-7.018638	4.148086	1.887461
H	-7.528979	4.893401	2.515666
H	-6.021826	4.517641	1.612598
H	-6.914848	3.220626	2.456454
C	-8.001313	5.050840	-0.033363
H	-8.611478	4.786943	-0.901672
H	-7.041645	5.465813	-0.372233
H	-8.532822	5.803293	0.568346
C	-8.459173	0.376337	-3.125427
H	-9.545857	0.269575	-3.256051
H	-7.941916	-0.295271	-3.824728
H	-8.166009	1.407388	-3.334203
C	-8.482934	-1.245355	-1.445697
H	-9.574845	-1.352630	-1.521908
H	-8.171263	-1.433774	-0.416980
H	-7.997483	-1.974504	-2.107154

TS2–7 – Quartet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -10171.754347

Ce	-2.814264	1.155381	0.052172
Ce	2.729071	-0.772641	-0.327377
O	3.479116	-2.374422	1.197105
O	-3.144705	-1.040723	-0.999870
O	-4.812350	0.439014	1.084023
O	1.847016	-2.440221	-1.571238
C	-2.300089	-2.618383	2.355609
C	0.468159	-4.088716	-0.576212
C	-3.595932	-2.271805	-0.837089
C	-5.332678	-0.284243	2.070821
C	-4.686172	-1.489476	2.480648
C	-2.167727	-3.052952	3.677937
H	-2.931854	-2.831165	4.414316
C	-5.247737	-2.282552	3.476939
H	-4.776348	-3.226095	3.736828
C	2.228214	-4.403689	1.153600
C	-1.244601	-2.860480	1.479980
H	-1.310077	-2.476885	0.465988
C	3.458681	-3.708353	1.270522
C	1.020587	-3.466202	-1.724043
C	-0.114023	-3.585278	1.833582
C	-7.046910	-0.746633	3.721260
H	-7.971363	-0.470713	4.218034
C	-1.047965	-3.802594	4.049649
H	-0.970059	-4.182123	5.065884
C	0.972303	-3.648619	0.781961
H	1.255505	-2.597763	0.669788
C	-3.477011	-1.922430	1.690946
H	-3.044764	-1.018257	1.265257
C	-6.418400	-1.918169	4.136832
C	-0.448593	-5.124603	-0.698507
H	-0.890471	-5.547575	0.202039
C	-0.036779	-4.095686	3.131838
H	0.798228	-4.729256	3.424369
C	2.182358	-5.783038	1.330408
H	1.227486	-6.289765	1.207186
C	-4.403957	-4.018966	0.701698
H	-4.560315	-4.342820	1.728705
C	-3.862733	-2.758855	0.477834
C	-0.818324	-5.621385	-1.945376
C	-0.227822	-5.040619	-3.065829
H	-0.486796	-5.449410	-4.037285
C	-4.733898	-4.868959	-0.345685
C	3.320437	-6.523670	1.634362
C	-4.476542	-4.400338	-1.632609
H	-4.727151	-5.057308	-2.459036
C	-6.560310	0.073930	2.699830
C	-3.908209	-3.156668	-1.922393
C	4.528691	-5.833543	1.723894
H	5.423115	-6.410230	1.937618
C	0.678373	-3.978512	-3.002859
C	4.640777	-4.453343	1.542968
O	-2.805448	1.769292	-2.179687
O	4.232036	0.718046	0.831569
O	4.053225	-0.224303	-2.186061
O	-2.781261	3.333798	0.751511
C	2.602726	3.204280	-2.048347
C	-1.079684	4.727590	-0.126019
C	4.289290	2.023141	1.102214
C	4.946495	0.676512	-2.557628
C	4.843527	2.012796	-2.087477
C	2.788827	3.779666	-3.304601
H	3.758823	3.724709	-3.789016
C	5.829899	2.956702	-2.360748
H	5.712192	3.958660	-1.951509
C	-2.264177	4.088438	-2.198129
C	1.342440	3.265742	-1.461789
H	1.194491	2.818258	-0.482617
C	-3.094814	3.018275	-2.594266
C	-2.089521	4.472539	0.838751
C	0.258703	3.865920	-2.091911
C	7.033522	1.335856	-3.618163
H	7.892048	1.085626	-4.233757
C	1.712913	4.395327	-3.944609
H	1.857958	4.840257	-4.925670
C	-1.051826	3.827661	-1.338846
H	-1.109537	2.797447	-0.969629
C	3.633347	2.403571	-1.284469
H	3.099595	1.475478	-1.090512
C	6.952134	2.639889	-3.121516
C	-0.235254	5.823944	-0.020292
H	0.539131	5.966884	-0.770851
C	0.451351	4.434700	-3.353871
H	-0.385163	4.897131	-3.868270
C	-2.553601	5.396622	-2.568990
H	-1.910685	6.192503	-2.198195
C	4.005897	4.324891	0.315587
H	3.725849	5.001719	-0.489794
C	3.980028	2.958767	0.076704

C	-0.372769	6.737371	1.021102
C	-1.434278	6.542979	1.898563
H	-1.581271	7.286273	2.675078
C	4.348492	4.835135	1.566943
C	-3.651857	5.702987	-3.364155
C	4.665216	3.917470	2.565142
H	4.930872	4.312175	3.540344
C	6.070067	0.350840	-3.380294
C	4.656823	2.530742	2.378544
C	-4.463012	4.642808	-3.758513
H	-5.328869	4.875552	-4.369693
C	-2.323575	5.466016	1.826367
C	-4.227695	3.314374	-3.396575
N	0.716556	0.120792	0.067549
N	-0.403034	0.540553	0.364674
K	-0.450402	0.153813	-2.450684
K	6.714829	0.374912	-0.235868
K	-6.240975	-1.111031	-0.801121
O	-8.123612	-2.842693	-0.002112
O	-8.310030	-1.090598	-2.696717
O	8.346500	2.339837	0.539458
O	9.094172	-0.889692	0.141934
Si	-0.185404	1.224058	3.076866
C	0.637690	-0.452246	3.156091
H	-0.072168	-1.225559	3.466406
H	1.463978	-0.377267	3.867556
H	1.021452	-0.704951	2.158544
C	0.769687	2.605583	2.273047
H	0.106338	3.278435	1.721977
H	1.484994	2.167070	1.571568
H	1.326239	3.193614	3.006294
C	-2.055734	1.155748	3.123080
H	-2.436792	1.308524	4.136037
H	-2.419338	0.181433	2.787333
H	-2.471996	1.972168	2.524788
K	2.890507	-2.586855	3.855164
C	-3.733529	-2.793670	-3.397716
C	-7.328068	1.328602	2.295344
C	-4.996565	-2.053505	-3.881821
H	-5.887221	-2.667833	-3.694206
H	-4.925318	-1.848329	-4.958029
H	-5.091403	-1.091808	-3.368810
C	5.998711	-3.763396	1.612236
C	1.378779	-3.482677	-4.262801
C	-6.472889	2.574057	2.585646
H	-6.254836	2.644315	3.657300
H	-7.010451	3.478227	2.275202
H	-5.530462	2.521315	2.038505
C	-1.803333	-6.748280	-2.070348
H	-1.504765	-7.613688	-1.461676
H	-1.890611	-7.083785	-3.112045
H	-2.800231	-6.434130	-1.732825
C	-5.281250	-6.247961	-0.105540
H	-4.470896	-6.982495	0.016114
H	-5.901708	-6.586185	-0.946910
H	-5.893845	-6.282769	0.805491
C	6.270960	-3.036820	0.280127
H	6.321022	-3.754928	-0.545704
H	7.222658	-2.493103	0.337726
H	5.456707	-2.336924	0.079101
C	3.249672	-8.011326	1.832847
H	2.587115	-8.274314	2.669768
H	4.241578	-8.428493	2.047146
H	2.858958	-8.514478	0.937259
C	-6.983984	-2.762254	5.243956
H	-6.857285	-3.833639	5.035656
H	-8.055043	-2.567405	5.384763
H	-6.485312	-2.556860	6.203341
C	-7.676701	1.318012	0.790698
H	-6.756401	1.341990	0.202651
H	-8.264380	2.211245	0.543438
H	-8.280782	0.433085	0.544048
C	-8.657367	1.484676	3.058572
H	-9.330644	0.637860	2.871579
H	-9.150022	2.400795	2.711162
H	-8.490468	1.580015	4.137865
C	-2.508791	-1.895202	-3.641753
H	-2.676222	-0.938817	-3.145865
H	-2.381679	-1.741416	-4.721595
H	-1.614968	-2.392680	-3.243231
C	7.161108	-4.745662	1.845708
H	7.068874	-5.256596	2.812082
H	8.101121	-4.177930	1.849885
H	7.215530	-5.494741	1.047142
C	6.035571	-2.729890	2.756326
H	5.286350	-1.954802	2.576671
H	7.020966	-2.248244	2.798019
H	5.865280	-3.223578	3.724515
C	-3.550041	-4.040606	-4.291255
H	-2.724240	-4.653760	-3.918064
H	-3.308892	-3.706244	-5.308275
H	-4.459504	-4.648966	-4.352488
C	2.870011	-3.875026	-4.158488
H	2.955997	-4.961544	-4.037079
H	3.324782	-3.379636	-3.296277
H	3.403226	-3.575015	-5.067675
C	1.270248	-1.951404	-4.440765
H	1.807243	-1.646437	-5.347689
H	1.721369	-1.449410	-3.580983
H	0.214639	-1.669829	-4.561651
C	0.811725	-4.119518	-5.545823
H	0.955331	-5.206192	-5.552609
H	1.345309	-3.701372	-6.408299
H	-0.257693	-3.898340	-5.658049
C	5.047260	1.602557	3.522991
C	6.181825	-1.013595	-4.046574
C	6.285682	0.769821	3.131290
H	7.116460	1.428367	2.847416
H	6.600813	0.141979	3.975203
H	6.020978	0.115943	2.298458
C	-5.173280	2.220116	-3.866504
C	-3.560596	5.449364	2.715950

C	4.977189	-1.175028	-4.999261
H	4.991473	-0.378870	-5.753939
H	5.030345	-2.145641	-5.506740
H	4.046396	-1.119771	-4.430492
C	0.564985	7.901064	1.168397
H	0.707259	8.429077	0.214872
H	0.188423	8.622927	1.904399
H	1.558765	7.573496	1.505739
C	4.359933	6.313553	1.830484
H	3.347306	6.734828	1.770877
H	4.751998	6.534055	2.831314
H	4.976432	6.852166	1.096798
C	-5.726041	1.446566	-2.650950
H	-6.192236	2.145372	-1.944790
H	-6.482188	0.723255	-2.979693
H	-4.895529	0.930712	-2.159974
C	-3.954744	7.118948	-3.764861
H	-3.171948	7.530058	-4.419095
H	-4.907743	7.180844	-4.305688
H	-4.021347	7.776020	-2.886402
C	7.996651	3.669212	-3.452232
H	8.080305	4.422658	-2.657435
H	8.983747	3.208317	-3.594861
H	7.750605	4.204965	-4.381245
C	6.172904	-2.153508	-3.009224
H	5.264918	-2.104687	-2.407433
H	6.210130	-3.124427	-3.519832
H	7.053320	-2.078451	-2.354934
C	7.464917	-1.170230	-4.883440
H	8.364742	-1.072232	-4.260806
H	7.465776	-2.171690	-5.330577
H	7.509917	-0.434977	-5.695614
C	3.881307	0.645736	3.839928
H	3.623862	0.093831	2.930494
H	4.181093	-0.040491	4.648585
H	3.009861	1.217972	4.178011
C	-6.387298	2.765806	-4.642117
H	-6.078453	3.284641	-5.556906
H	-7.024134	1.920351	-4.931204
H	-6.979446	3.451045	-4.023226
C	-4.414031	1.261644	-4.807462
H	-3.585012	0.795294	-4.270187
H	-5.085932	0.480602	-5.183674
H	-4.018939	1.825436	-5.661540
C	5.389131	2.354670	4.821735
H	4.533784	2.941499	5.176308
H	5.642100	1.618619	5.595227
H	6.251452	3.019110	4.685778
C	-4.805321	5.466419	1.798423
H	-4.811847	6.387382	1.202837
H	-4.784170	4.607805	1.122195
H	-5.718632	5.428806	2.405485
C	-3.599358	4.210351	3.628324
H	-4.457886	4.277555	4.309494
H	-3.706367	3.311109	3.026643
H	-2.679436	4.142026	4.222725
C	-3.654611	6.684825	3.632842
H	-3.671385	7.615154	3.052695
H	-4.589986	6.618951	4.202526
H	-2.821471	6.718885	4.346022
C	-8.288259	-3.907819	-0.934492
H	-9.184998	-4.498918	-0.695286
H	-7.407240	-4.563583	-0.931683
H	-8.400296	-3.447436	-1.920337
C	-7.973957	-3.343887	1.325211
H	-8.869848	-3.906731	1.627710
H	-7.835363	-2.484950	1.985749
H	-7.089727	-3.990777	1.396315
C	-8.376683	-0.737142	-4.072886
H	-9.162174	-1.314226	-4.583422
H	-7.406338	-0.971676	-4.516758
H	-8.582149	0.335767	-4.197610
C	-9.546865	-0.805446	-2.046012
H	-10.379723	-1.312118	-2.556156
H	-9.740932	0.277079	-2.031860
H	-9.463900	-1.188983	-1.025822
C	7.759657	3.626288	0.738739
H	7.566133	4.116056	-0.225272
H	8.422169	4.261473	1.345449
H	6.811678	3.479943	1.261000
C	9.578825	2.446454	-0.162798
H	9.948283	1.428144	-0.312860
H	10.310886	3.027618	0.417956
H	9.431898	2.928679	-1.139335
C	9.704653	-1.995167	-0.514815
H	9.508548	-2.933756	0.023502
H	10.790943	-1.846376	-0.597364
H	9.265743	-2.057485	-1.514212
C	9.563488	-0.764877	1.481656
H	9.264021	-1.636435	2.082180
H	9.114644	0.142107	1.896380
H	10.658968	-0.670842	1.505906
Cl	0.123602	1.783327	5.242754
K	0.066661	-0.964397	6.614507

TS11–2 – Quartet

(Optimised at the PBE0-D3BJ/BS1′ level of theory)

SCF Energy (a.u.): -10526.097583

Ce	-3.861477	0.918291	1.008290
Ce	3.301163	-0.619358	-0.184014
O	3.905725	-2.939327	-0.169304
O	-2.997783	-0.307637	-0.790635
O	-5.512443	-0.613140	1.367903
O	1.940598	-1.363035	-1.913825
C	-2.378370	-3.409980	1.188642
C	0.653074	-3.360964	-1.822518
C	-3.529467	-1.365337	-1.400265
C	-5.810484	-1.830142	1.832636
C	-4.903204	-2.898524	1.599194
C	-2.197903	-4.112333	2.382869
H	-2.980888	-4.134560	3.132817
C	-5.248507	-4.191086	1.981807

H	-4.560640	-5.005757	1.767973
C	2.242536	-4.638728	-0.441822
C	-1.310787	-3.353202	0.290690
H	-1.454796	-2.824403	-0.645522
C	3.600119	-4.170306	-0.486057
C	1.167244	-2.245070	-2.529119
C	-0.077072	-3.968939	0.523558
C	-7.287939	-3.390767	2.924706
H	-8.206101	-3.600411	3.464067
C	-1.005669	-4.798323	2.602603
H	-0.881329	-5.375102	3.515583
C	1.096100	-3.640195	-0.391305
H	1.490789	-2.704170	0.031802
C	-3.618661	-2.582744	0.860014
H	-3.336014	-1.572133	1.169501
C	-6.440752	-4.462421	2.652064
C	-0.240216	-4.238421	-2.440630
H	-0.633134	-5.074216	-1.865266
C	0.036173	-4.741407	1.681906
H	0.955215	-5.281737	1.880753
C	1.967963	-5.996070	-0.590975
H	0.931271	-6.321723	-0.526967
C	-4.427205	-3.636824	-1.256704
H	-4.666976	-4.501412	-0.641504
C	-3.871485	-2.518905	-0.640899
C	-0.676599	-4.050274	-3.741763
C	-0.132351	-2.972871	-4.445331
H	-0.440953	-2.840600	-5.477734
C	-4.680280	-3.671336	-2.623357
C	2.962890	-6.942859	-0.844665
C	-4.341563	-2.536677	-3.360822
H	-4.525236	-2.564872	-4.429004
C	-7.018942	-2.077831	2.528958
C	-3.782783	-1.381489	-2.805762
C	4.267402	-6.464678	-0.994712
H	5.039440	-7.181979	-1.258126
C	0.790868	-2.083407	-3.902010
C	4.617810	-5.118937	-0.836582
O	-4.715835	2.402409	-0.364944
O	3.976683	1.646322	0.837103
O	4.619211	0.573188	-1.842887
O	-3.275697	2.601036	2.284040
C	1.257047	3.069326	-1.884255
C	-1.619732	4.016095	1.347881
C	3.786741	2.944184	0.816503
C	4.682488	1.597703	-2.666113
C	3.739850	2.670349	-2.577418
C	0.855230	3.303977	-3.199670
H	1.565995	3.185595	-4.007856
C	3.856507	3.770638	-3.424822
H	3.157958	4.595945	-3.311020
C	-3.353800	4.365538	-0.402674
C	0.292139	3.194512	-0.869134
H	0.598557	3.028010	0.161925
C	-4.612266	3.732453	-0.496503
C	-2.316202	3.507839	2.472300
C	-1.027448	3.581636	-1.136227
C	5.752663	2.813491	-4.488065
H	6.532542	2.888526	-5.239249
C	-0.454451	3.686134	-3.480684
H	-0.746572	3.871380	-4.511244
C	-2.089522	3.598671	-0.039473
H	-2.377883	2.542695	0.012884
C	2.682133	2.682982	-1.478244
H	2.625015	1.663945	-1.087151
C	4.835414	3.861450	-4.406969
C	-0.609473	4.954548	1.529051
H	-0.071878	5.334743	0.663083
C	-1.388628	3.833135	-2.464175
H	-2.405568	4.138007	-2.689108
C	-3.255596	5.743937	-0.583014
H	-2.275740	6.208272	-0.492478
C	2.997452	4.924916	-0.426614
H	2.479653	5.325489	-1.296187
C	3.149850	3.550353	-0.317342
C	-0.253326	5.400793	2.801050
C	-0.957314	4.893301	3.890153
H	-0.678172	5.247114	4.877429
C	3.488369	5.801769	0.537310
C	-4.366296	6.530095	-0.854615
C	4.093794	5.221196	1.644668
H	4.455154	5.890745	2.423284
C	5.728465	1.701246	-3.646835
C	4.238573	3.841561	1.843328
C	-5.609186	5.894082	-0.901101
H	-6.485478	6.510761	-1.075761
C	-1.987381	3.958523	3.770188
C	-5.771206	4.523494	-0.717562
N	1.782535	-0.603531	1.372523
K	-0.218824	-0.185533	-0.930344
K	6.377941	2.088810	-0.112540
K	-6.565110	-0.714684	-1.252746
O	-8.273967	-2.739521	-1.259386
O	-7.827392	-0.608614	-3.663154
O	7.447700	4.519264	-0.593511
O	7.957101	0.428666	1.324123
Si	0.710045	0.036321	2.503551
C	-1.074814	0.391093	1.832265
H	-1.487013	-0.530561	1.401932
H	-1.088641	1.231558	1.125638
H	-1.650474	0.696098	2.711852
C	1.159927	1.718274	3.258973
H	0.282638	2.235852	3.662507
H	1.605560	2.363254	2.494655
H	1.890958	1.630484	4.069643
C	0.137458	-1.089349	3.946288
H	-0.537060	-0.519132	4.597385
H	0.934392	-1.488180	4.578091
H	-0.428470	-1.944249	3.554605
Si	3.795376	-1.938164	3.315859
C	5.055636	-1.125272	2.205667
H	4.741013	-0.114991	1.921764

H	5.980158	-1.012965	2.777642
H	5.282547	-1.753979	1.340407
C	3.487406	-0.959382	4.875260
H	3.013609	-1.585078	5.637651
H	2.835958	-0.105282	4.683767
H	4.440113	-0.590184	5.265773
C	2.516793	-3.179543	2.798042
H	1.562047	-2.681083	2.649903
H	2.412728	-3.986292	3.535414
H	2.789828	-3.557962	1.810326
K	4.164733	-5.797614	2.050789
C	-3.496785	-0.175939	-3.700554
C	-7.991810	-0.946111	2.846838
C	-4.467633	0.975479	-3.369652
H	-5.502246	0.669145	-3.575103
H	-4.243204	1.845474	-4.001348
H	-4.364960	1.292228	-2.327020
C	6.064961	-4.669287	-1.023128
C	1.479843	-1.059924	-4.797925
C	-7.304759	0.112202	3.740096
H	-7.003054	-0.336947	4.693443
H	-7.998780	0.938212	3.940999
H	-6.419081	0.510711	3.240255
C	-1.681062	-4.963292	-4.383790
H	-1.966896	-5.771883	-3.698569
H	-1.286074	-5.420704	-5.302482
H	-2.596890	-4.417104	-4.650803
C	-5.272277	-4.886544	-3.279372
H	-6.147946	-5.253700	-2.725602
H	-4.544176	-5.708617	-3.326994
H	-5.586918	-4.666524	-4.307996
C	6.135595	-3.496667	-2.025675
H	5.751740	-3.811623	-3.002996
H	7.177852	-3.172025	-2.146374
H	5.533931	-2.658943	-1.672771
C	2.629159	-8.396680	-1.036455
H	3.533598	-9.018422	-1.006593
H	2.143371	-8.567591	-2.008391
H	1.940124	-8.760524	-0.261430
C	-6.785915	-5.862460	3.076306
H	-7.789235	-5.904484	3.518347
H	-6.075606	-6.241848	3.824817
H	-6.762176	-6.559278	2.226193
C	-8.487273	-0.262063	1.551864
H	-7.658073	0.265483	1.076967
H	-9.264285	0.473644	1.794596
H	-8.908739	-1.007121	0.863876
C	-9.242015	-1.442496	3.598078
H	-9.810235	-2.163096	2.995854
H	-9.889521	-0.582123	3.805236
H	-8.975395	-1.906463	4.554870
C	-2.056067	0.337322	-3.524578
H	-1.959332	0.847261	-2.565354
H	-1.827966	1.069429	-4.307739
H	-1.346743	-0.494695	-3.608813
C	6.970524	-5.788625	-1.571740
H	6.600850	-6.157386	-2.535786
H	7.050731	-6.631185	-0.872410
H	7.977217	-5.379556	-1.721976
C	6.664810	-4.216939	0.326234
H	6.027361	-3.457522	0.781878
H	7.667193	-3.796151	0.171334
H	6.775059	-5.071861	1.011629
C	-3.661439	-0.511151	-5.196967
H	-2.984526	-1.321194	-5.496090
H	-3.409790	0.382880	-5.779608
H	-4.694139	-0.790205	-5.442896
C	2.944364	-1.514742	-4.957233
H	2.988556	-2.509695	-5.417193
H	3.418874	-1.548540	-3.974068
H	3.488421	-0.799952	-5.586186
C	1.484821	0.369975	-4.227198
H	2.005582	1.034035	-4.929192
H	2.016423	0.399817	-3.276926
H	0.466013	0.746970	-4.096064
C	0.849876	-0.978201	-6.202205
H	0.931083	-1.929634	-6.740974
H	1.389717	-0.216195	-6.777490
H	-0.206433	-0.683609	-6.145933
C	4.847969	3.447210	3.195045
C	6.797590	0.615671	-3.797071
C	4.987241	1.937284	3.429483
H	5.732658	1.498932	2.760765
H	5.317327	1.774546	4.465412
H	4.036997	1.429516	3.262370
C	-7.160694	3.893348	-0.694624
C	-2.750214	3.454884	4.991537
C	6.152137	-0.715265	-4.225254
H	5.676318	-0.606405	-5.204897
H	6.918573	-1.499136	-4.289215
H	5.397064	-1.007261	-3.494492
C	0.862902	6.386944	2.990500
H	0.700793	7.299400	2.398548
H	0.953516	6.680356	4.044230
H	1.822497	5.958283	2.672245
C	3.337563	7.289516	0.398658
H	2.282419	7.593153	0.462545
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C	-4.246429	8.011238	-1.077545
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H	-3.264403	8.378049	-0.753896
H	-4.363323	8.270378	-2.140601
C	4.909109	5.038986	-5.337824
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C	7.547507	0.364173	-2.471781

H	6.828080	0.024085	-1.722476
H	8.300044	-0.421356	-2.618663
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C	7.866677	0.972259	-4.848119
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C	3.952160	3.998612	4.333249
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H	3.879236	5.090318	4.291926
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H	-8.181368	5.404195	-1.910350
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C	-7.289272	2.819134	-1.796368
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H	-8.259052	2.307208	-1.703461
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C	6.261861	4.054903	3.355465
H	6.246171	5.147048	3.280669
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H	6.935672	3.669193	2.578014
C	-4.246881	3.823371	4.863463
H	-4.362358	4.913557	4.838585
H	-4.659181	3.402023	3.943166
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C	-2.616031	1.922201	5.139166
H	-3.130912	1.592425	6.051144
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C	-2.231364	4.078157	6.301425
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H	-1.179752	3.818752	6.476064
C	-8.050288	-3.863365	-0.410058
H	-6.994837	-3.855743	-0.129916
H	-8.290825	-4.798062	-0.938337
H	-8.651898	-3.790216	0.504686
C	-9.641462	-2.637988	-1.632117
H	-9.970256	-3.541690	-2.166643
H	-9.726156	-1.771252	-2.293646
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C	-7.678454	-1.831043	-4.381475
H	-6.816842	-1.778211	-5.061318
H	-8.585523	-2.051310	-4.964171
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C	-8.060005	0.473759	-4.558747
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H	-7.226753	0.582370	-5.268170
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C	6.581467	4.876094	-1.676002
H	6.970476	5.759900	-2.203569
H	5.564818	5.081682	-1.314570
H	6.552332	4.036072	-2.375214
C	7.550796	5.603154	0.322406
H	8.220596	5.289030	1.128016
H	6.565874	5.852764	0.740768
H	7.972047	6.490018	-0.174854
C	8.558773	0.736392	2.575455
H	9.655341	0.685076	2.506528
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C	8.302255	-0.889624	0.911687
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