Accurate computed singlet-triplet energy differences for cobalt systems: implication for two-state reactivity

Electronic Supplementary Information (ESI)

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Contents

1 Full computational details

1.1 Calculation of semicore correlation

In the multireference calculations, we exclude the core orbitals (built on the $1s2s2p$ for Cobalt and the $1s$ for Carbon) of the subset that is reoptimised during the CASSCF procedure. They are also excluded from the following dynamical correlation treatment (MRCISD or PT2). We evaluated the influence of $3s3p$ semicore correlation as detailed in Figure 1. In the multireference case, semicore electrons are either kept frozen in addition to all the other closed shell (*nosp* calculations), or included in addition to the active electrons (*sp* calculations). In coupled cluster calculations, we either froze all lower energy electrons, core and semicore (*nosp* calculations), or correlated semicore electrons in addition to all other higher energy electrons (*sp* calculations).

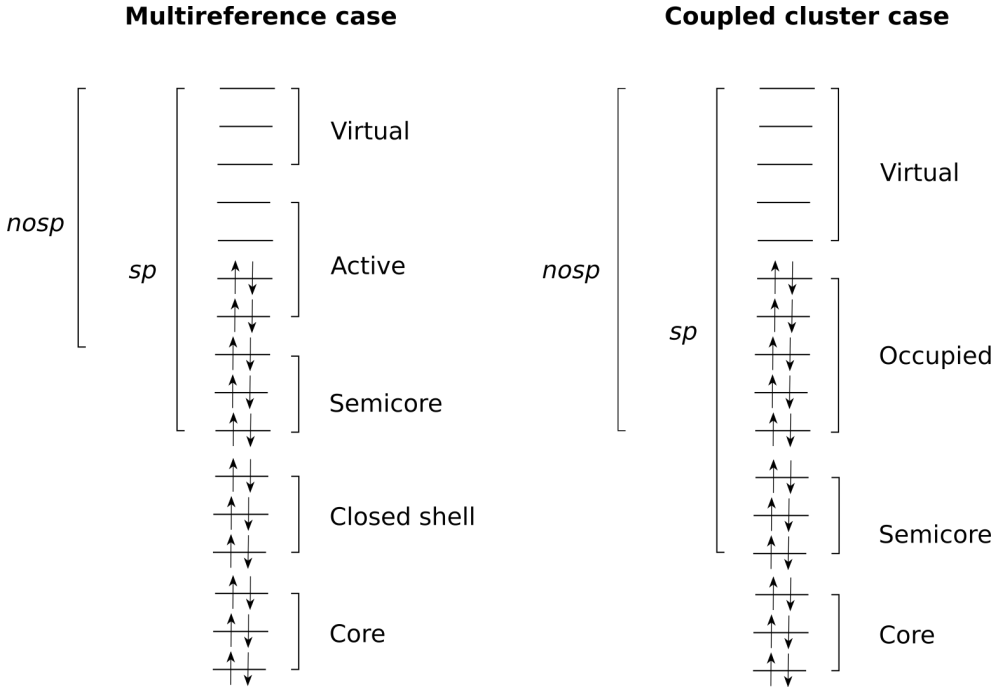

Figure 1: Details on the selection of the different orbital subspaces for wave function methods.

2 MRCISD size-consistency corrections

Table 1: MRCISD ΔE_{ST} values (kcal/mol) for a series of cobalt and rhodium complexes with B1 (respectively B4) basis set using several size-consistency corrections (fixed coefficients were used to calculate the corrections except for degenerate roots of Co^+ where we use the relaxed coefficients)

	Co^+	$[Co(C_2H_4)]^+$	CpCo	$[CpCo(C_2H_4)]$
exp	31.32	-	-	-
$CAS(i,j)_{MRCISD}$	(8,5)	(10,8)	(12,9)	(14,11)
MRCISD uncorrected sp	33.25	33.72	33.67	12.41
MRCISD uncorrected nosp	36.08	34.93	33.29	11.73
Davidson-Silver sp	32.42	32.61	30.42	11.84
Davidson-Silver nosp	32.50	34.43	30.80	12.52
Pople sp	31.98	32.24	30.33	11.43
Pople nosp	35.43	33.93	30.67	11.78
Davidson sp	32.50	32.75	30.89	11.94
Davidson nosp	36.16	34.48	31.12	12.37
	Rh^+	$[Rh(C_2H_4)]^+$	CpRh	$[CpRh(C_2H_4)]$
exp	28.56	-	-	-
$CAS(i,j)_{MRCISD}$	(8,5)	(10,8)	(14,11)	(14,11)
MRCISD uncorrected sp	26.51	13.62	13.71	-5.55
MRCISD uncorrected nosp	27.56	8.23	13.86	-9.08
Davidson-Silver sp	25.00	11.73	13.20	-5.54
Davidson-Silver nosp	26.80	5.82	13.74	-9.07
Pople sp	24.61	11.43	12.68	-6.12
Pople nosp	26.35	5.88	13.11	-9.72
Davidson sp	25.20	11.99	13.26	-5.58
Davidson nosp	26.87	6.06	13.73	-9.14

3 Experimental value of M^+ energy splitting (M = Co, Rh)

Since the triplet ground state has three possible values of the total angular momentum J, we use a degeneracy weighted average expression of the energy (Equation 1) to compute ΔE_{ST} and assess the validity of our results.[1]

$$\bar{E}(^{2S+1}L) = \frac{\sum_{J=|L-S|}^{L+S} (2J+1) E(^{2S+1}L_J)}{\sum_{J=|L-S|}^{L+S} (2J+1)} \tag{1}$$

4 Relativistic effects

In Table 2, we report the ΔE_{ST} with and without taking into account scalar relativistic effects within the second order Douglas-Kroll-Hess formalism. We define Δ_{rel}, representing the influence of relativistic effects on ΔE_{ST} as follows (Equation 2):

$$\Delta_{rel} = \Delta E_{ST}^{rel} - \Delta E_{ST}^{nonrel} \tag{2}$$

Table 2: ΔE_{ST} with and without scalar relativistic effects and Δ_{rel} in kcal/mol, $3s3p$ electrons are correlated

	Co^+	$[Co(C_2H_4)]^+$	CpCo	$[CpCo(C_2H_4)]$
ΔE_{ST} MRCISD non rel	32.16	33.11	30.78	12.01
ΔE_{ST} CCSD(T) non rel	-	-	30.99	12.28
ΔE_{ST} MRCISD rel	31.98	32.24	30.33	11.43
ΔE_{ST} CCSD(T) rel	-	-	30.49	11.77
Δ_{rel} MRCISD	-0.18	-0.87	-0.45	-0.58
Δ_{rel} CCSD(T)	-	-	-0.50	-0.50

5 Basis set quality

5.1 Choice of basis set for multireference and coupled-cluster calculations

We report here the value of ΔE_{ST} computed with several basis sets in Table 3. Performances of B1 and B2 basis sets were evaluated with respect to higher quality basis sets calculations. As we can see in Figure 2, reducing the basis quality on carbon and hydrogen atom has a very small impact on the energy.

Table 3: ΔE_{ST} (kcal/mol) for a series of basis sets with the number of basis functions for complex CpCo, $3s3p$ electrons are correlated

	Co^+	$[Co(C_2H_4)]^+$	$CpCo$	B.S. Size ($CpCo$)
MRCISD				
B1	31.98	32.24	30.33	367
B2	31.98	32.24	30.33	302
cc-pwCVTZ-DK	32.18	32.26	30.76	387
aug-cc-pwCVTZ-DK	31.98	32.26	30.26	537
cc-pwCVQZ-DK	31.94	32.21	30.20	719
CCSD(T)				
B1	-	-	30.49	367
B2	-	-	30.46	302
cc-pwCVTZ-DK	-	-	31.07	387
aug-cc-pwCVTZ-DK	-	-	30.54	537
cc-pwCVQZ-DK	-	-	30.56	719

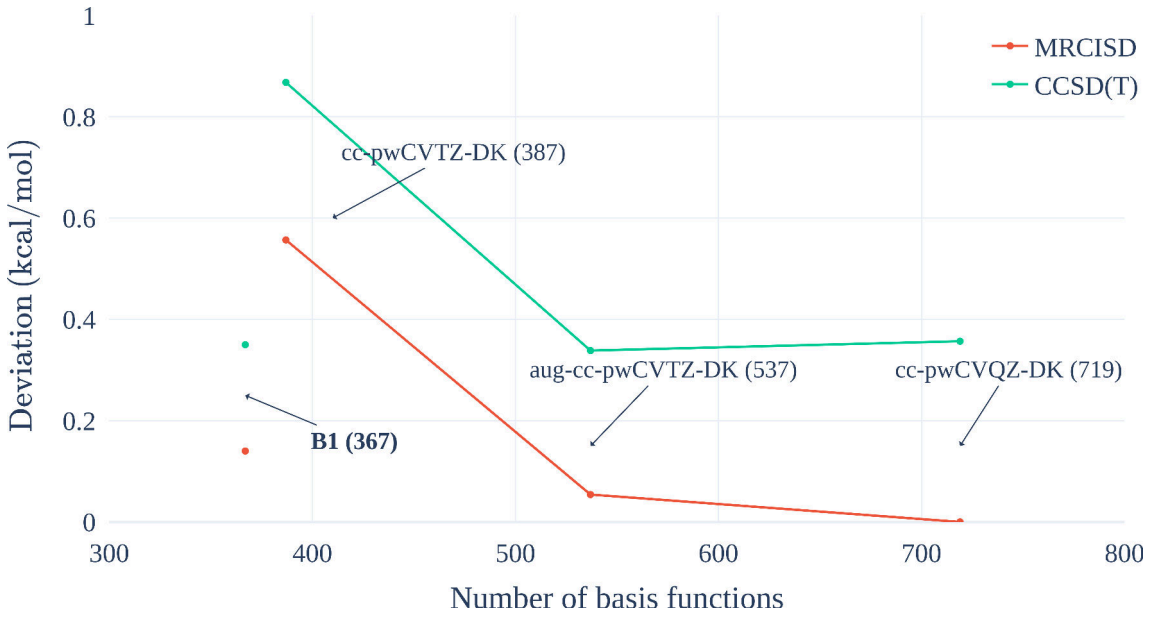

Figure 2: Deviation from MRCISD at the highest dimensional basis set (cc-pwCVQZ-DK) for complex CpCo

5.2 Choice of basis set for f12-methods

We used the non-relativistic counterpart of B1 basis, B3, in the f12- calculations. In the case of correlation consistent basis set B3, we used a value of 1.2 for the exponent of the Slater-type correlation factor based on the work of Giner et. al.[2] For B5 basis set we used a value of 1.4. Results for complexes CpCo and [CpCo(C_2H_4)] for all basis sets are available in Table 4

Table 4: Auxiliary basis sets for f12-CCSD(T) and f12-BCCD(T) calculations

B3	Basis	CBAS	CABS	JKBAS
Co	aug-cc-pwCVTZ	aug-cc-pVTZ	aug-cc-pVTZ	universal
C	cc-pwCVTZ	cc-pwCVQZ	cc-pwCVTZ	aug-cc-pVQZ
H	cc-pVDZ	cc-pVTZ	cc-pVDZ	cc-pVTZ
B5	Basis	CBAS	CABS	JKBAS
Co	def2-QZVP	def2-QZVPP	def2-QZVPP	universal
C	def2-QZVP	def2-QZVPP	def2-QZVPP	def2-QZVPP
H	def2-SVP	def2-TZVP	def2-TZVP	def2-TZVPP

6 Active spaces for cobalt systems

Active spaces of OpenMolcas CASSCF/RASSCF calculations.

6.1 $[Co(C_2H_4)]^+$

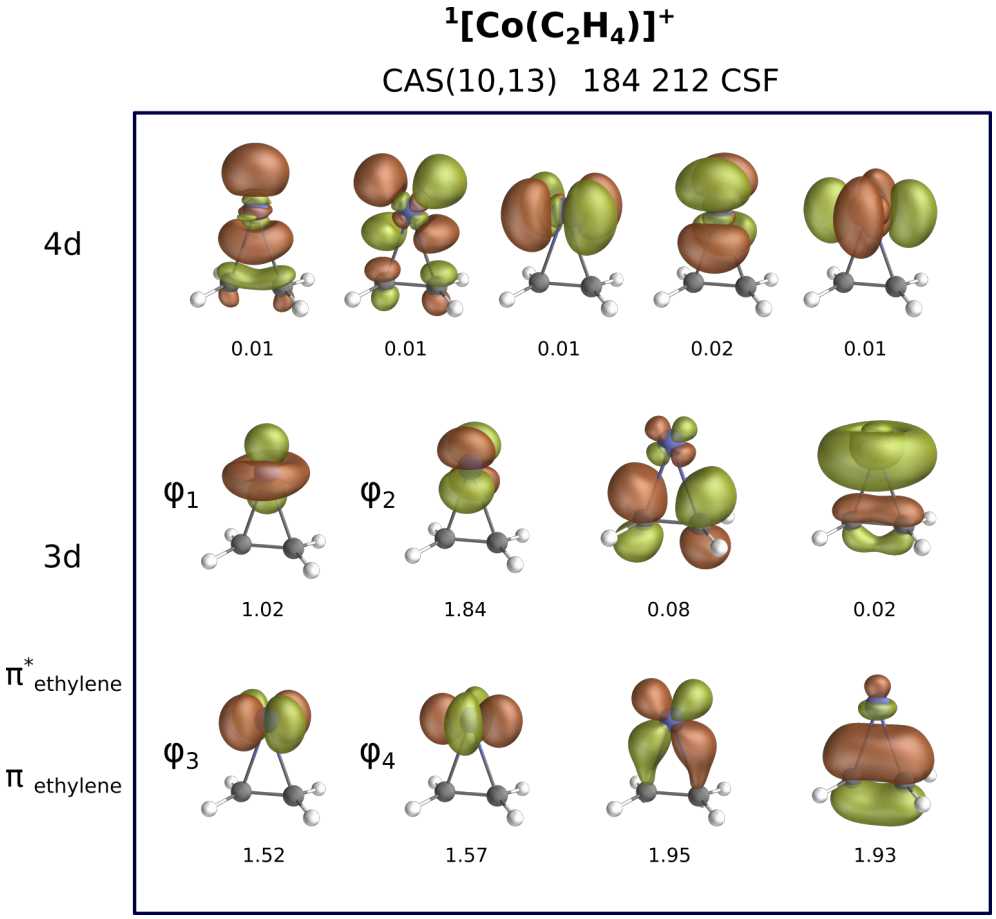

Figure 3: Active space of $[Co(C_2H_4)]^+$ (singlet state, C_{2v}), isovalue=0.07

Table 5: Largest contributions to the CASSCF wave function for $[Co(C_2H_4)]^+$, the three main singlet configurations from a state specific singlet ground state CASSCF calculation are given (C_{2v})

Configuration	Occupation	Weight
Singlet configuration 1	$\ldots(\varphi_1)^0(\varphi_2)^2(\varphi_3)^2(\varphi_4)^2\ldots\rangle$	0.45
Singlet configuration 2	$\ldots(\varphi_1)^2(\varphi_2)^2(\varphi_3)^0(\varphi_4)^2\ldots\rangle$	0.21
Singlet configuration 3	$\ldots(\varphi_1)^2(\varphi_2)^2(\varphi_3)^2(\varphi_4)^0\ldots\rangle$	0.19

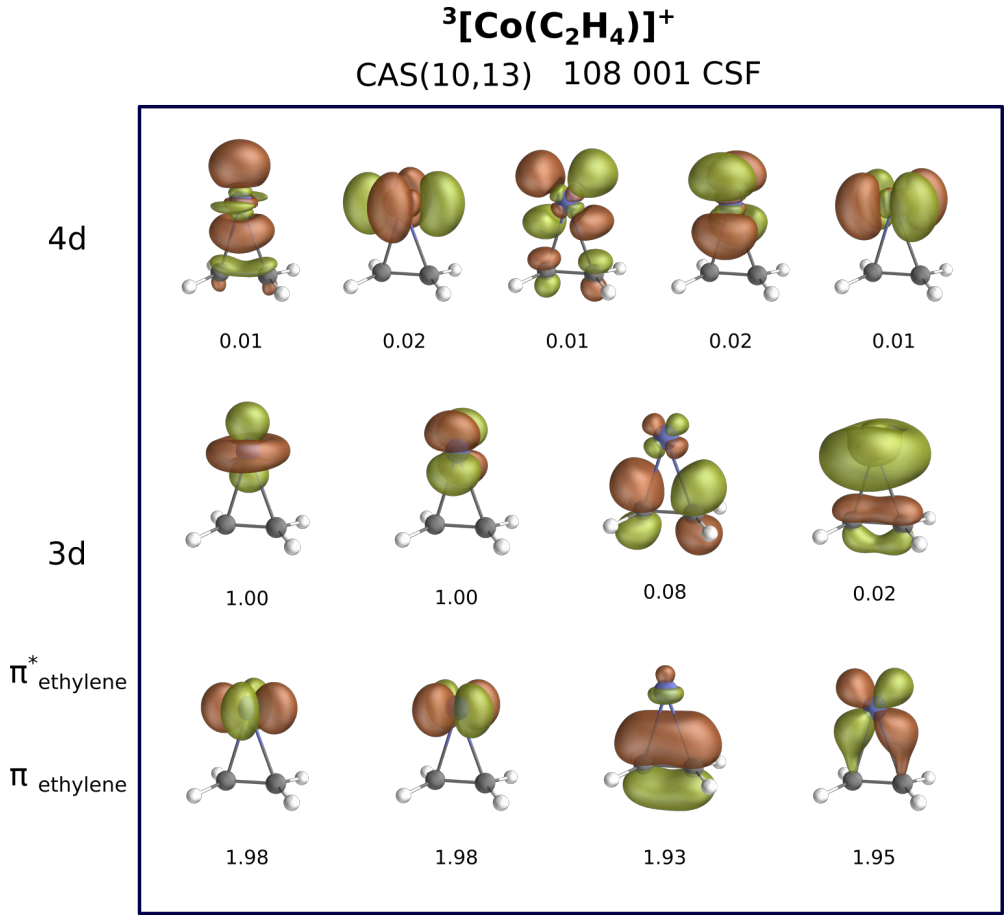

Figure 4: Active space of $[Co(C_2H_4)]^+$ (A_2 triplet state, C_{2v}), isovalue=0.07

Table 6: Largest contributions to the CASSCF wave function for $[Co(C_2H_4)]^+$ (A_2 triplet state, C_{2v})

Configuration	Weight
Main triplet	0.92
Diexcitation $\pi_{ethylene} \rightarrow \pi^*_{ethylene}$	0.02

6.2 CpCo

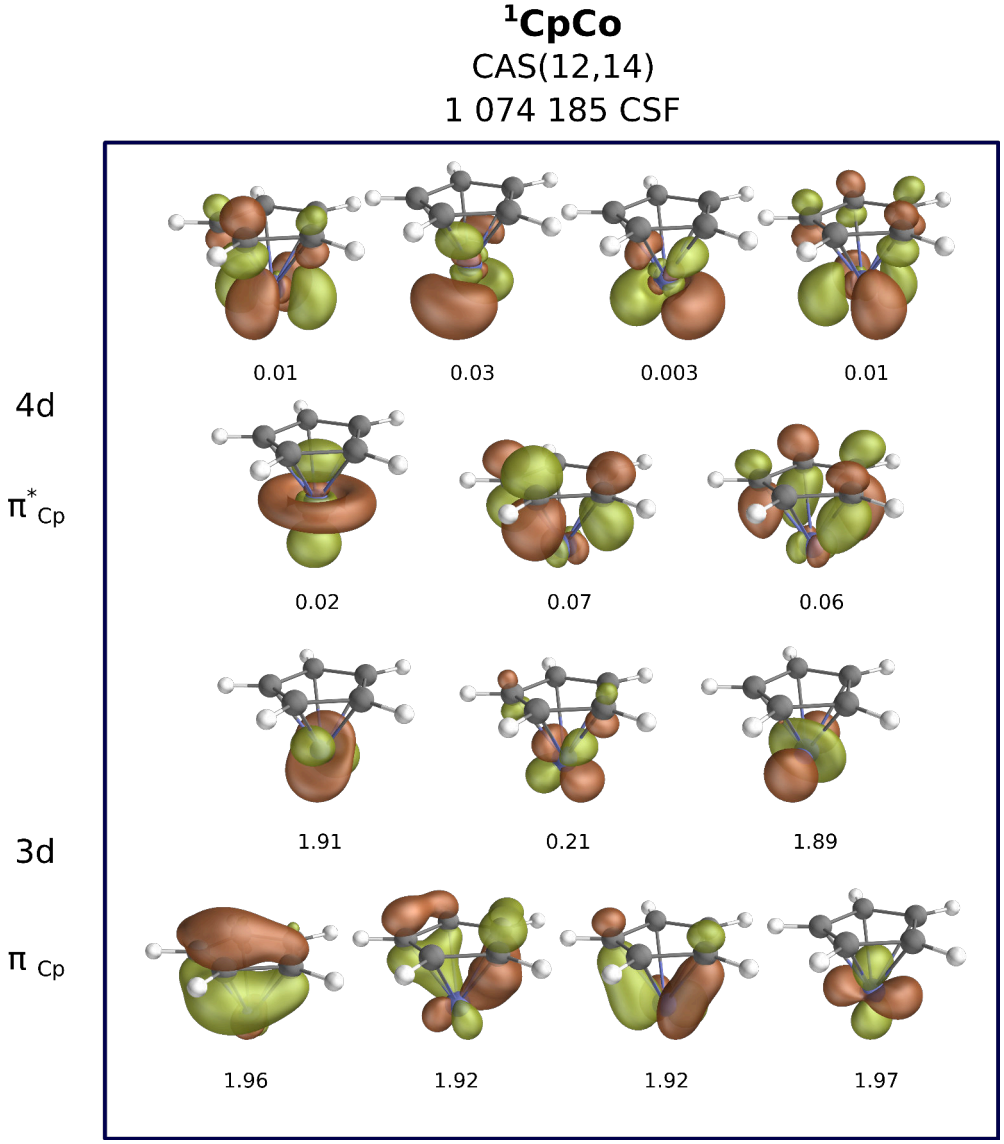

Figure 5: Active space of CpCo (singlet state, C_s), isovalue=0.07

Table 7: Largest contributions to the CASSCF wave function for CpCo (singlet state, C_s)

Configuration	Weight
Main singlet	0.81
Diexcitation $3d$ (1.89) $\rightarrow$ $3d$ (0.21)	0.03
Diexcitation $3d$ (1.91) $\rightarrow$ $3d$ (0.21)	0.02
Diexcitation $3d$ (1.92) $\rightarrow$ $3d$ (0.21)	0.01

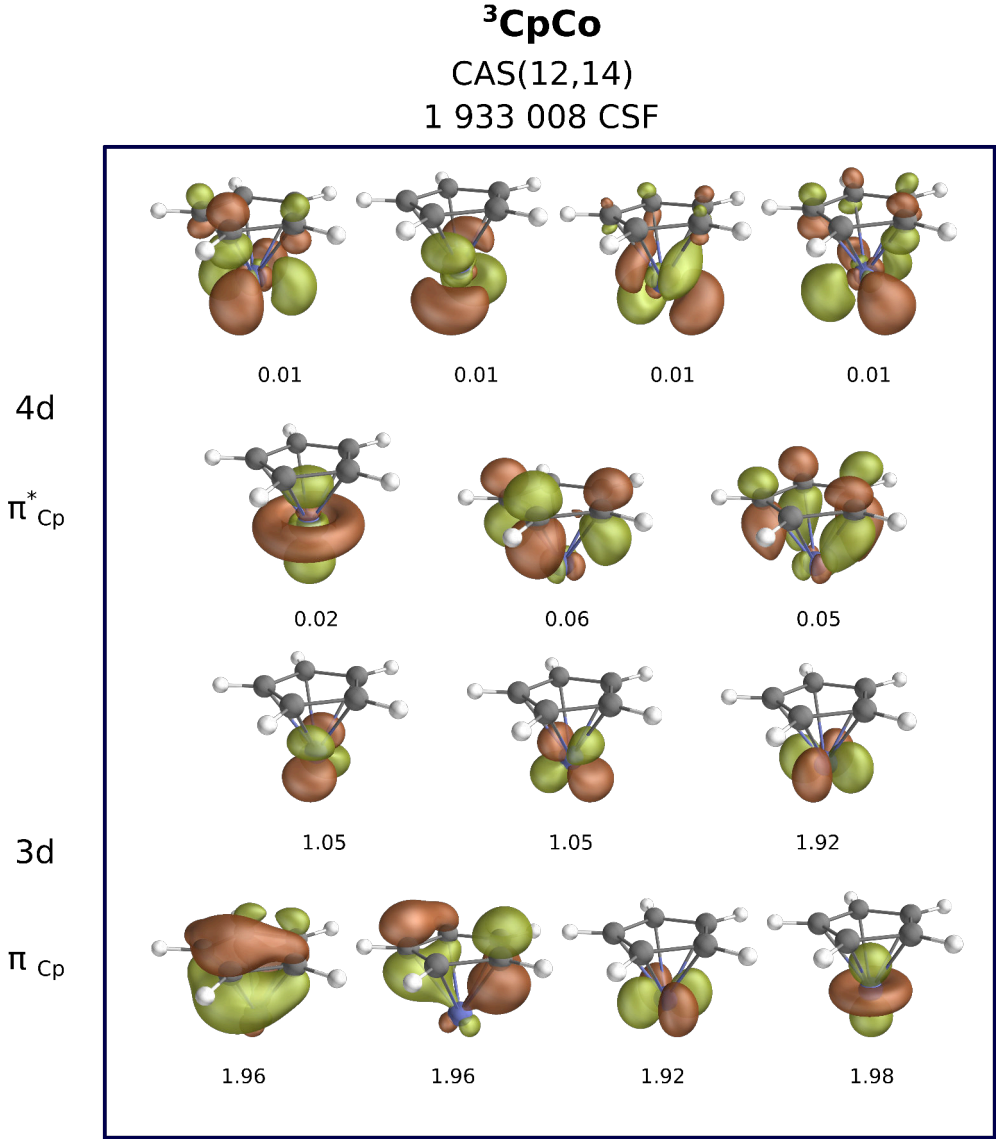

Figure 6: Active space of CpCo ($A^{''}$ triplet state, C_s), isovalue=0.07

Table 8: Largest contributions to the CASSCF wave function for CpCo ($A^{''}$ triplet state, C_s)

Configuration	Weight
Main triplet	0.87
Diexcitation, from two possible $3d$ (1.92) $\rightarrow$ $3d$ (1.05)	0.04

6.3 $[CpCo(C_2H_4)]$

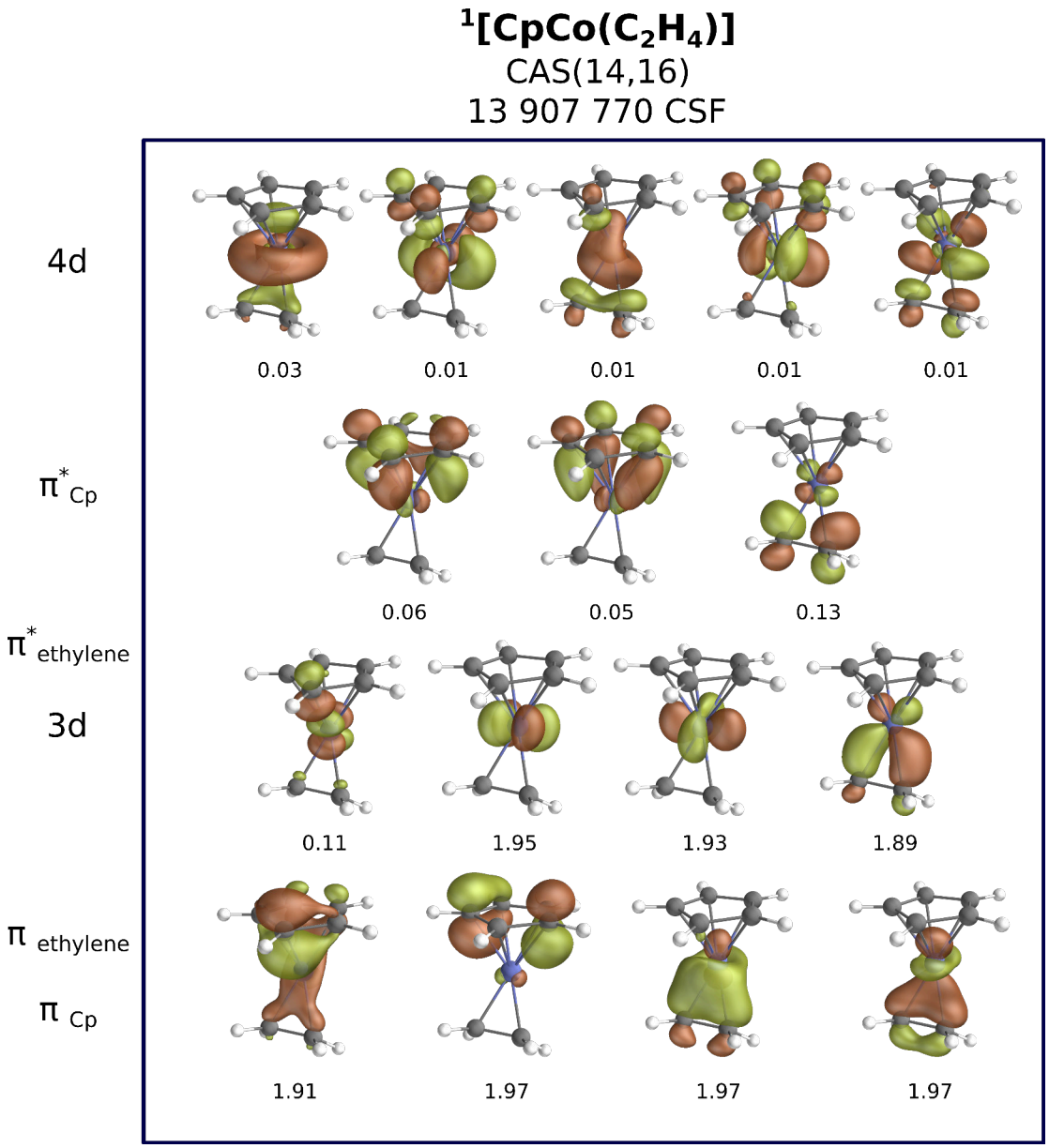

Figure 7: Active space of $[CpCo(C_2H_4)]$ (singlet state, C_s), isovalue=0.07

Table 9: Largest contributions to the CASSCF wave function for $[CpCo(C_2H_4)]$ (singlet state, C_s)

Configuration	Weight
Main singlet	0.82
Diexcitation $3d$ (1.89) $\rightarrow$ $3d$ (0.13)	0.03

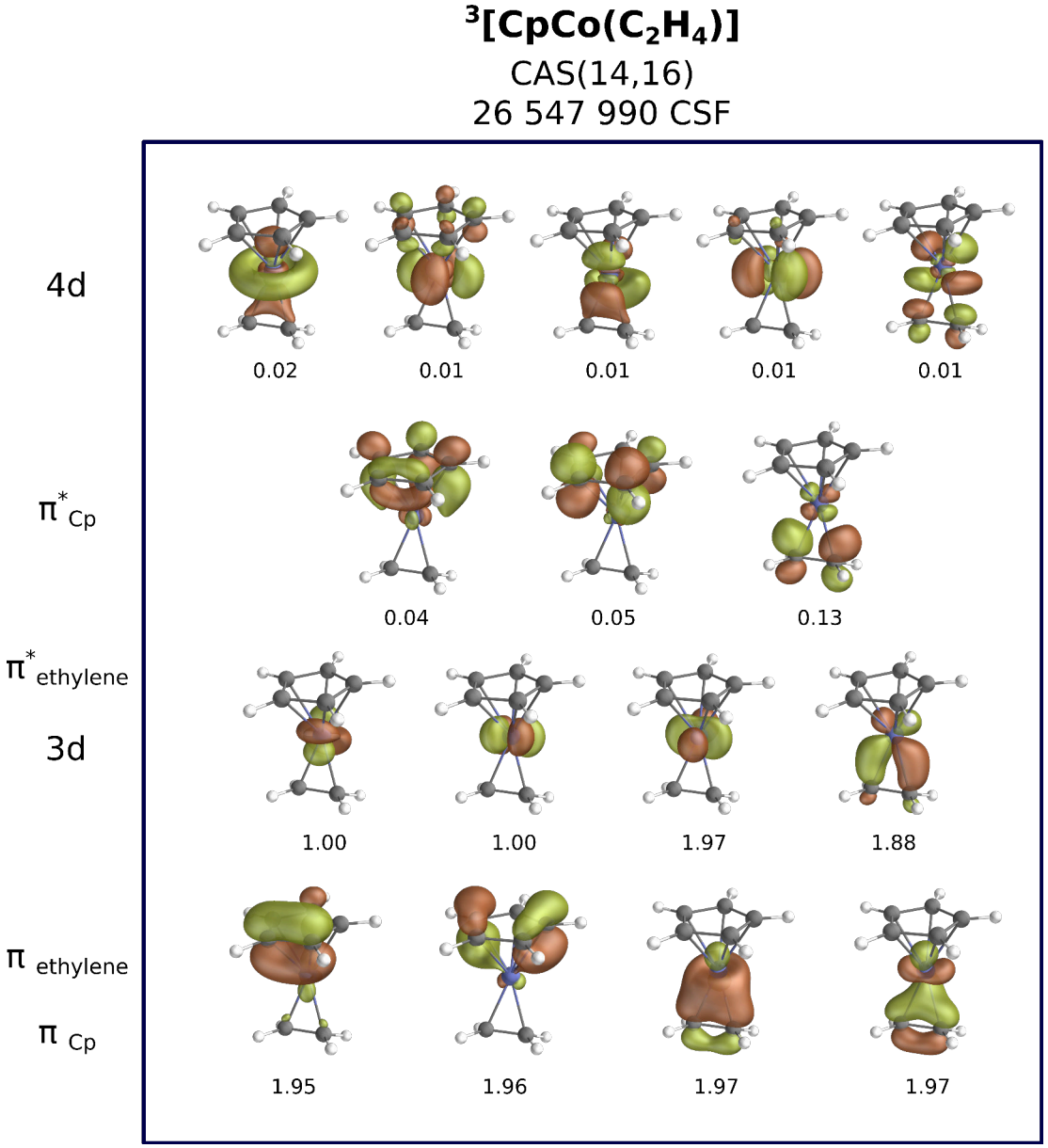

Figure 8: Active space of [CpCo(C_2H_4)] (A'' triplet state, C_s), isovalue=0.07

Table 10: Largest contributions to the CASSCF wave function for [CpCo(C_2H_4)] (A'' triplet state, C_s)

Configuration	Weight
Main triplet	0.85
Diexcitation $[\pi^*_{ethylene} - Co] \rightarrow [\pi^*_{ethylene} - Co]^*$	0.03

6.4 Intermediate I

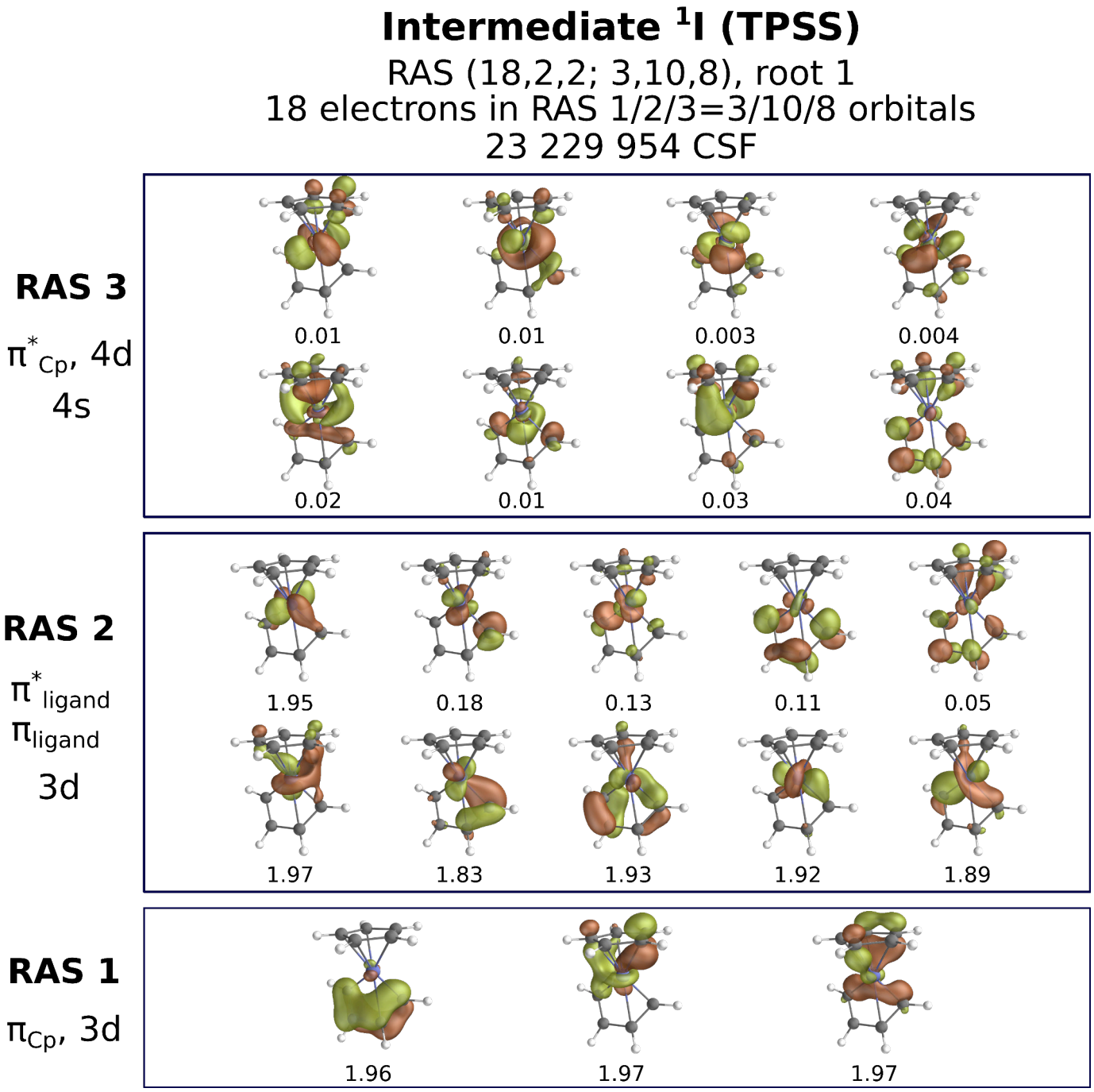

Figure 9: Active space of intermediate **I** (singlet state, root 1), TPSS-D3 geometry, isovalue=0.07

Table 11: Largest contributions to the root 1 of CASSCF wave function for **I** (singlet state, C_1, SA-CASSCF 2 roots, TPSS-D3 geometry)

Configuration	Weight
Main singlet	0.73
Diexcitation $[3d-C2]$ (1.83)$\rightarrow$ $[3d-C2]^*$(0.18)	0.01
Diexcitation $[3d-C1]$ (1.89)$\rightarrow$ $[3d-C1]^*$ (0.13)	0.01

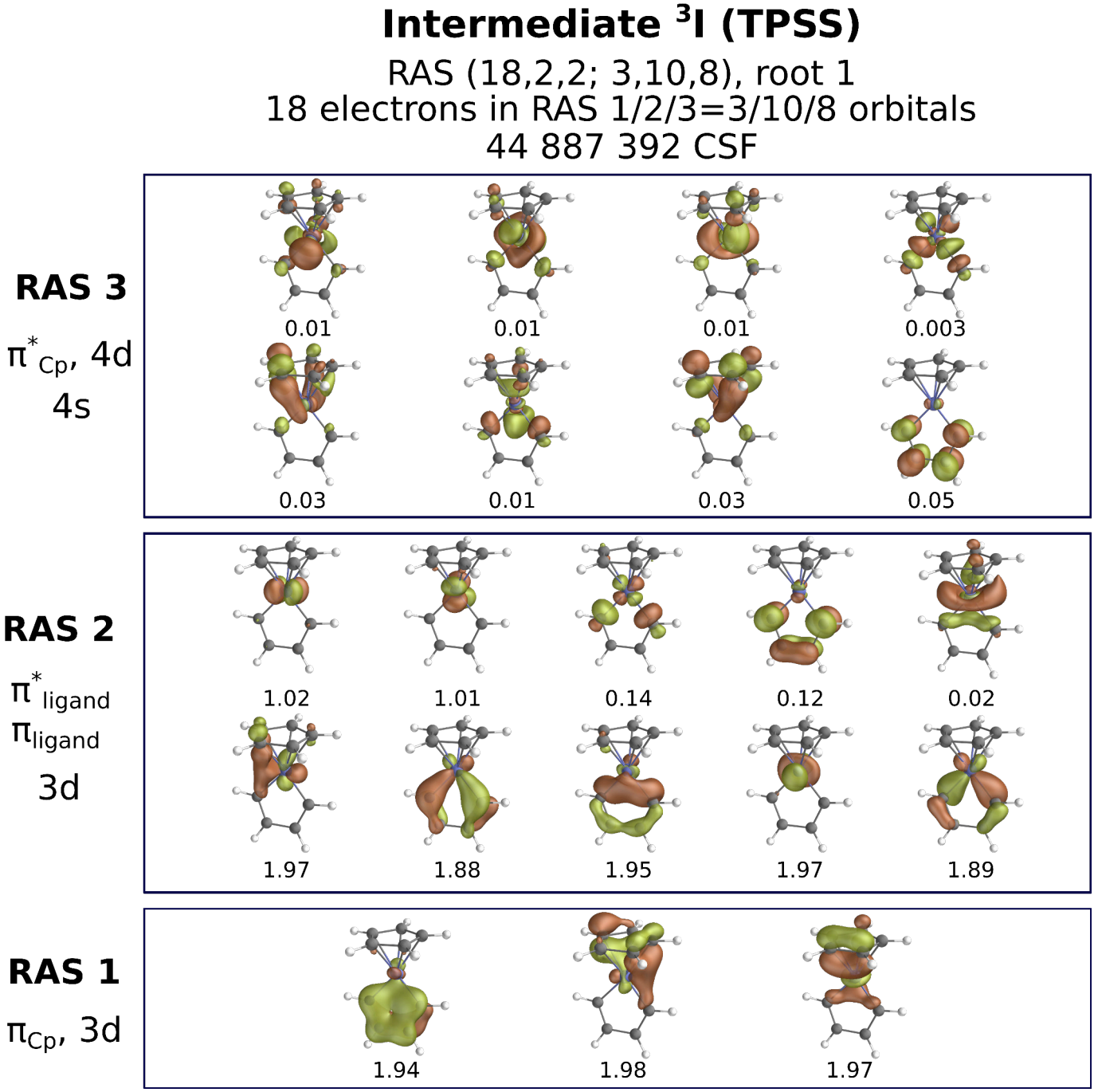

Figure 10: Active space of intermediate **I** (triplet state, root 1), TPSS-D3 geometry, isovalue=0.07

Table 12: Largest contributions to the root 1 of CASSCF wave function for **I** (triplet state, C_1, SA-CASSCF 2 roots, TPSS-D3 geometry)

Configuration	Weight
Main triplet	0.76
Diexcitation $[3d - C]$ (1.88)→ $[3d - C]^*$(0.14)	0.02
Diexcitation π (1.89)→ π^*(0.12)	0.01

6.5 Intermediate II

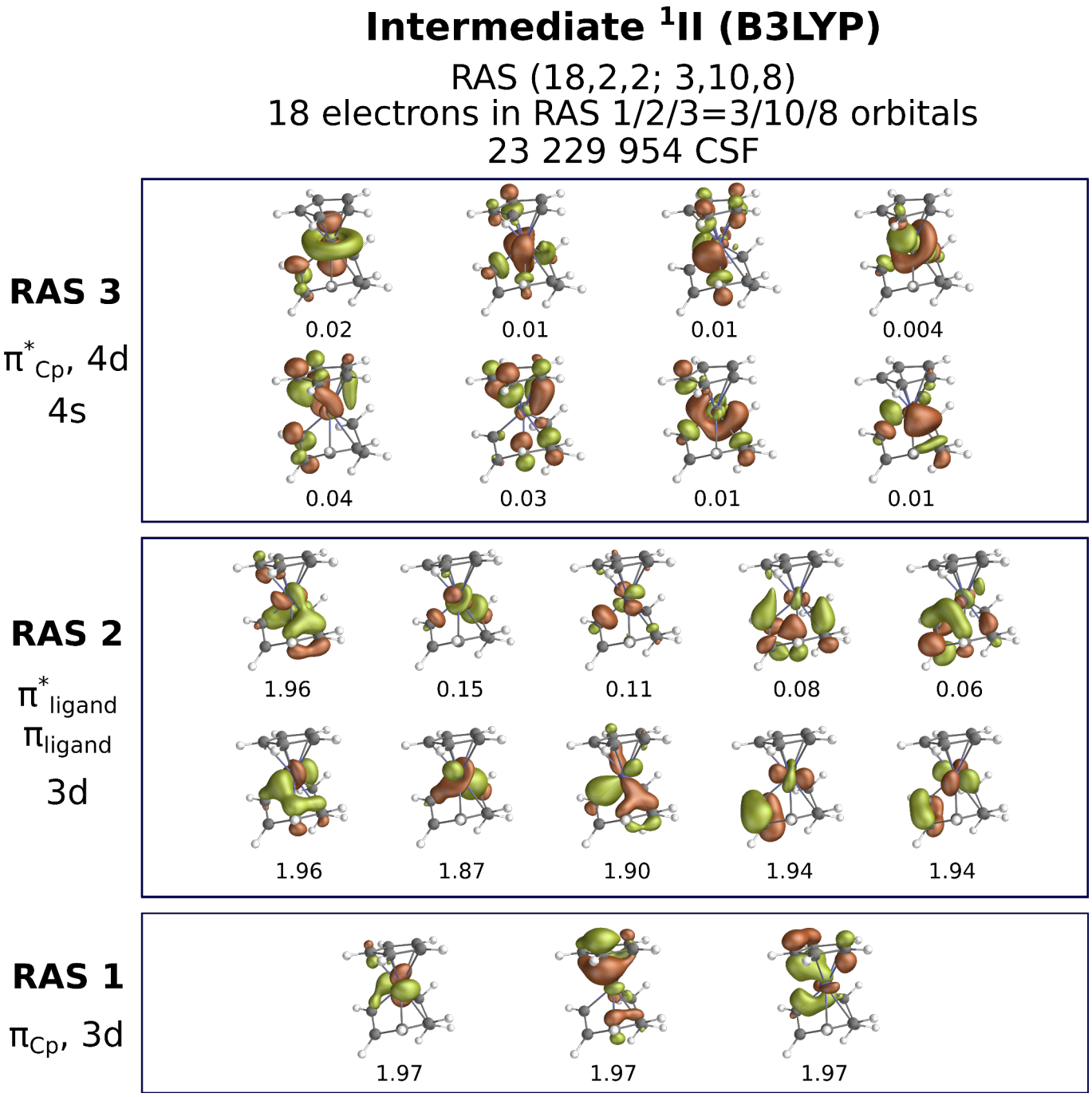

Figure 11: Active space of intermediate **II** (singlet state), isovalue=0.07, B3LYP-D3 geometry

Table 13: Largest contributions to the CASSCF wave function for **II** (singlet state, C_1, B3LYP-D3 geometry)

Configuration	Weight
Main singlet	0.76
Diexcitation $[3d-C2]$ (1.87)→ $[3d-C2]^*$(0.15)	0.03

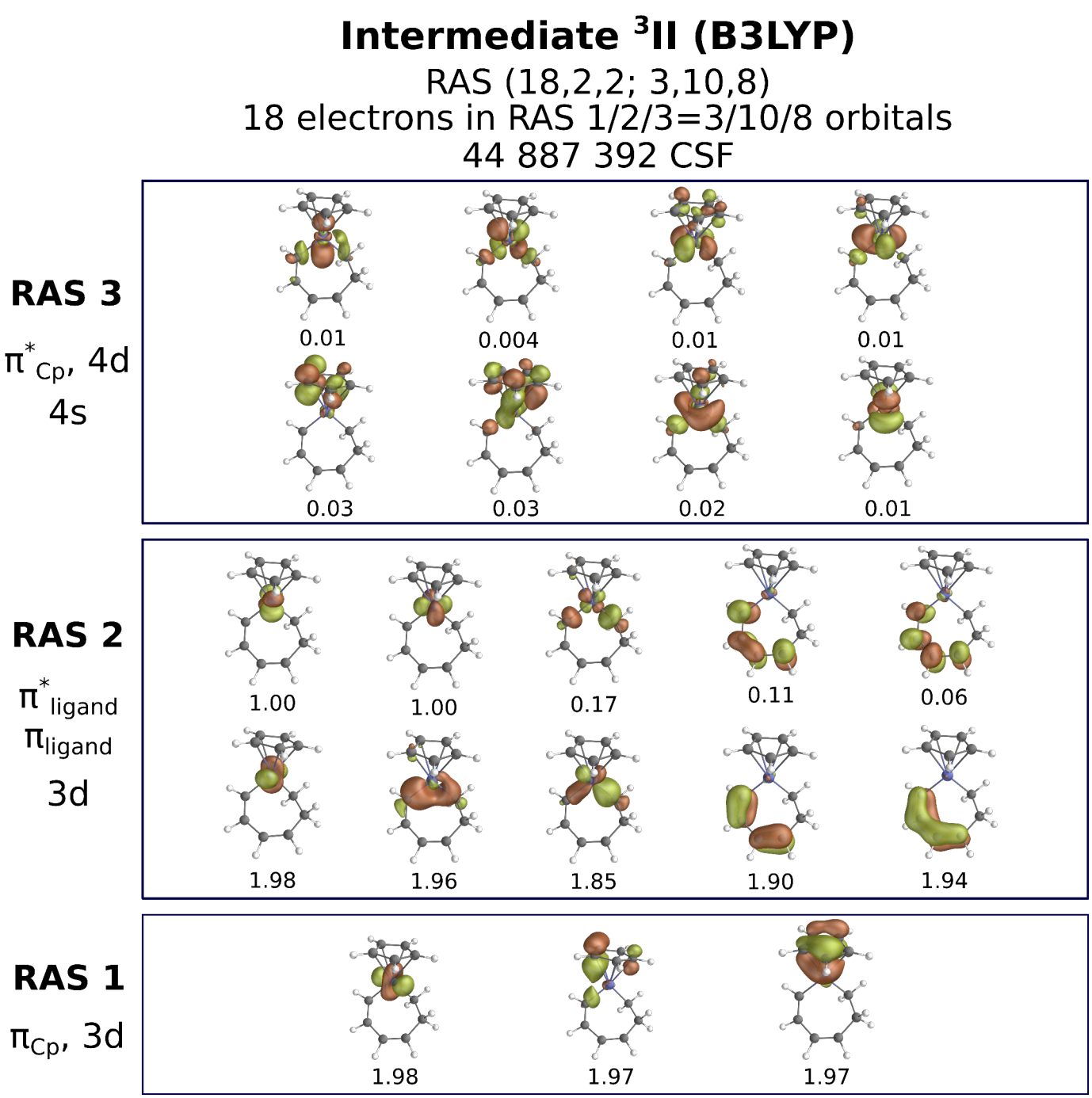

Figure 12: Active space of intermediate **II** (triplet state), isovalue=0.07, B3LYP-D3 geometry

Table 14: Largest contributions to the CASSCF wave function for **II** (triplet state, C_1, B3LYP-D3 geometry)

Configuration	Weight
Main triplet	0.77
Diexcitation $[3d-C]$ (1.85)→ $[3d-C]^*$(0.17)	0.04

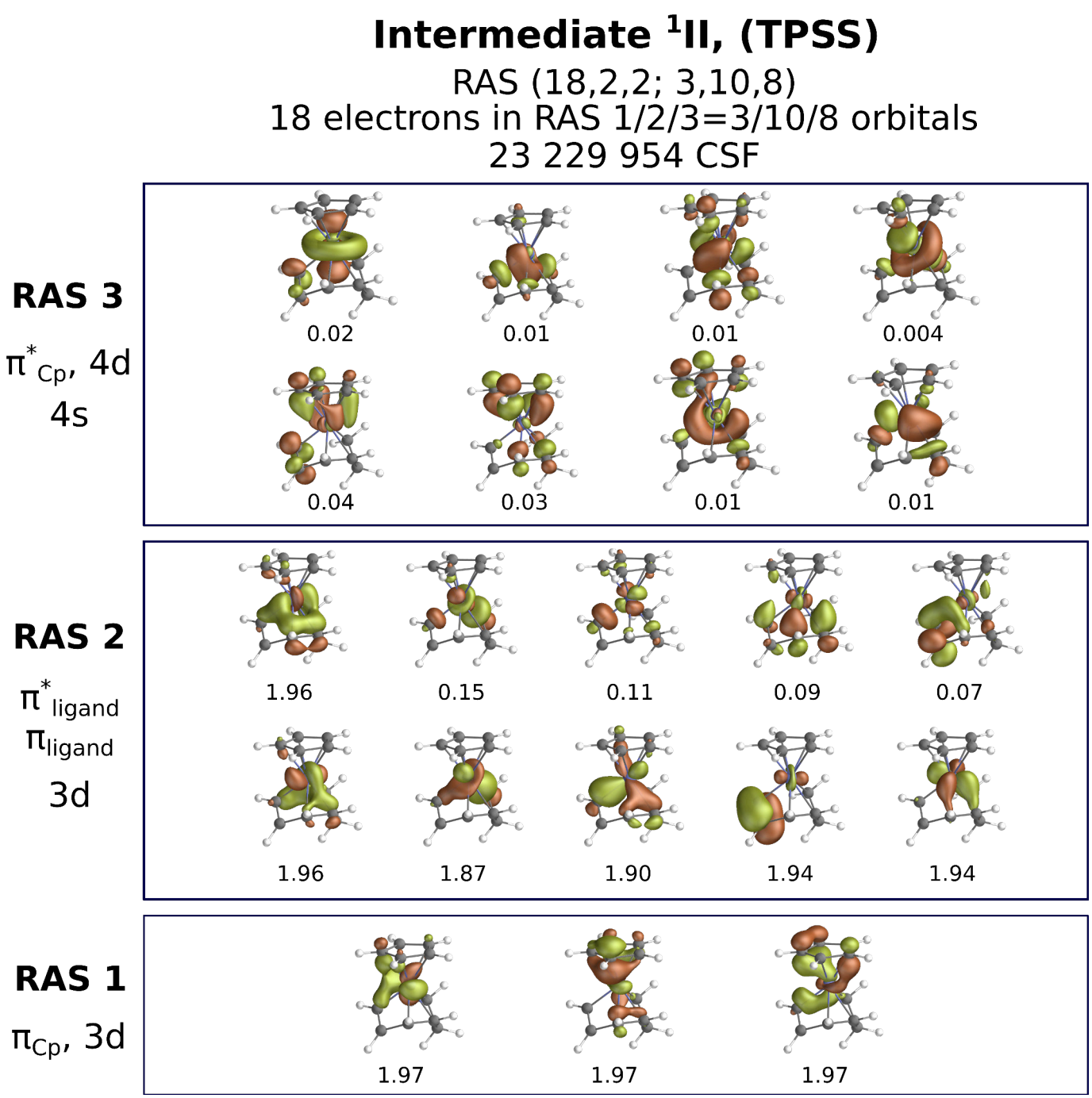

Figure 13: Active space of intermediate **II** (singlet state), isovalue=0.07, TPSS-D3 geometry

Table 15: Largest contributions to the CASSCF wave function for **II** (singlet state, C_1, TPSS-D3 geometry)

Configuration	Weight
Main singlet	0.76
Diexcitation $[3d-C2]$ (1.87)$\rightarrow$ $[3d-C2]^*$(0.15)	0.03

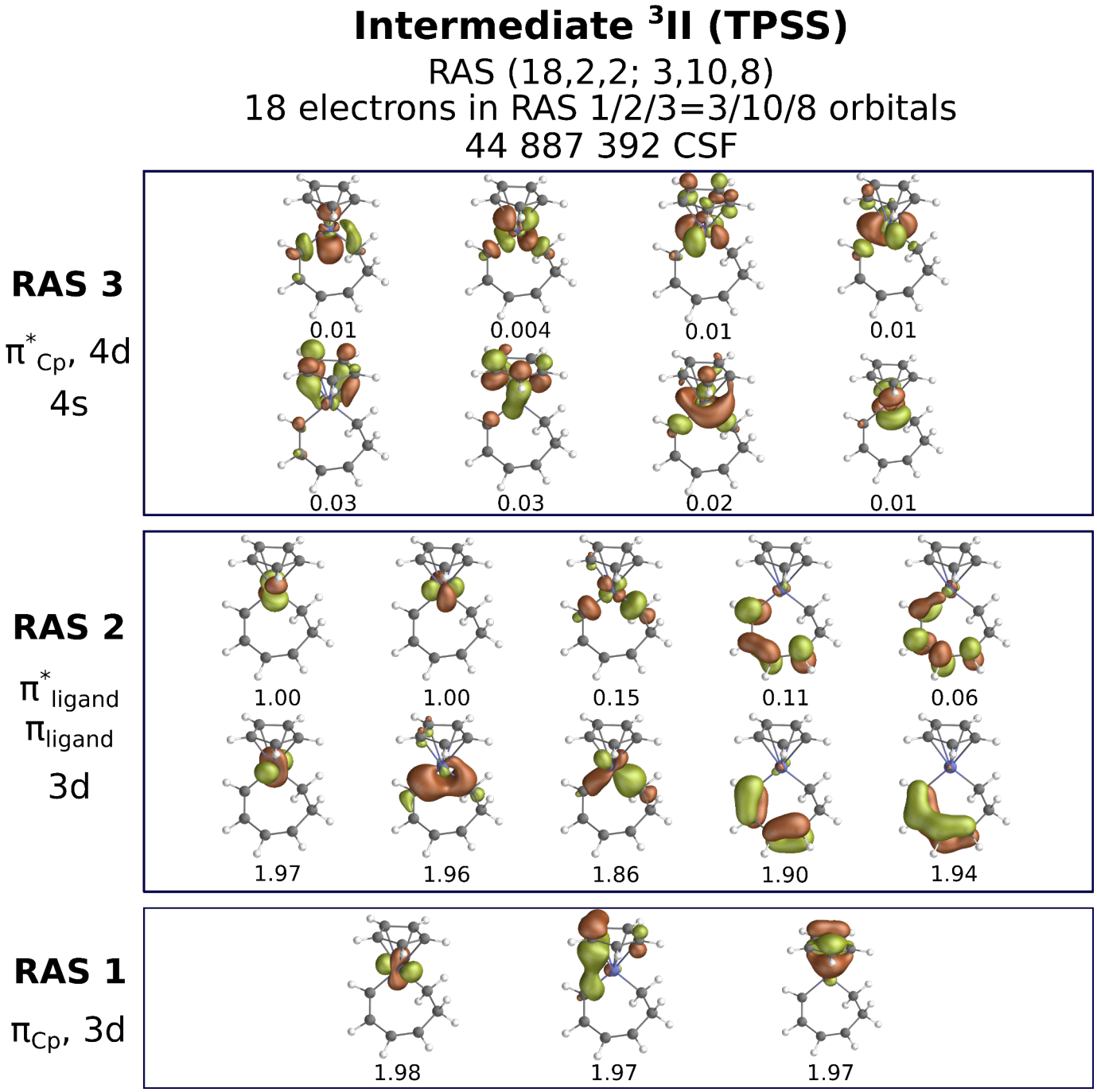

Figure 14: Active space of intermediate **II** (triplet state), isovalue=0.07, TPSS-D3 geometry

Table 16: Largest contributions to the CASSCF wave function for **II** (triplet state, C_1, TPSS-D3 geometry)

Configuration	Weight
Main triplet	0.77
Diexcitation $[3d-C]$ (1.86)→ $[3d-C]^*$(0.15)	0.03

We selected active orbitals for ^{1}**II** and ^{3}**II** with the aim of keeping RAS1, RAS2 and RAS3 of similar nature despite the structural differences between the complexes in the singlet and triplet states: overall, all orbitals of same character are kept in the same active subspaces for each spin state. In RAS1, we have a $3d$ orbital and two π orbitals of the Cp ligand in both cases. In RAS2 the metal-ligand bond differs from the singlet to the triplet. In the singlet case, two $3d$ orbitals bond asymmetrically with the terminal carbon atoms of the alkenyl chain whereas in the triplet case, only one $3d$ orbital is involved and all other $3d$ orbitals are non-bonding. The two π orbitals of the alkenyl ligand are bonding with the metal center in the singlet case and remain localised on the ligand in the triplet case (as for the corresponding π^* orbitals). Orbitals that differ significantly in occupation number from singlet to triplet state are kept in RAS2. In RAS3 two π^* orbitals of Cp, five $4d$ orbitals (double shell) and a $4s$ orbital are present in both cases.

7 Active spaces for rhodium systems

7.1 $[Rh(C_2H_4)]^+$

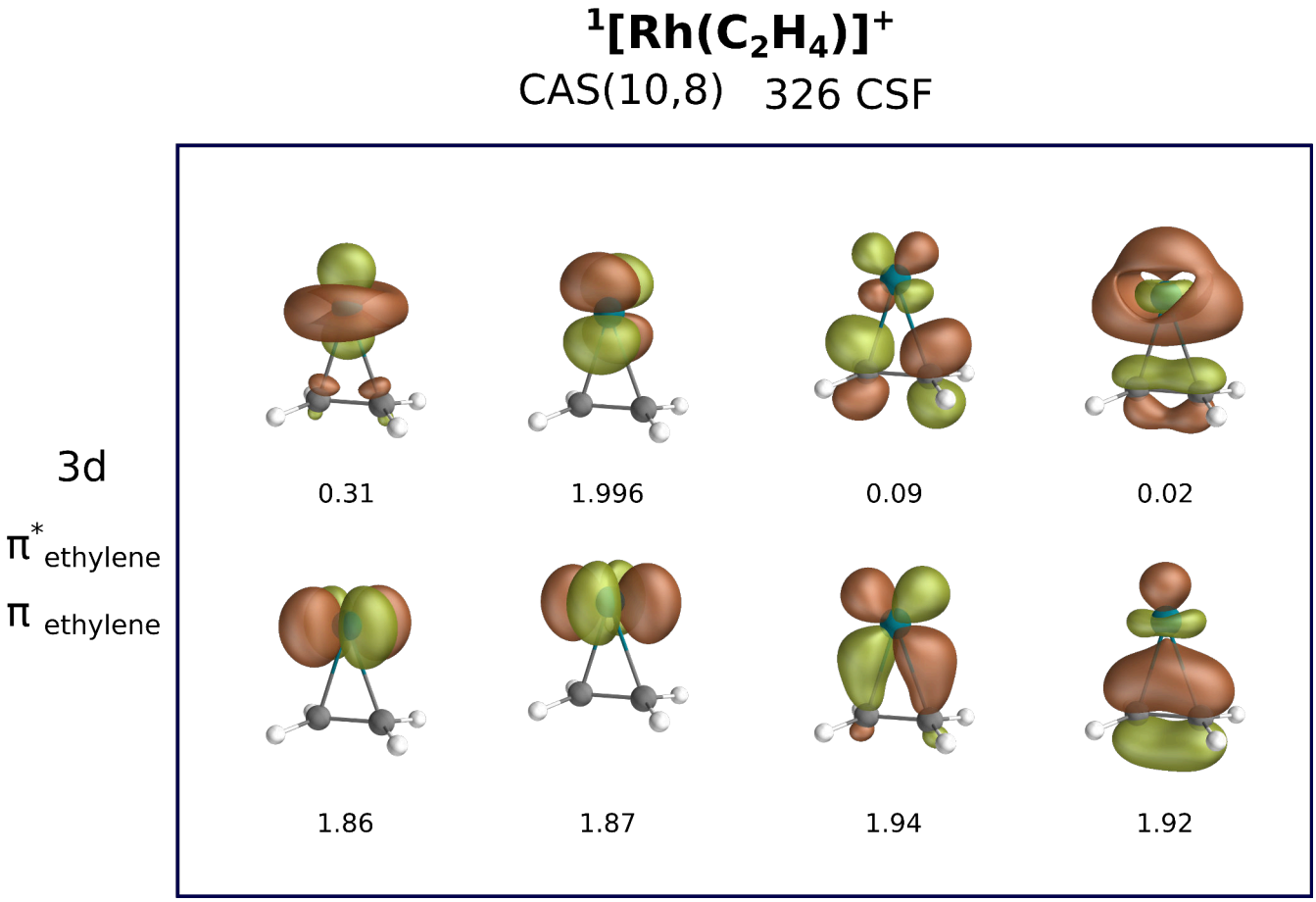

Figure 15: Active space of $[Rh(C_2H_4)]^+$ (singlet state, C_{2v}), isovalue=0.07

Table 17: Largest contributions to the CASSCF wave function for $[Rh(C_2H_4)]^+$ (singlet state, C_{2v})

Configuration	Weight
Singlet 1	0.80
Singlet 2	0.07
Singlet 3	0.06

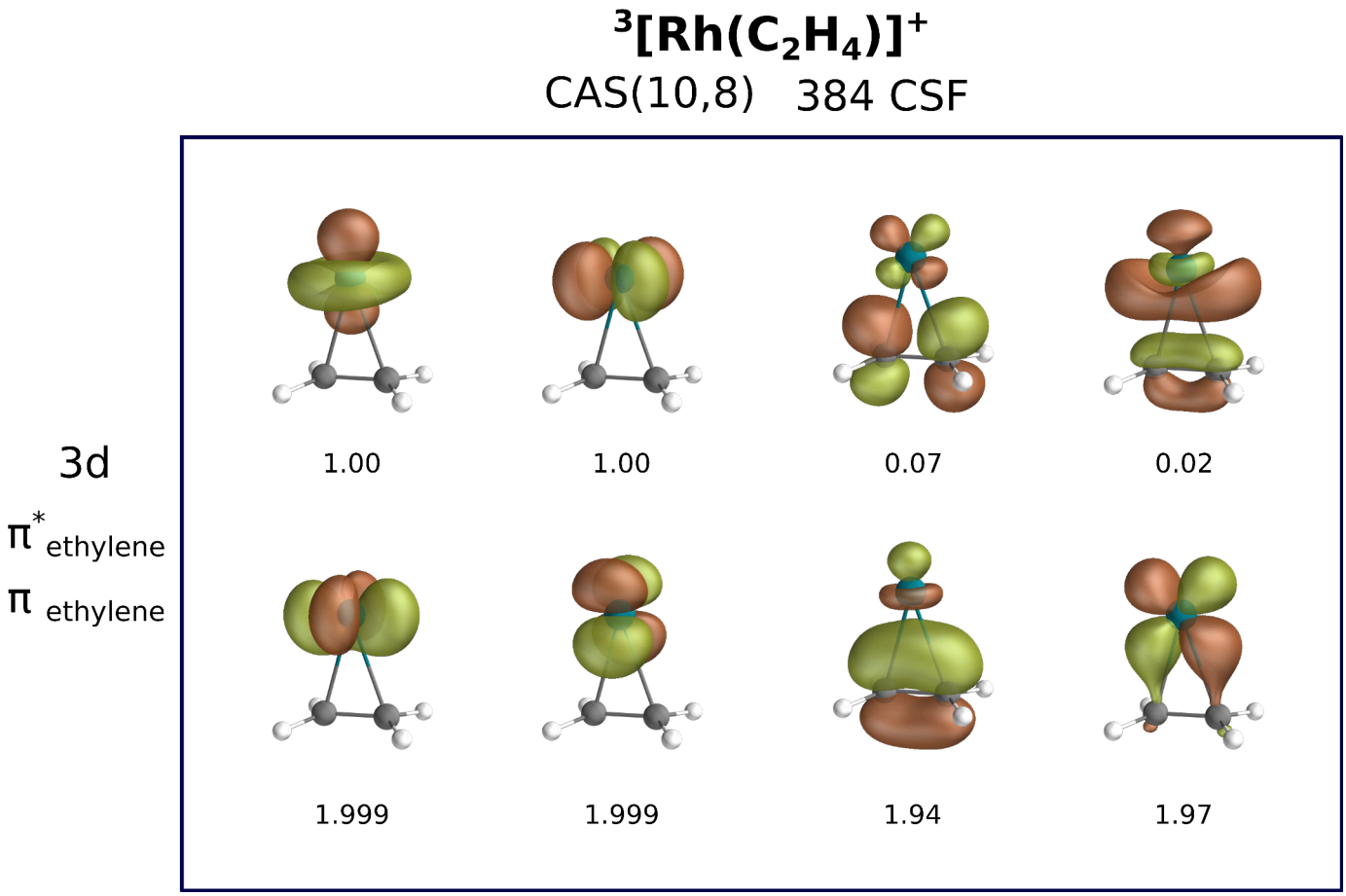

Figure 16: Active space of $[Rh(C_2H_4)]^+$ (A_2 triplet state, C_{2v}), isovalue=0.07

Table 18: Largest contributions to the CASSCF wave function for $[Rh(C_2H_4)]^+$ (A_2 triplet state, C_{2v})

Configuration	Weight
Main triplet	0.95
Diexcitation $\pi_{ethylene} \rightarrow \pi^*_{ethylene}$	0.02

7.2 CpRh

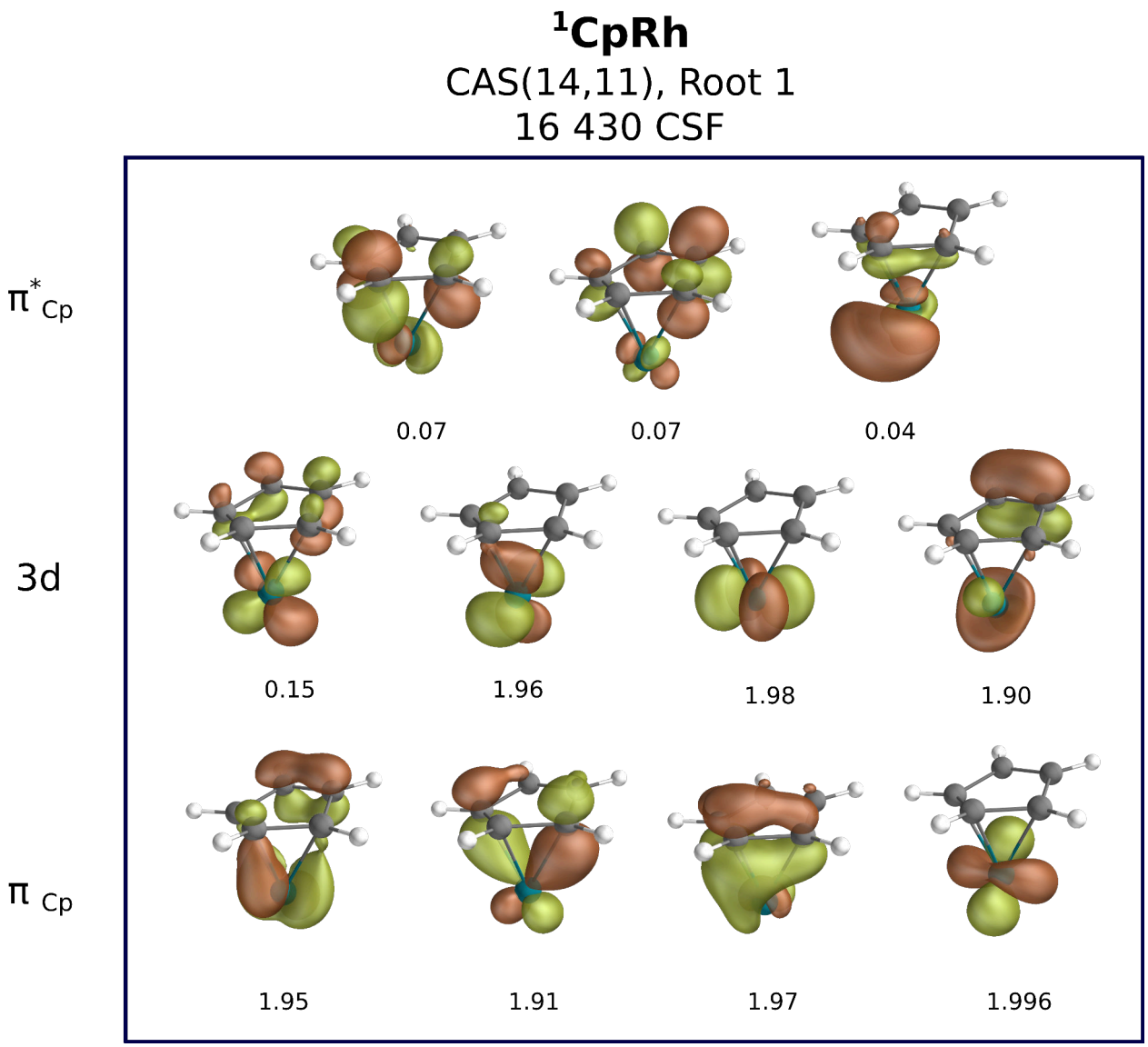

Figure 17: Active space of the first root of CpRh (singlet state, C_s), isovalue=0.07, SA-CASSCF on 2 roots

Table 19: Largest contributions to the CASSCF wave function for CpRh (singlet state, C_s), root 1, SA-CASSCF 2 roots

Configuration	Weight
Main singlet	0.84
Diexcitation $[\pi - 3d]$ (1.91) $\rightarrow$ $[\pi - 3d]^*$ (0.15)	0.02
Diexcitation $[\pi - 3d]$ (1.90)$\rightarrow$ $[\pi - 3d]^*$ (0.15)	0.01

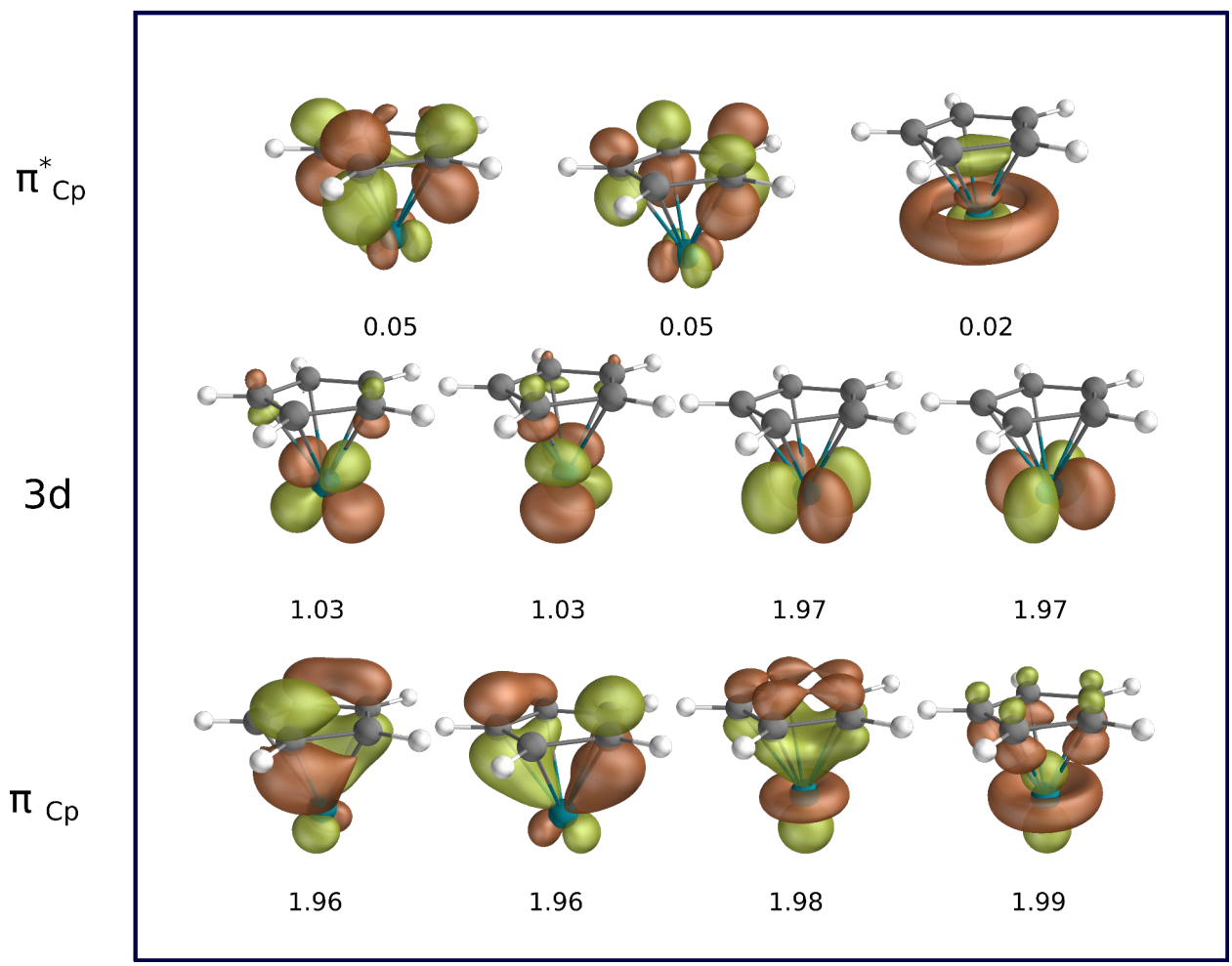

Figure 18: Active space of CpRh ($A^{''}$ triplet state, C_s), isovalue=0.07

Table 20: Largest contributions to the CASSCF wave function for CpRh ($A^{''}$ triplet state, C_s)

Configuration	Weight
Main triplet	0.91
Diexcitation, from two 3*d* (1.97, 1.97) → 3*d* (1.03, 1.03)	0.01

7.3 [CpRh(C_2H_4)]

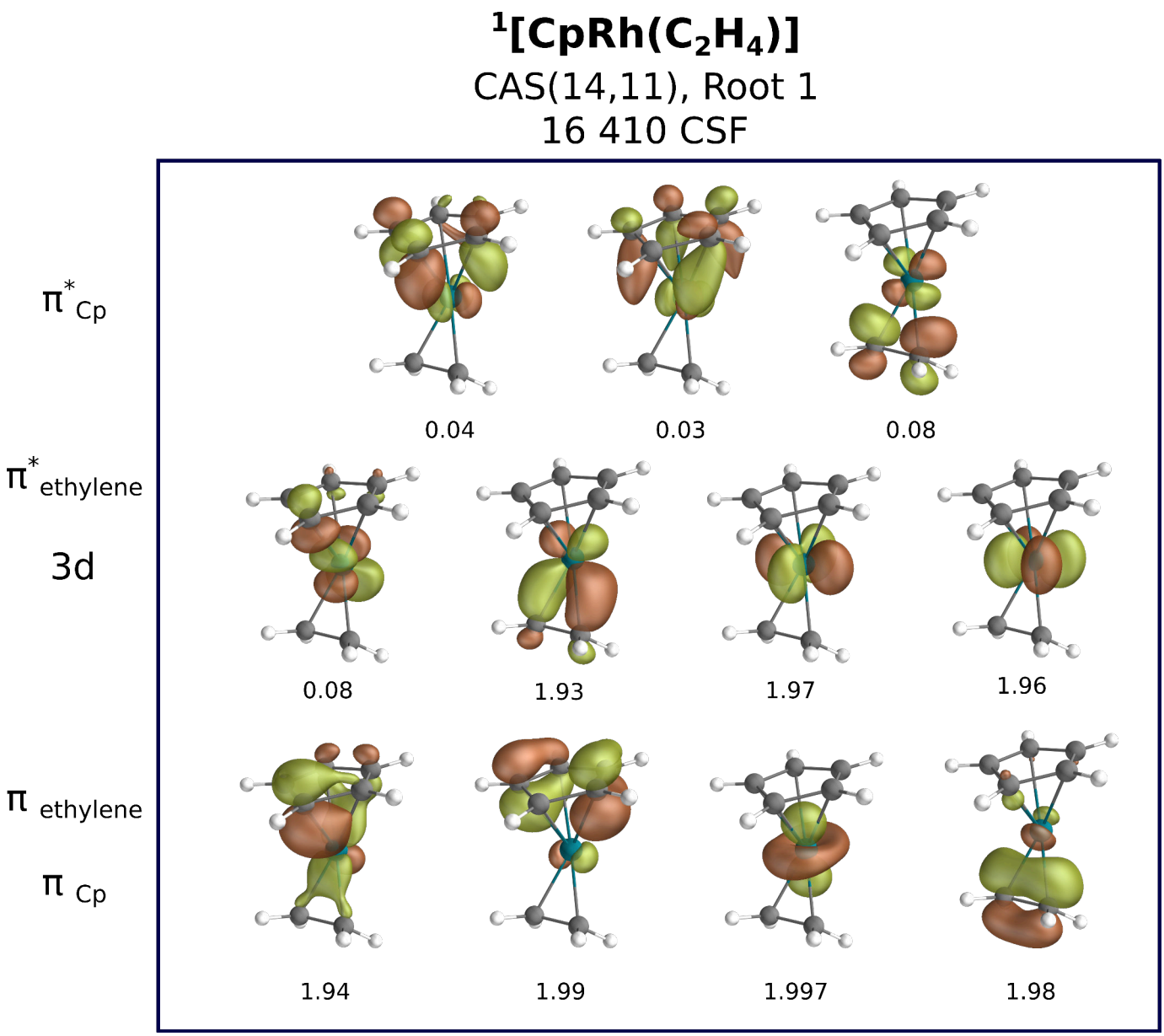

Figure 19: Active space of the first root of [CpRh(C_2H_4)] (singlet state, C_s), isovalue=0.07, SA-CASSCF on 2 roots

Table 21: Largest contributions to the CASSCF wave function for [CpRh(C_2H_4)] (singlet state, C_s)

Configuration	Weight
Main singlet	0.89
Diexcitation $[\pi_{ethylene} - 3d]$ (1.93) $\rightarrow$ $[\pi_{ethylene} - 3d]^*$ (0.08)	0.02

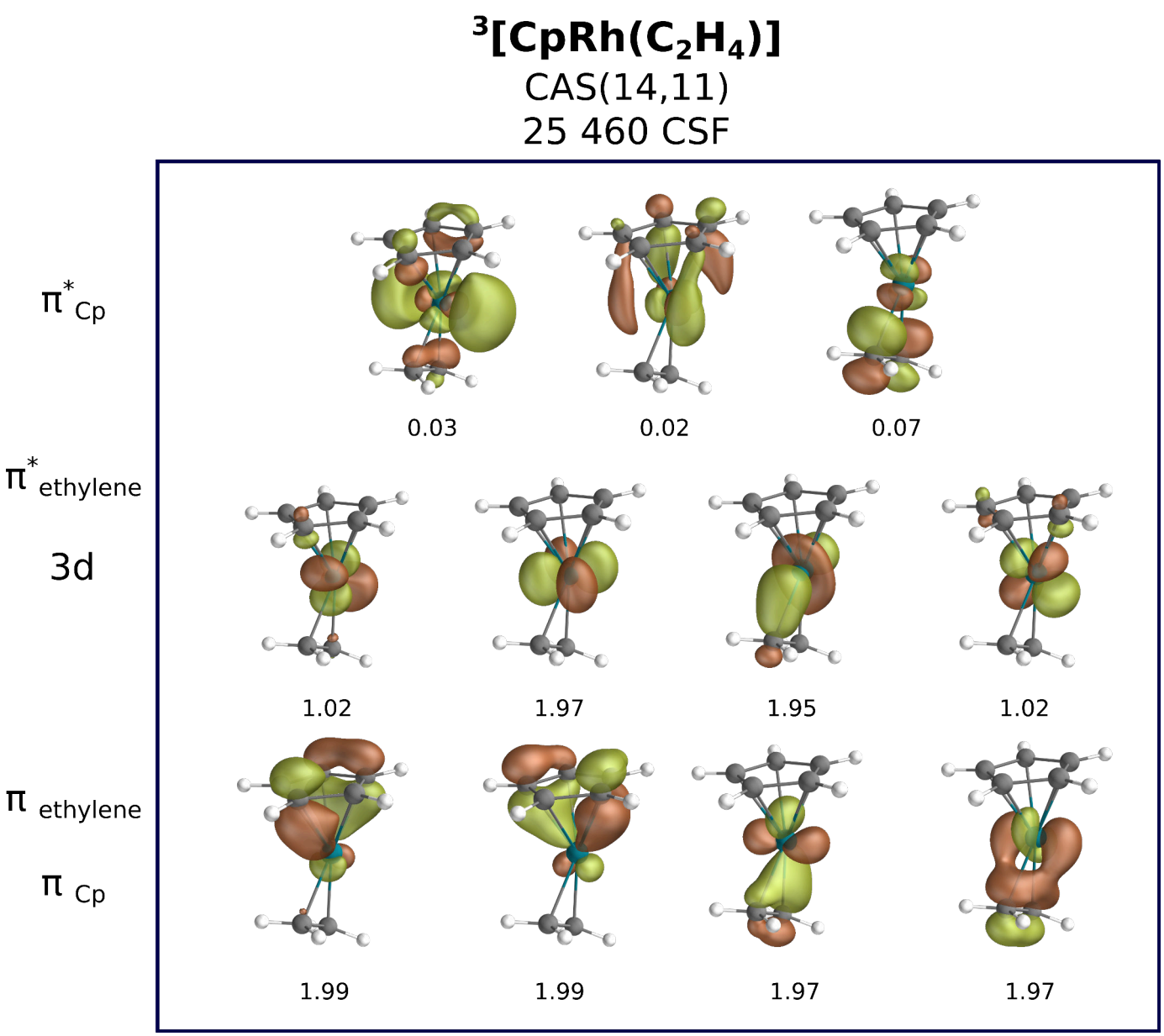

Figure 20: Active space of [CpRh(C_2H_4)] ($A^{''}$ triplet state, C_s), isovalue=0.07

Table 22: Largest contributions to the CASSCF wave function for [CpRh(C_2H_4)] ($A^{''}$ triplet state, C_s)

Configuration	Weight
Main triplet	0.92
Diexcitation $[\pi_{ethylene} - 3d]$ (1.95) $\rightarrow$ $[\pi_{ethylene} - 3d]^*$ (0.07)	0.009

8 Structural parameters

8.1 Evolution of selected geometrical parameters with the choice of density functional

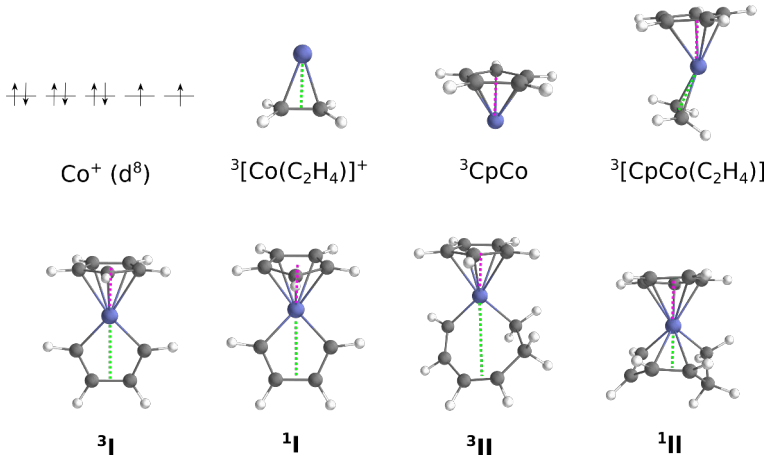

Figure 21: Co - π = green line, Co - Cp = pink line

Table 23: Selected geometry parameters for cobalt complexes (Å). Co - π is the distance between Co and the middle of the C-C bond of the ligand (see the green line in Figure 21). Co - Cp is the distance between the Co and the centroid of the Cp ring.

	Co - π		Co - Cp	
	singlet	triplet	singlet	triplet
B3LYP-D3				
$[Co(C_2H_4)]^+$	1.94	1.99	-	-
CpCo	-	-	1.68	1.75
$[CpCo(C_2H_4)]$	1.84	1.91	1.71	1.88
I C_s	2.63	2.65	1.74	1.85
II	2.08	3.37	1.77	1.90
PBE0-D3				
$[Co(C_2H_4)]^+$	1.89	1.95	-	-
CpCo	-	-	1.64	1.71
$[CpCo(C_2H_4)]$	1.82	1.88	1.67	1.87
I C_s	2.62	2.65	1.69	1.82
II	2.01	3.30	1.72	1.84
TPSS-D3				
$[Co(C_2H_4)]^+$	-	-	-	-
CpCo	-	-	1.60	1.65
$[CpCo(C_2H_4)]$	1.82	1.88	1.64	1.86
I (singlet C_1, triplet C_s)	2.27	2.67	1.68	1.76
II	1.97	3.31	1.71	1.80
PBE-D3				
$[Co(C_2H_4)]^+$	-	-	-	-
CpCo	-	-	1.60	1.65
$[CpCo(C_2H_4)]$	1.82	1.88	1.65	1.78
I (singlet C_1, triplet C_s)	2.27	2.67	1.69	1.77
II	1.97	3.31	1.72	1.81
TPSSh-D3				
$[Co(C_2H_4)]^+$	1.85	1.93	-	-
CpCo	-	-	1.61	1.67
$[CpCo(C_2H_4)]$	1.82	1.88	1.65	1.86
I (singlet C_1, triplet C_s)	2.29	2.66	1.68	1.79
II	1.98	3.30	1.71	1.82

	Co - π		Co - Cp	
	singlet	triplet	singlet	triplet
BP86-D3				
$[Co(C_2H_4)]^+$	-	-	-	-
CpCo	-	-	1.61	1.66
$[CpCo(C_2H_4)]$	1.83	1.89	1.65	1.86
I (singlet C_1, triplet C_s)	2.28	2.66	1.69	1.77
II	1.97	3.32	1.72	1.81
CAM-B3LYP				
$[Co(C_2H_4)]^+$	1.93	1.98	-	-
CpCo	-	-	1.67	1.74
$[CpCo(C_2H_4)]$	1.87	1.89	1.70	1.87
I C_s	2.62	2.64	1.71	1.84
II	2.10	3.35	1.76	1.86
M06				
$[Co(C_2H_4)]^+$	1.92	1.95	-	-
CpCo	-	-	1.66	1.71
$[CpCo(C_2H_4)]$	1.83	1.90	1.68	1.82
I C_s	2.63	2.64	1.69	1.79
II	2.02	3.26	1.72	1.82
M06-L				
$[Co(C_2H_4)]^+$	-	-	-	-
CpCo	-	-	1.58	1.64
$[CpCo(C_2H_4)]$	1.81	1.87	1.63	1.79
I (singlet C_1, triplet C_s)	2.25	-	1.67	-
II	1.97	3.31	1.71	1.80

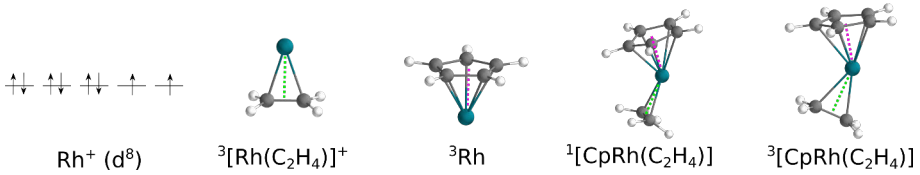

Figure 22: Rh - π = green line, Rh - Cp = pink line

Table 24: Selected geometry parameters for rhodium complexes (Å). Rh - π is the distance between Rh and the middle of the C-C bond of the ligand (see the green line in Figure 22). Rh - Cp is the distance between the Rh and the centroid of the Cp ring.

	Rh - π		Rh - Cp	
	singlet	triplet	singlet	triplet
B3LYP-D3				
$[Rh(C_2H_4)]^+$	1.97	2.10	-	-
CpRh	-	-	2.00	1.94
$[Rh(C_2H_4)]$	1.96	2.07	1.91	1.99
PBE0-D3				
$[Rh(C_2H_4)]^+$	1.93	2.04	-	-
CpRh	-	-	1.82	1.87
$[CpRh(C_2H_4)]$	1.93	2.03	1.85	1.92
TPSS-D3				
$[Rh(C_2H_4)]^+$	-	-	-	-
CpRh	-	-	1.96	1.85
$[CpRh(C_2H_4)]$	1.95	2.04	1.85	1.92
PBE-D3				
$[Rh(C_2H_4)]^+$	-	-	-	-
CpRh	-	-	1.98	1.85
$[CpRh(C_2H_4)]$	1.95	2.03	1.85	1.92

	Rh - π		Rh - Cp	
	singlet	triplet	singlet	triplet
TPSSh-D3				
$[Rh(C_2H_4)]^+$	1.93	2.04	-	-
CpRh	-	-	1.82	1.86
$[CpRh(C_2H_4)]$	1.95	2.04	1.85	1.92
BP86-D3				
$[Rh(C_2H_4)]^+$	-	-	-	-
CpRh	-	-	2.00	1.86
$[CpRh(C_2H_4)]$	1.95	2.03	1.86	1.93
CAM-B3LYP				
$[Rh(C_2H_4)]^+$	1.97	2.09	-	-
CpRh	-	-	1.86	1.92
$[CpRh(C_2H_4)]$	1.95	2.07	1.88	1.99
M06				
$[Rh(C_2H_4)]^+$	1.95	2.07	-	-
CpRh	-	-	1.86	1.91
$[CpRh(C_2H_4)]$	1.96	2.05	1.88	1.96
M06-L				
$[Rh(C_2H_4)]^+$	-	-	-	-
CpRh	-	-	1.80	1.85
$[CpRh(C_2H_4)]$	1.94	2.03	1.83	1.91

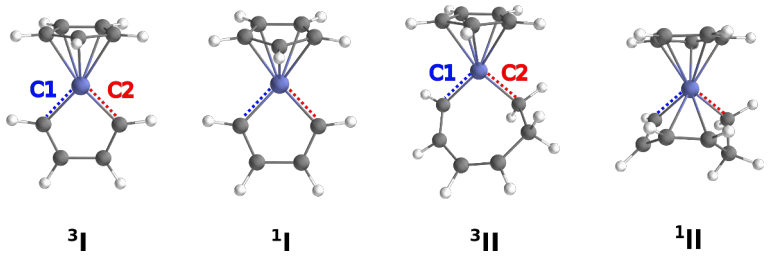

Figure 23: Co - C1 = blue line, Co - C2 = red line

Table 25: Distance between cobalt and terminal carbon atoms C1 and C2 of the ligand (Å) (corresponding to the red and blue lines in Figure 23)

	Co - C1		Co - C2	
	singlet	triplet	singlet	triplet
B3LYP-D3				
I C_s	1.93	1.93	1.93	1.93
II	1.92	1.92	1.99	1.97
PBE0-D3				
I C_s	1.92	1.92	1.92	1.92
II	1.90	1.91	1.97	1.95
TPSS-D3				
I (singlet C_1, triplet C_s)	1.91	1.89	1.81	1.89
II	1.92	1.89	2.01	1.96
PBE-D3				
I (singlet C_1, triplet C_s)	1.91	1.88	1.81	1.88
II	1.92	1.88	2.01	1.95
TPSSh-D3				
I (singlet C_1, triplet C_s)	1.91	1.91	1.82	1.91
II	1.92	1.90	1.99	1.96
BP86-D3				
I (singlet C_1, triplet C_s)	1.91	1.88	1.81	1.88
II	1.92	1.88	2.01	1.95
CAM-B3LYP				
I C_s	1.92	1.93	1.92	1.93
II	1.91	1.91	1.96	1.95
M06				
I C_s	1.93	1.91	1.93	1.91
II	1.92	1.91	1.98	1.96
M06-L				
I (singlet C_1, triplet C_s)	1.91	-	1.81	-
II	1.92	1.91	2.00	1.96

References

[1] A. Fouqueau, S. Mer, M. E. Casida, L. M. Lawson Daku, A. Hauser, T. Mineva and F. Neese, *J. Chem. Phys.*, 2004, **120**, 9473–9486.

[2] E. Giner, D. P. Tew, Y. Garniron and A. Alavi, *J. Chem. Theory Comput.*, 2018, **14**, 6240–6252.

9 Energies and coordinates

9.1 Energies

9.1.1 DFT Energies

Table 26: Energies (in hartree) of DFT optimised structures for cobalt model systems

Singlet	Co^+	$[Co(C_2H_4)]^+$	CpCo	$[CpCo(C_2H_4)]$
M06	-1382.32606	-1460.96679	-1576.12178	-1654.75949
TPSSh-D3	-1382.39119	-1461.12543	-1576.38461	-1655.11315
PBE0-D3	-1382.14436	-1460.75516	-1575.86364	-1654.47439
B3LYP-D3	-1382.31611	-1460.97679	-1576.13848	-1654.79484
CAM-B3LYP	-1382.46289	-1461.11996	-1576.29114	-1654.94419
M06-L	-	-	-1576.26826	-1654.97200
TPSS-D3	-	-	-1576.44741	-1655.18801
PBE-D3	-	-	-1575.87576	-1654.48478
BP86-D3	-	-	-1576.61028	-1655.33831
Triplet	Co^+	$[Co(C_2H_4)]^+$	CpCo	$[CpCo(C_2H_4)]$
M06	-1382.41347	-1461.03965	-1576.17020	-1654.78582
TPSSh-D3	-1382.49435	-1461.20842	-1576.43828	-1655.13582
PBE0-D3	-1382.24733	-1460.84351	-1575.92712	-1654.51092
B3LYP-D3	-1382.41269	-1461.05951	-1576.19571	-1654.82786
CAM-B3LYP	-1382.55847	-1461.20214	-1576.35135	-1654.97955
M06-L	-	-	-1576.31743	-1654.99410
TPSS-D3	-	-	-1576.49260	-1655.19940
PBE-D3	-	-	-1575.91765	-1654.49322
BP86-D3	-	-	-1576.65267	-1655.34747

Table 27: Energies (in hartree) of DFT optimised structures for target systems

Singlet	**I**	**II**
M06	-1730.86894	-1809.48657
TPSSh-D3	-1731.29831	-1809.99552
PBE0-D3	-1730.55657	-1809.14490
B3LYP-D3	-1730.92648	-1809.55123
CAM-B3LYP	-1731.07305	-1809.69648
M06-L	-1731.13771	-1809.80512
TPSS-D3	-1731.38818	-1810.09139
PBE-D3	-1730.57529	-1809.14820
BP86-D3	-1731.52671	-1810.21847
Triplet	**I**	**II**
M06	-1730.88764	-1809.48515
TPSSh-D3	-1731.31600	-1809.98565
PBE0-D3	-1730.58533	-1809.15377
B3LYP-D3	-1730.95170	-1809.56418
CAM-B3LYP	-1731.09941	-1809.71007
M06-L	-1731.15033	-1809.79909
TPSS-D3	-1731.39802	-1810.06965
PBE-D3	-1730.58332	-1809.12705
BP86-D3	-1731.53547	-1810.19811

Table 28: Energies (in hartree) of DFT optimised structures for rhodium systems

Singlet	Rh^+	$[Rh(C_2H_4)]^+$	CpRh	$[CpRh(C_2H_4)]$
M06	-110.13555	-188.80986	-304.15321	-382.59414
TPSSh-D3	-110.09272	-188.84965	-304.09851	-382.82387
PBE0-D3	-110.12350	-188.76427	-303.86748	-382.47938
B3LYP-D3	-110.11665	-188.80067	-303.95768	-382.60991
CAM-B3LYP	-110.09787	-188.77867	-303.94344	-382.59679
M06-L	-	-	-303.95990	-382.85215
TPSS-D3	-	-	-304.13131	-382.86701
PBE-D3	-	-	-303.89058	-382.49482
BP86-D3	-	-	-304.25211	-382.97265
Triplet	Rh^+	$[Rh(C_2H_4)]^+$	CpRh	$[CpRh(C_2H_4)]$
M06	-110.20111	-188.82713	-304.17667	-382.58379
TPSSh-D3	-110.17308	-188.88502	-304.12358	-382.81129
PBE0-D3	-110.20246	-188.79948	-303.89488	-382.46909
B3LYP-D3	-110.18962	-188.83349	-303.98224	-382.60137
CAM-B3LYP	-110.16981	-188.81266	-303.97069	-382.59127
M06-L	-	-	-303.98004	-382.83847
TPSS-D3	-	-	-304.15396	-382.85251
PBE-D3	-	-	-303.91039	-382.47943
BP86-D3	-	-	-304.27184	-382.95863

9.1.2 Wave function methods single-point energies

Table 29: Single-point energies (in hartree) of wave function methods for cobalt model systems

Singlet	Co^+	$[Co(C_2H_4)]^+$	CpCo	$[CpCo(C_2H_4)]$
RHF molpro	-	-	-1584.03539	-1662.15928
CASSCF molpro	-1391.48961	-1469.80716	-1584.27934	-1662.45909
CASSCF molcas	-1391.63317	-1469.80716	-1584.27911	-1662.45917
MRCISD sp	-1392.20673	-1470.39683	-1584.89872	-1663.10874
MRCISD nosp	-1391.78104	-1469.97655	-1584.48583	-1662.69881
CASPT2 sp	-1392.22694	-1470.41728	-1584.91884	-1663.11915
CASPT2 nosp	-1391.78888	-1469.98301	-1584.49034	-1662.69588
CCSD sp	-	-	-1585.68996	-1664.22160
CCSD nosp	-	-	-1585.26763	-1663.80076
CCSD(T) sp	-	-	-1585.78267	-1664.33903
CCSD(T) nosp	-	-	-1585.34898	-1663.90529
f12-CCSD(T) sp B3	-	-	-1575.40540	-1653.96154
f12-CCSD(T) sp B5	-	-	-1575.37113	-1653.93101
f12-BCCD(T) sp B3	-	-	-1575.40969	-1653.96749
f12-BCCD(T) sp B5	-	-	-1575.37703	-1653.93875
Triplet	Co^+	$[Co(C_2H_4)]^+$	CpCo	$[CpCo(C_2H_4)]$
ROHF molpro	-	-	-1584.05475	-1651.61709
CASSCF molpro	-1391.55290	-1469.86670	-1584.33721	-1662.48966
CASSCF molcas	-1391.69538	-1469.86670	-1584.33721	-1662.48969
MRCISD sp	-1392.25770	-1470.44821	-1584.94705	-1663.12695
MRCISD nosp	-1391.83750	-1470.03062	-1584.53470	-1662.71759
CASPT2 sp	-1392.27501	-1470.46673	-1584.96745	-1663.14533
CASPT2 nosp	-1391.84413	-1470.03619	-1584.53852	-1662.71693
CCSD sp	-	-	-1585.78955	-1664.25271
CCSD nosp	-	-	-1585.33965	-1663.83209
CCSD(T) sp	-	-	-1585.88664	-1664.35779
CCSD(T) nosp	-	-	-1585.42468	-1663.92530
f12-CCSD(T) sp B3	-	-	-1575.45362	-1653.98193
f12-CCSD(T) sp B5	-	-	-1575.42258	-1653.95228
f12-BCCD(T) sp B3	-	-	-1575.45651	-1653.98262
f12-BCCD(T) sp B5	-	-	-1575.42481	-1653.95484

Table 30: Single-point energies (in hartree) of wave function methods for cobalt target systems

Singlet geometry	**I** B3LYP-D3	**I** TPSS-D3	**II** B3LYP-D3	**II** TPSS-D3
RHF molpro	-1737.89398	-1737.85599	-1815.99644	-1815.96859
RASSCF molcas	-	-1738.23065	-1816.35932	-1816.35200
RASPT2 sp	-	-1738.96541	-1817.07937	-1817.07439
RASPT2 nosp	-	-1738.53323	-1816.64862	-1816.64678
CCSD sp	-1740.22555	-1740.22141	-1818.72320	-1818.72247
CCSD nosp	-1739.80434	-1739.80085	-1818.30236	-1818.30213
CCSD(T) sp	-1740.36363	-1740.36811	-1818.88353	-1818.88760
CCSD(T) nosp	-1739.92975	-1739.93454	-1818.44959	-1818.45382
Triplet geometry	**I** B3LYP-D3	**I** TPSS-D3	**II** B3LYP-D3	**II** TPSS-D3
ROHF molpro	-1737.93250	-1737.91901	-1816.08763	-1816.07813
RASSCF molcas	-	-1738.25660	-1816.38366	-1816.37481
RASPT2 sp	-	-1738.97823	-1817.07447	-1817.07056
RASPT2 nosp	-	-1738.54616	-1816.64170	-1816.63766
CCSD sp	-1740.22306	-1740.22908	-1818.72856	-1818.72881
CCSD nosp	-1739.80382	-1739.80996	-1818.30867	-1818.30882
CCSD(T) sp	-1740.37259	-1740.37652	-1818.86860	-1818.87062
CCSD(T) nosp	-1739.94339	-1739.94630	-1818.43616	-1818.43798

Table 31: Single-point energies (in hartree) of wave function methods for rhodium systems

Singlet	Rh^+	$[Rh(C_2H_4)]^+$	CpRh	$[CpRh(C_2H_4)]$
RHF molpro	-	-	-301.59258	-379.70065
CASSCF molpro	-109.09707	-187.24330	-301.69227	-379.80521
CASSCF molcas	-109.09707	-187.24330	-301.69210	-379.80526
MRCISD sp	-109.71411	-187.88787	-302.41910	-380.51569
MRCISD nosp	-109.33981	-187.51777	-302.05218	-380.15467
CASPT2 sp	-109.73583	-187.90658	-302.44139	-380.52866
CASPT2 nosp	-109.35298	-187.52899	-302.06052	-380.15980
CCSD sp	-	-	-303.14271	-381.58067
CCSD nosp	-	-	-302.77181	-381.25848
CCSD(T) sp	-	-	-303.23209	-381.68796
CCSD(T) nosp	-	-	-302.84762	-381.35355
Triplet	Rh^+	$[Rh(C_2H_4)]^+$	CpRh	$[CpRh(C_2H_4)]$
ROHF molpro	-	-	-301.65305	-379.72329
CASSCF molpro	-109.14851	-187.27687	-301.72047	-379.80051
CASSCF molcas	-109.14851	-187.27687	-301.72047	-379.80056
MRCISD sp	-109.75332	-187.90608	-302.43930	-380.50593
MRCISD nosp	-109.38180	-187.52714	-302.07308	-380.13918
CASPT2 sp	-109.77192	-187.92477	-302.45882	-380.52417
CASPT2 nosp	-109.39339	-187.53499	-302.07927	-380.14415
CCSD sp	-	-	-303.17194	-381.63494
CCSD nosp	-	-	-302.80025	-381.26100
CCSD(T) sp	-	-	-303.25307	-381.73993
CCSD(T) nosp	-	-	-302.86858	-381.35188

9.2 Coordinates

Coordinates are given for every DFT optimised system in this study. Geometries are displayed from the smallest system to the biggest for cobalt and rhodium systems (in that order). Singlet states are given first, followed by triplets.

9.2.1 M06

```
7
E(RM06) =  -1460.96679779
Co    0.000000    0.000000    0.723275
C     0.000000    0.684473   -1.192935
H    -0.926516    1.244214   -1.303299
H     0.926516    1.244214   -1.303299
C    -0.000000   -0.684473   -1.192935
H     0.926516   -1.244214   -1.303299
H    -0.926516   -1.244214   -1.303299

7
E(UM06) =  -1461.03965849
Co   -0.000000    0.000000    0.735950
C    -0.000000    0.685502   -1.212422
H    -0.924624    1.246616   -1.330397
H     0.924624    1.246616   -1.330397
C    -0.000000   -0.685502   -1.212422
H     0.924624   -1.246616   -1.330397
H    -0.924624   -1.246616   -1.330397

11
E(RM06) =  -1576.12178356
Co   -0.934353   -0.046394    0.000000
C     0.807200   -1.196919    0.000000
C     0.697559   -0.344824    1.129609
C     0.697559   -0.344824   -1.129609
H     0.921856   -2.269109    0.000000
C     0.697559    1.032146    0.699628
H     0.676909   -0.666872    2.162139
C     0.697559    1.032146   -0.699628
H     0.676909   -0.666872   -2.162139
H     0.683622    1.894568    1.348918
H     0.683622    1.894568   -1.348918

11
E(UM06) =  -1576.17020468
Co    0.968303    0.000218    0.000000
C    -0.743718    1.210205   -0.000000
C    -0.743394    0.373827    1.151089
C    -0.743394    0.373827   -1.151089
H    -0.768402    2.289870   -0.000000
C    -0.743394   -0.979350    0.711444
H    -0.768168    0.707448    2.177963
C    -0.743394   -0.979350   -0.711444
H    -0.768168    0.707448   -2.177963
H    -0.767845   -1.852798    1.346131
H    -0.767845   -1.852798   -1.346131

17
E(RM06) =  -1654.75949778
Co    0.395944    0.258731   -0.000000
C     0.339144    2.083805    0.704910
H    -0.561987    2.301897    1.269967
H     1.261021    2.304220    1.241745
C     0.339144    2.083805   -0.704910
H     1.261021    2.304220   -1.241745
H    -0.561987    2.301897   -1.269967
C    -0.779846   -0.997731    1.164323
C    -1.437019   -0.486486    0.000000
C     0.339144   -1.708757    0.717347
H    -1.060683   -0.810361    2.188848
C    -0.779846   -0.997731   -1.164323
H    -2.311479    0.149211   -0.000000
C     0.339144   -1.708757   -0.717347
H     1.092539   -2.167681    1.340812
H    -1.060683   -0.810361   -2.188848
H     1.092539   -2.167681   -1.340812
```

```
17
E(UM06) =  -1654.78582192
Co     0.410818   -0.207005   -0.136508
C      2.381717   -0.557468    0.112927
H      2.563369   -1.018188    1.077602
H      2.732780   -1.121940   -0.746847
C      2.150799    0.810718   -0.000011
H      2.317051    1.322089   -0.943687
H      2.133487    1.450327    0.875681
C     -1.238216    0.302812    1.256245
C     -1.220341    1.280090    0.234415
C     -1.439367   -0.958118    0.655160
H     -1.102364    0.485021    2.311765
C     -1.413208    0.625901   -1.002339
H     -1.070952    2.340362    0.373482
C     -1.548301   -0.761046   -0.751870
H     -1.516209   -1.901635    1.174678
H     -1.446796    1.099040   -1.972385
H     -1.740944   -1.523265   -1.491738

19
E(RM06) =  -1730.86920698
C      0.015251   -2.596301    0.735613
C      0.015251   -2.596301   -0.735613
C     -0.013283   -1.385258    1.290221
C     -0.013283   -1.385258   -1.290221
Co    -0.301372    0.022115    0.000000
C      0.572737    1.503577   -1.154975
H      0.867429    1.335820   -2.179444
C     -0.658470    1.994187   -0.716309
H     -1.484447    2.289928   -1.346047
C     -0.658470    1.994187    0.716309
H     -1.484447    2.289928    1.346047
C      1.330818    1.131335    0.000000
H      2.313694    0.686473    0.000000
C      0.572737    1.503577    1.154975
H      0.867429    1.335820    2.179444
H     -0.001981   -1.232013    2.368378
H      0.040813   -3.526765    1.302262
H      0.040813   -3.526765   -1.302262
H     -0.001981   -1.232013   -2.368378

19
E(UM06) =  -1730.88764127
C      0.059022    2.661450    0.721925
C      0.059022    2.661450   -0.721925
C     -0.006096    1.435545    1.280722
C     -0.006096    1.435545   -1.280722
Co    -0.231863    0.038233    0.000000
C     -0.219394   -1.772280   -1.141683
H     -0.543764   -1.818656   -2.170402
C      1.112988   -1.541560   -0.700867
H      1.963022   -1.343172   -1.335544
C      1.112988   -1.541560    0.700867
H      1.963022   -1.343172    1.335544
C     -1.034194   -1.951746    0.000000
H     -2.095873   -2.147307    0.000000
C     -0.219394   -1.772280    1.141683
H     -0.543764   -1.818656    2.170402
H      0.052504    1.288828    2.358059
H      0.129791    3.586810    1.293072
H      0.129791    3.586810   -1.293072
H      0.052504    1.288828   -2.358059

25
E(RM06) =  -1809.48657421
C      1.774965   -1.650972   -0.253660
C      1.452631   -0.938071    1.002490
C      0.942878   -1.165235   -1.160394
C      1.578731    0.423149    1.121434
Co    -0.112992    0.030576   -0.091349
C     -1.719959    0.359869    1.265625
H     -1.597268    0.670816    2.292977
C     -1.836052    1.212748    0.158990
H     -1.814816    2.291523    0.182919
```

```
C    -1.898231    0.404100   -1.011622
H    -1.976779    0.757738   -2.028175
C    -1.760635   -0.988764    0.803796
H    -1.689034   -1.874648    1.416359
C    -1.889117   -0.955374   -0.594986
H    -1.910463   -1.814300   -1.248533
C     1.003557    1.472245   -0.875280
H     1.228032    1.316082   -1.930464
C     2.180739    1.303381    0.057790
H     0.481836    2.420568   -0.740787
H     0.859710   -1.438813   -2.209038
H     1.293328    0.880460    2.064954
H     1.094375   -1.497848    1.865901
H     2.530154   -2.431154   -0.335376
H     2.559383    2.238175    0.479077
H     3.015298    0.793388   -0.428485

25
E(UM06) =  -1809.48515559
C    -2.064432    1.637204   -0.163503
C    -2.798434    0.626440    0.587279
C    -0.797320    1.600211   -0.580568
C    -2.673316   -0.702524    0.665537
Co    0.377144    0.111041   -0.324832
C     1.811064   -1.228898    0.586305
H     1.598337   -2.279571    0.721230
C     2.389668   -0.638859   -0.574004
H     2.697220   -1.165020   -1.465022
C     2.469276    0.747999   -0.357151
H     2.839863    1.483336   -1.054858
C     1.553599   -0.206394    1.520011
H     1.088894   -0.327518    2.486812
C     1.933277    1.016545    0.928812
H     1.812996    1.994432    1.370435
C    -0.852619   -1.195570   -1.114044
H    -1.377701   -0.720922   -1.943343
C    -1.789714   -1.682486   -0.034309
H    -0.247193   -2.018564   -1.500871
H    -0.400449    2.466316   -1.109379
H    -3.365595   -1.188982    1.350517
H    -3.603962    1.043308    1.189296
H    -2.639203    2.549203   -0.341702
H    -1.219294   -2.221313    0.737356
H    -2.453107   -2.454808   -0.456203

7
E(RM06) =  -188.809867081
Rh    0.000000   -0.000000    0.520109
C     0.000000    0.697442   -1.428013
H    -0.926919    1.250655   -1.567189
H     0.926919    1.250655   -1.567189
C    -0.000000   -0.697442   -1.428013
H     0.926919   -1.250655   -1.567189
H    -0.926919   -1.250655   -1.567189

7
E(UM06) =  -188.827138860
Rh    0.000000   -0.000000    0.550535
C     0.000000    0.687591   -1.516661
H    -0.923020    1.248727   -1.643538
H     0.923020    1.248727   -1.643538
C    -0.000000   -0.687591   -1.516661
H     0.923020   -1.248727   -1.643538
H    -0.923020   -1.248727   -1.643538

11
E(RM06) =  -303.959900454
Rh   -0.810255   -0.100083    0.000000
C     1.207180   -1.104982    0.000000
C     0.997539   -0.262451    1.119334
C     0.997539   -0.262451   -1.119334
H     1.366911   -2.170351    0.000000
C     0.997539    1.135602    0.688364
H     1.001872   -0.580207    2.153529
C     0.997539    1.135602   -0.688364
H     1.001872   -0.580207   -2.153529
```

```
H     0.953410    1.993290    1.341582
H     0.953410    1.993290   -1.341582

11
E(UM06) =  -303.980045503
Rh   -0.837850   -0.000089    0.000000
C     1.073982   -1.208387   -0.000000
C     1.074024   -0.373341    1.149387
C     1.074024   -0.373341   -1.149387
H     1.096705   -2.287735   -0.000000
C     1.074024    0.977816    0.710341
H     1.096537   -0.706870    2.175911
C     1.074024    0.977816   -0.710341
H     1.096537   -0.706870   -2.175911
H     1.096502    1.851047    1.344753
H     1.096502    1.851047   -1.344753

17
E(RM06) =  -382.594146403
Rh    0.366752    0.259246   -0.000000
C     0.216140    2.211564    0.708013
H    -0.694054    2.408902    1.266148
H     1.124179    2.489398    1.241695
C     0.216140    2.211564   -0.708013
H     1.124179    2.489398   -1.241695
H    -0.694054    2.408902   -1.266148
C    -0.883493   -1.193695    1.172117
C    -1.514945   -0.633419    0.000000
C     0.216140   -1.915686    0.722291
H    -1.175596   -1.022769    2.195926
C    -0.883493   -1.193695   -1.172117
H    -2.414374   -0.032789    0.000000
C     0.216140   -1.915686   -0.722291
H     0.952847   -2.405006    1.342015
H    -1.175596   -1.022769   -2.195926
H     0.952847   -2.405006   -1.342015

17
E(UM06) =  -382.583799517
Rh    0.410112   -0.202165    0.000000
C     2.518266    0.202314    0.000000
H     2.922045   -0.210024    0.920640
H     2.922045   -0.210024   -0.920640
C     1.865407    1.422860    0.000000
H     1.747303    1.989917   -0.916942
H     1.747303    1.989917    0.916942
C    -1.547603    0.253553    1.148161
C    -1.535139    1.081354    0.000000
C    -1.547603   -1.095329    0.709045
H    -1.547966    0.587636    2.174150
C    -1.547603    0.253553   -1.148161
H    -1.513387    2.160790    0.000000
C    -1.547603   -1.095329   -0.709045
H    -1.566588   -1.968138    1.344001
H    -1.547966    0.587636   -2.174150
H    -1.566588   -1.968138   -1.344001
```

9.2.2 TPSSh-D3

```
7
Energy = -1461.125436668
Co    0.0000000    0.0000000   -1.6786185
C    -0.0000000   -0.7036259    0.1692956
H    -0.9207720   -1.2611206    0.3350068
H     0.9207720   -1.2611206    0.3350068
C    -0.0000000    0.7036259    0.1692956
H     0.9207720    1.2611206    0.3350068
H    -0.9207720    1.2611206    0.3350068

7
Energy = -1461.208424962
Co    0.0000000    0.0000000   -1.7302436
C     0.0000000   -0.6937294    0.1966365
H    -0.9248074   -1.2514601    0.3342427
```

```
H     0.9248074   -1.2514601    0.3342427
C     0.0000000    0.6937294    0.1966365
H     0.9248074    1.2514601    0.3342427
H    -0.9248074    1.2514601    0.3342427

11
Energy = -1576.384613224
Co    0.0460394    1.4694317    0.0000000
C    -1.2543090   -0.1328904    0.0000000
C    -0.3863466   -0.0934048    1.1339317
C    -0.3863466   -0.0934048   -1.1339317
H    -2.3313447   -0.1907584    0.0000000
C     1.0009089   -0.1930742    0.7037650
H    -0.7040154   -0.0312007    2.1671691
C     1.0009089   -0.1930742   -0.7037650
H    -0.7040154   -0.0312007   -2.1671691
H     1.8592602   -0.2552118    1.3561730
H     1.8592602   -0.2552118   -1.3561730

11
Energy = -1576.438282968
Co    0.0538475    1.5347315    0.0000000
C    -1.2226506   -0.0959850    0.0000000
C    -0.3812621   -0.1255524    1.1590373
C    -0.3812621   -0.1255524   -1.1590373
H    -2.3027676   -0.0872493    0.0000000
C     0.9803827   -0.1732590    0.7162356
H    -0.7157563   -0.1436812    2.1859004
C     0.9803827   -0.1732590   -0.7162356
H    -0.7157563   -0.1436812   -2.1859004
H     1.8524210   -0.2332560    1.3507980
H     1.8524210   -0.2332560   -1.3507980

17
Energy = -1655.113154154
Co   -0.1917371    0.4848097    0.0000000
C    -1.9913790    0.2162554    0.7136029
H    -2.1266216   -0.7051317    1.2729315
H    -2.3299235    1.1060667    1.2467535
C    -1.9913790    0.2162554   -0.7136029
H    -2.3299235    1.1060667   -1.2467535
H    -2.1266216   -0.7051317   -1.2729315
C     1.1716968   -0.5126707    1.1722819
C     0.7468405   -1.2362734    0.0000000
C     1.7521327    0.6857216    0.7222495
H     1.0213076   -0.8143906    2.1969111
C     1.1716968   -0.5126707   -1.1722819
H     0.2247306   -2.1826202    0.0000000
C     1.7521327    0.6857216   -0.7222495
H     2.1128700    1.4911913    1.3454982
H     1.0213076   -0.8143906   -2.1969111
H     2.1128700    1.4911913   -1.3454982

17
Energy = -1655.135821040
Co   -0.3922524    0.5118283    0.0000000
C    -2.1652676   -0.1161717    0.7033881
H    -2.0811962   -1.0413687    1.2643160
H    -2.6307644    0.7065717    1.2442356
C    -2.1652676   -0.1161717   -0.7033881
H    -2.6307644    0.7065717   -1.2442356
H    -2.0811962   -1.0413687   -1.2643160
C     1.2520389   -0.9251167    0.7085740
C     1.2520389   -0.9251167   -0.7085740
C     1.4696353    0.4065798    1.1515728
H     1.0810245   -1.7811883    1.3437090
C     1.4696353    0.4065798   -1.1515728
H     1.0810245   -1.7811883   -1.3437090
C     1.6159842    1.2391370    0.0000000
H     1.5370191    0.7286842    2.1801665
H     1.5370191    0.7286842   -2.1801665
H     1.8512890    2.2930538    0.0000000

19
Energy = -1731.298316341
C    -0.5315739    2.0578941    1.0509321
```

```
C     0.9431339    2.1510616    0.9511607
C    -1.2463978    1.4726685    0.0450411
C     1.4243099    1.2633712    0.0745921
Co   -0.0713171    0.0890067   -0.0485277
C     1.0749376   -1.6315251   -0.3017031
H     2.1284386   -1.6901947   -0.0788717
C     0.0195194   -1.9199385    0.5875387
H     0.1315091   -2.2285392    1.6164209
C    -1.2232866   -1.6708268   -0.0776867
H    -2.2065001   -1.7807393    0.3524108
C     0.4969980   -1.1501067   -1.5213553
H     1.0348422   -0.8111085   -2.3926600
C    -0.9274236   -1.2086504   -1.3812507
H    -1.6425938   -0.8862220   -2.1220204
H    -2.3302494    1.4825215   -0.0387475
H    -1.0327227    2.4501739    1.9395232
H     1.4913412    2.8851979    1.5405963
H     2.4670349    1.1259558   -0.1953928

19
Energy = -1731.316009161
C     0.4042242    2.5791305   -0.7244468
C     0.4042242    2.5791305    0.7244468
C     0.3428799    1.3406206   -1.2787464
C     0.3428799    1.3406206    1.2787464
Co    0.3490300   -0.0769476    0.0000000
C     0.0223372   -1.8533185    1.1475914
H     0.3364507   -1.9522261    2.1755116
C    -1.2518078   -1.3878445    0.7054909
H    -2.0528870   -1.0417571    1.3398584
C    -1.2518078   -1.3878445   -0.7054909
H    -2.0528870   -1.0417571   -1.3398584
C     0.7997873   -2.1666192    0.0000000
H     1.8120405   -2.5418127    0.0000000
C     0.0223372   -1.8533185   -1.1475914
H     0.3364507   -1.9522261   -2.1755116
H     0.2835340    1.2033072   -2.3587701
H     0.4348399    3.5047776   -1.2987082
H     0.4348399    3.5047776    1.2987082
H     0.2835340    1.2033072    2.3587701


25
Energy = -1809.995525389
C    -1.9013750    1.4230933    0.0316963
C    -0.8354412    1.3449998    1.0660095
C    -1.5120771    0.5741566   -0.9149571
C    -0.5594220    0.1587602    1.7335511
Co    0.1779157    0.0058270   -0.2129905
C     2.2580813    0.2616562    0.1071623
H     2.7241580    0.3709599    1.0748164
C     2.0060172   -0.9572632   -0.5546058
H     2.2384413   -1.9420958   -0.1805784
C     1.3133515   -0.6645285   -1.7709702
H     0.9648940   -1.3832199   -2.4962784
C     1.7666909    1.3300556   -0.7114204
H     1.8052044    2.3821725   -0.4757220
C     1.1987358    0.7577707   -1.8700469
H     0.7113407    1.2967259   -2.6675321
C    -0.7936803   -1.6594371    0.2989300
H    -1.5145290   -1.9929177   -0.4486978
C    -1.4009618   -1.0923679    1.5727521
H    -0.0568616   -2.4415184    0.4900511
H    -2.0089284    0.3279304   -1.8504366
H     0.2280188    0.1600295    2.4814272
H    -0.2670408    2.2345054    1.3326044
H    -2.7709501    2.0768494    0.0872748
H    -1.3216386   -1.7480741    2.4444870
H    -2.4499440   -0.8240700    1.4334738

25
Energy = -1809.985650324
C    -1.0137306    2.2601376    0.5947615
C    -0.2526618    2.0683622    1.8268025
C    -1.0866871    1.4485519   -0.4762780
C     0.1862125    0.9591451    2.4498913
```

```
Co   -0.2417790   -0.2474746   -0.6463757
C     1.2843554   -1.7052616   -1.0815923
H     1.6880991   -2.3566022   -0.3212544
C     0.1305982   -1.9712414   -1.8863212
H    -0.4834084   -2.8575705   -1.8374608
C    -0.0647208   -0.8649575   -2.7450248
H    -0.8672641   -0.7430306   -3.4563006
C     1.7976112   -0.4403666   -1.4547011
H     2.6430370    0.0615021   -1.0095155
C     0.9497040    0.0907531   -2.4601467
H     1.0447418    1.0652649   -2.9140684
C    -0.9460415   -0.9314706    1.0446836
H    -1.9585310   -0.5527318    1.1942328
C    -0.0082199   -0.5050015    2.1686380
H    -0.9805677   -2.0233338    0.9851569
H    -1.6868214    1.7915991   -1.3217069
H     0.7725969    1.1345045    3.3503559
H    -0.0036324    3.0026910    2.3272411
H    -1.5302982    3.2214606    0.5480346
H     0.9864729   -0.9474930    2.0101156
H    -0.3590651   -0.9574366    3.1108330

7
Energy = -188.8496529039
Rh    0.0000000    0.0000000   -1.7438314
C     0.0000000   -0.7053003    0.1894029
H    -0.9272726   -1.2548405    0.3412564
H     0.9272726   -1.2548405    0.3412564
C     0.0000000    0.7053003    0.1894029
H     0.9272726    1.2548405    0.3412564
H    -0.9272726    1.2548405    0.3412564

7
Energy = -188.8850284710
Rh    0.0000000    0.0000000   -1.8260061
C     0.0000000   -0.6954483    0.2105135
H    -0.9239899   -1.2518423    0.3512448
H     0.9239899   -1.2518423    0.3512448
C     0.0000000    0.6954483    0.2105135
H     0.9239899    1.2518423    0.3512448
H    -0.9239899    1.2518423    0.3512448

11
Energy = -304.0985119178
Rh    0.0239722    1.6651235    0.0000000
C    -1.2592766   -0.1728093    0.0000000
C    -0.3877980   -0.0671305    1.1255856
C    -0.3877980   -0.0671305   -1.1255856
H    -2.3353247   -0.2371539    0.0000000
C     1.0106491   -0.2257535    0.6950841
H    -0.7028127   -0.0318045    2.1607735
C     1.0106491   -0.2257535   -0.6950841
H    -0.7028127   -0.0318045   -2.1607735
H     1.8652761   -0.3028916    1.3503869
H     1.8652761   -0.3028916   -1.3503869

11
Energy = -304.1235899207
Rh    0.0599173    1.7093222    0.0000000
C    -1.2223850   -0.1094909    0.0000000
C    -0.3814230   -0.1390041    1.1581631
C    -0.3814230   -0.1390041   -1.1581631
H    -2.3025564   -0.1091459    0.0000000
C     0.9792518   -0.1867576    0.7157840
H    -0.7160717   -0.1647764    2.1848553
C     0.9792518   -0.1867576   -0.7157840
H    -0.7160717   -0.1647764   -2.1848553
H     1.8507550   -0.2548046    1.3503102
H     1.8507550   -0.2548046   -1.3503102

17
Energy = -382.8238792456
Rh   -0.2620979    0.5638288    0.0000000
C    -2.1782485    0.2236740    0.7166436
H    -2.2948732   -0.7032348    1.2706721
H    -2.5630284    1.0969010    1.2440321
```

```
C    -2.1782485    0.2236740   -0.7166436
H    -2.5630284    1.0969010   -1.2440321
H    -2.2948732   -0.7032348   -1.2706721
C     1.2800463   -0.5084249    1.1797190
C     0.7929048   -1.2051816    0.0000000
C     1.8903207    0.6661088    0.7260985
H     1.1500975   -0.8205378    2.2042477
C     1.2800463   -0.5084249   -1.1797190
H     0.2958956   -2.1656189    0.0000000
C     1.8903207    0.6661088   -0.7260985
H     2.3023343    1.4489995    1.3462885
H     1.1500975   -0.8205378   -2.2042477
H     2.3023343    1.4489995   -1.3462885

17
Energy = -382.8112901487
Rh   -0.4103616    0.5130633    0.0000000
C    -2.5553320    0.3631670    0.0000000
H    -2.9254138    0.8062227    0.9201690
H    -2.9254138    0.8062227   -0.9201690
C    -2.0178234   -0.9259431    0.0000000
H    -1.9703498   -1.5027287   -0.9177091
H    -1.9703498   -1.5027287    0.9177091
C     1.4160568   -0.2264093    1.1566405
C     1.2719011   -1.0451940    0.0000000
C     1.6295730    1.1123247    0.7141944
H     1.3725865   -0.5586115    2.1826172
C     1.4160568   -0.2264093   -1.1566405
H     1.0839046   -2.1085396    0.0000000
C     1.6295730    1.1123247   -0.7141944
H     1.7914030    1.9709253    1.3491215
H     1.3725865   -0.5586115   -2.1826172
H     1.7914030    1.9709253   -1.3491215
```

9.2.3 PBE0-D3

```
7
Energy = -1460.755166962
Co    0.0000000    0.0000000   -1.6946623
C     0.0000000   -0.6904577    0.1932276
H    -0.9252742   -1.2490048    0.3270518
H     0.9252742   -1.2490048    0.3270518
C     0.0000000    0.6904577    0.1932276
H     0.9252742    1.2490048    0.3270518
H    -0.9252742    1.2490048    0.3270518

7
Energy = -1460.843516066
Co    0.0000000    0.0000000   -1.7428708
C     0.0000000   -0.6876188    0.2055798
H    -0.9252179   -1.2471581    0.3329278
H     0.9252179   -1.2471581    0.3329278
C     0.0000000    0.6876188    0.2055798
H     0.9252179    1.2471581    0.3329278
H    -0.9252179    1.2471581    0.3329278

11
Energy = -1575.863645571
Co    0.0457897    1.4993064    0.0000000
C    -1.2423355   -0.1344084    0.0000000
C    -0.3827539   -0.0966993    1.1320033
C    -0.3827539   -0.0966993   -1.1320033
H    -2.3202504   -0.1728540    0.0000000
C     0.9917088   -0.1941599    0.7023224
H    -0.7027760   -0.0527833    2.1646544
C     0.9917088   -0.1941599   -0.7023224
H    -0.7027760   -0.0527833   -2.1646544
H     1.8522192   -0.2523795    1.3519697
H     1.8522192   -0.2523795   -1.3519697

11
Energy = -1575.927120868
Co    0.0550852    1.5715358    0.0000000
C    -1.2160315   -0.0988687    0.0000000
```

```
C    -0.3795318   -0.1286085    1.1531970
C    -0.3795318   -0.1286085   -1.1531970
H    -2.2960674   -0.0906972    0.0000000
C     0.9751155   -0.1758610    0.7123366
H    -0.7142310   -0.1493037    2.1797814
C     0.9751155   -0.1758610   -0.7123366
H    -0.7142310   -0.1493037   -2.1797814
H     1.8471542   -0.2372117    1.3465809
H     1.8471542   -0.2372117   -1.3465809

17
Energy = -1654.474398693
Co   -0.2075772    0.4832079    0.0000000
C    -2.0048858    0.2245319    0.7082751
H    -2.1345616   -0.6948367    1.2711670
H    -2.3326209    1.1174321    1.2416447
C    -2.0048858    0.2245319   -0.7082751
H    -2.3326209    1.1174321   -1.2416447
H    -2.1345616   -0.6948367   -1.2711670
C     1.1826432   -0.5204002    1.1640343
C     0.7686965   -1.2435477    0.0000000
C     1.7461638    0.6834230    0.7177387
H     1.0321037   -0.8218412    2.1888134
C     1.1826432   -0.5204002   -1.1640343
H     0.2599253   -2.1967725    0.0000000
C     1.7461638    0.6834230   -0.7177387
H     2.1006353    1.4902473    1.3426332
H     1.0321037   -0.8218412   -2.1888134
H     2.1006353    1.4902473   -1.3426332

17
Energy = -1654.510924285
Co   -0.3979861    0.4742303    0.0000000
C    -2.1845786   -0.1088652    0.6994099
H    -2.1158259   -1.0341615    1.2618262
H    -2.6250319    0.7263126    1.2412329
C    -2.1845786   -0.1088652   -0.6994099
H    -2.6250319    0.7263126   -1.2412329
H    -2.1158259   -1.0341615   -1.2618262
C     1.2753468   -0.9271379    0.7056083
C     1.2753468   -0.9271379   -0.7056083
C     1.4719454    0.4038376    1.1467936
H     1.1252877   -1.7870411    1.3410938
C     1.4719454    0.4038376   -1.1467936
H     1.1252877   -1.7870411   -1.3410938
C     1.6077858    1.2337535    0.0000000
H     1.5367603    0.7270068    2.1753033
H     1.5367603    0.7270068   -2.1753033
H     1.8223929    2.2921139    0.0000000

19
Energy = -1730.556572066
C     0.6629461    2.4371805   -0.7376030
C     0.6629461    2.4371805    0.7376030
C     0.3204970    1.2692052   -1.2882960
C     0.3204970    1.2692052    1.2882960
Co   -0.3772402    0.0350461    0.0000000
C    -0.0412737   -1.6522499    1.1546154
H     0.2921082   -1.5946960    2.1789551
C    -1.3690366   -1.7027101    0.7160781
H    -2.2454426   -1.7017143    1.3471073
C    -1.3690366   -1.7027101   -0.7160781
H    -2.2454426   -1.7017143   -1.3471073
C     0.7983047   -1.5622403    0.0000000
H     1.8732711   -1.4734538    0.0000000
C    -0.0412737   -1.6522499   -1.1546154
H     0.2921082   -1.5946960   -2.1789551
H     0.2975121    1.1194489   -2.3668149
H     0.9355218    3.3258597   -1.3060711
H     0.9355218    3.3258597    1.3060711
H     0.2975121    1.1194489    2.3668149

19
Energy = -1730.585337799
C     0.4319101    2.5957343   -0.7272950
C     0.4319101    2.5957343    0.7272950
```

```
C     0.3417383    1.3764845   -1.2880771
C     0.3417383    1.3764845    1.2880771
Co    0.2949759   -0.0507452    0.0000000
C     0.0136765   -1.8595483    1.1421106
H     0.3307512   -1.9483967    2.1702239
C    -1.2746087   -1.4466237    0.7016952
H    -2.0884777   -1.1327311    1.3370138
C    -1.2746087   -1.4466237   -0.7016952
H    -2.0884777   -1.1327311   -1.3370138
C     0.7980859   -2.1475364    0.0000000
H     1.8231663   -2.4860579    0.0000000
C     0.0136765   -1.8595483   -1.1421106
H     0.3307512   -1.9483967   -2.1702239
H     0.2991644    1.2350489   -2.3666260
H     0.4877317    3.5222018   -1.2983610
H     0.4877317    3.5222018    1.2983610
H     0.2991644    1.2350489    2.3666260

25
Energy = -1809.144906958
C    -1.9023049    1.4207434    0.0432308
C    -0.8605770    1.3407510    1.0944021
C    -1.5015003    0.5879710   -0.9077392
C    -0.5875297    0.1650103    1.7524463
Co    0.1712583    0.0024391   -0.2170847
C     2.2666067    0.2628590    0.0920868
H     2.7341054    0.3794516    1.0583883
C     2.0194784   -0.9553587   -0.5589405
H     2.2543485   -1.9371558   -0.1782148
C     1.3246975   -0.6738101   -1.7697609
H     0.9762724   -1.3989401   -2.4886567
C     1.7698605    1.3202298   -0.7279615
H     1.8058475    2.3742256   -0.4997725
C     1.2074345    0.7401120   -1.8795334
H     0.7178920    1.2720047   -2.6806513
C    -0.7937573   -1.6389869    0.2935247
H    -1.5201972   -1.9763111   -0.4468944
C    -1.4005283   -1.0925942    1.5703730
H    -0.0620806   -2.4273518    0.4787252
H    -1.9974386    0.3654325   -1.8492377
H     0.2050624    0.1650853    2.4951100
H    -0.2890470    2.2281960    1.3614787
H    -2.7729617    2.0725743    0.0906630
H    -1.3103841   -1.7565675    2.4340058
H    -2.4545576   -0.8400096    1.4400128

25
Energy = -1809.153777420
C    -1.0247329    2.2502667    0.6046828
C    -0.2353130    2.0692407    1.8190467
C    -1.1244894    1.4324335   -0.4484332
C     0.1965628    0.9657943    2.4437407
Co   -0.2570536   -0.2564300   -0.6423482
C     1.2905075   -1.7142358   -1.1002094
H     1.6921947   -2.3748116   -0.3463939
C     0.1477458   -1.9734611   -1.9140676
H    -0.4625231   -2.8633654   -1.8822819
C    -0.0449307   -0.8612299   -2.7549951
H    -0.8409327   -0.7339386   -3.4729356
C     1.8028739   -0.4497919   -1.4541026
H     2.6456109    0.0472341   -0.9980762
C     0.9623154    0.0912348   -2.4526092
H     1.0602965    1.0700444   -2.8970921
C    -0.9556548   -0.9100174    1.0590590
H    -1.9675713   -0.5329296    1.2077869
C    -0.0231736   -0.4898136    2.1771083
H    -0.9912963   -2.0009716    0.9907984
H    -1.7526650    1.7547907   -1.2801883
H     0.8040030    1.1410435    3.3299183
H     0.0414960    3.0066492    2.2979242
H    -1.5427476    3.2104435    0.5594489
H     0.9649497   -0.9506902    2.0328888
H    -0.3854722   -0.9274888    3.1213302

7
Energy = -188.7642740338
```

```
Rh     0.0000000     0.0000000    -1.7394073
C      0.0000000    -0.6999095     0.1898535
H     -0.9274395    -1.2502806     0.3399250
H      0.9274395    -1.2502806     0.3399250
C      0.0000000     0.6999095     0.1898535
H      0.9274395     1.2502806     0.3399250
H     -0.9274395     1.2502806     0.3399250

7
Energy = -188.7994883048
Rh     0.0000000     0.0000000    -1.8288407
C      0.0000000    -0.6904780     0.2137631
H     -0.9243751    -1.2478594     0.3503286
H      0.9243751    -1.2478594     0.3503286
C      0.0000000     0.6904780     0.2137631
H      0.9243751     1.2478594     0.3503286
H     -0.9243751     1.2478594     0.3503286

11
Energy = -303.8674848192
Rh     0.0240636     1.6670992     0.0000000
C     -1.2520370    -0.1750037     0.0000000
C     -0.3856911    -0.0689065     1.1213895
C     -0.3856911    -0.0689065    -1.1213895
H     -2.3286552    -0.2287394     0.0000000
C      1.0048921    -0.2273227     0.6927291
H     -0.7016710    -0.0351511     2.1561762
C      1.0048921    -0.2273227    -0.6927291
H     -0.7016710    -0.0351511    -2.1561762
H      1.8607843    -0.3002977     1.3467910
H      1.8607843    -0.3002977    -1.3467910

11
Energy = -303.8948869828
Rh     0.0602128     1.7169722     0.0000000
C     -1.2169445    -0.1118160     0.0000000
C     -0.3797959    -0.1411918     1.1529169
C     -0.3797959    -0.1411918    -1.1529169
H     -2.2970389    -0.1087563     0.0000000
C      0.9747220    -0.1887251     0.7125424
H     -0.7143814    -0.1642342     2.1796239
C      0.9747220    -0.1887251    -0.7125424
H     -0.7143814    -0.1642342    -2.1796239
H      1.8463406    -0.2540488     1.3470788
H      1.8463406    -0.2540488    -1.3470788

17
Energy = -382.4793875566
Rh    -0.2663999     0.5672868     0.0000000
C     -2.1701461     0.2219846     0.7124684
H     -2.2824620    -0.7042554     1.2680970
H     -2.5530412     1.0951974     1.2408004
C     -2.1701461     0.2219846    -0.7124684
H     -2.5530412     1.0951974    -1.2408004
H     -2.2824620    -0.7042554    -1.2680970
C      1.2758995    -0.5078830     1.1742693
C      0.7886967    -1.1992396     0.0000000
C      1.8836936     0.6633576     0.7228957
H      1.1440248    -0.8186264     2.1989946
C      1.2758995    -0.5078830    -1.1742693
H      0.2906938    -2.1591322     0.0000000
C      1.8836936     0.6633576    -0.7228957
H      2.2955360     1.4457677     1.3438140
H      1.1440248    -0.8186264    -2.1989946
H      2.2955360     1.4457677    -1.3438140

17
Energy = -382.4690953449
Rh    -0.4174963     0.5087572     0.0000000
C     -2.5498913     0.3625170     0.0000000
H     -2.9158158     0.8088076     0.9204316
H     -2.9158158     0.8088076    -0.9204316
C     -2.0210265    -0.9227309     0.0000000
H     -1.9740690    -1.4994109    -0.9178038
H     -1.9740690    -1.4994109     0.9178038
C      1.4168119    -0.2260797     1.1515771
```

```
C     1.2772191   -1.0429738    0.0000000
C     1.6250079    1.1080646    0.7112700
H     1.3731063   -0.5578722    2.1777416
C     1.4168119   -0.2260797   -1.1515771
H     1.0963396   -2.1076042    0.0000000
C     1.6250079    1.1080646   -0.7112700
H     1.7823864    1.9675079    1.3462031
H     1.3731063   -0.5578722   -2.1777416
H     1.7823864    1.9675079   -1.3462031
```

9.2.4 B3LYP-D3

```
7
Energy = -1460.976790592
Co    0.0000000    0.0000000   -1.7327062
C     0.0000000   -0.6898240    0.2038393
H    -0.9246765   -1.2485493    0.3312569
H     0.9246765   -1.2485493    0.3312569
C     0.0000000    0.6898240    0.2038393
H     0.9246765    1.2485493    0.3312569
H    -0.9246765    1.2485493    0.3312569

7
Energy = -1461.059519036
Co    0.0000000    0.0000000   -1.7794448
C     0.0000000   -0.6879814    0.2129658
H    -0.9237717   -1.2477683    0.3383783
H     0.9237717   -1.2477683    0.3383783
C     0.0000000    0.6879814    0.2129658
H     0.9237717    1.2477683    0.3383783
H    -0.9237717    1.2477683    0.3383783

11
Energy = -1576.138482607
Co    0.0410037    1.5342167    0.0000000
C    -1.2434639   -0.1387620    0.0000000
C    -0.3837928   -0.0981071    1.1349313
C    -0.3837928   -0.0981071   -1.1349313
H    -2.3198742   -0.1703484    0.0000000
C     0.9944605   -0.2001890    0.7024374
H    -0.7040008   -0.0595331    2.1661863
C     0.9944605   -0.2001890   -0.7024374
H    -0.7040008   -0.0595331   -2.1661863
H     1.8545002   -0.2547240    1.3503409
H     1.8545002   -0.2547240   -1.3503409

11
Energy = -1576.195715705
Co    0.0562927    1.6043345    0.0000000
C    -1.2192100   -0.1039255    0.0000000
C    -0.3800363   -0.1332267    1.1548210
C    -0.3800363   -0.1332267   -1.1548210
H    -2.2975415   -0.0954112    0.0000000
C     0.9767596   -0.1809281    0.7140339
H    -0.7138923   -0.1485290    2.1802135
C     0.9767596   -0.1809281   -0.7140339
H    -0.7138923   -0.1485290   -2.1802135
H     1.8473984   -0.2398151    1.3476880
H     1.8473984   -0.2398151   -1.3476880

17
Energy = -1654.794841778
Co   -0.2235091    0.4806164    0.0000000
C    -2.0489058    0.2340591    0.7091575
H    -2.1830150   -0.6848299    1.2705503
H    -2.3718643    1.1262892    1.2448011
C    -2.0489058    0.2340591   -0.7091575
H    -2.3718643    1.1262892   -1.2448011
H    -2.1830150   -0.6848299   -1.2705503
C     1.2132278   -0.5264463    1.1669105
C     0.7969544   -1.2520422    0.0000000
C     1.7688772    0.6817365    0.7203279
H     1.0645147   -0.8287344    2.1900961
C     1.2132278   -0.5264463   -1.1669105
```

```
H     0.3012831   -2.2107353    0.0000000
C     1.7688772    0.6817365   -0.7203279
H     2.1198013    1.4890063    1.3439825
H     1.0645147   -0.8287344   -2.1900961
H     2.1198013    1.4890063   -1.3439825

17
Energy = -1654.827864635
Co   -0.3920968    0.4824754    0.0000000
C    -2.2036525   -0.1138765    0.6992693
H    -2.1306276   -1.0379327    1.2613239
H    -2.6440087    0.7186130    1.2433995
C    -2.2036525   -0.1138765   -0.6992693
H    -2.6440087    0.7186130   -1.2433995
H    -2.1306276   -1.0379327   -1.2613239
C     1.2814083   -0.9255919    0.7075276
C     1.2814083   -0.9255919   -0.7075276
C     1.4867244    0.4059462    1.1493652
H     1.1223472   -1.7828004    1.3417009
C     1.4867244    0.4059462   -1.1493652
H     1.1223472   -1.7828004   -1.3417009
C     1.6244777    1.2374223    0.0000000
H     1.5499639    0.7290309    2.1763392
H     1.5499639    0.7290309   -2.1763392
H     1.8433090    2.2933251    0.0000000

19
Energy = -1730.926483282
C     0.6439572    2.4702505   -0.7405662
C     0.6439572    2.4702505    0.7405662
C     0.3125091    1.3014731   -1.3002692
C     0.3125091    1.3014731    1.3002692
Co   -0.3804392    0.0516521    0.0000000
C    -0.0691555   -1.6845582    1.1578933
H     0.2643577   -1.6318972    2.1808395
C    -1.3976041   -1.7265318    0.7183941
H    -2.2734139   -1.7206620    1.3474905
C    -1.3976041   -1.7265318   -0.7183941
H    -2.2734139   -1.7206620   -1.3474905
C     0.7733478   -1.5944904    0.0000000
H     1.8485949   -1.5264597    0.0000000
C    -0.0691555   -1.6845582   -1.1578933
H     0.2643577   -1.6318972   -2.1808395
H     0.2962711    1.1502332   -2.3772355
H     0.9089134    3.3640237   -1.3029683
H     0.9089134    3.3640237    1.3029683
H     0.2962711    1.1502332    2.3772355

19
Energy = -1730.951705597
C     0.4643260    2.6219337   -0.7290977
C     0.4643260    2.6219337    0.7290977
C     0.3308474    1.4069874   -1.3001023
C     0.3308474    1.4069874    1.3001023
Co    0.2338111   -0.0211428    0.0000000
C     0.0080248   -1.8771354    1.1446908
H     0.3280028   -1.9552398    2.1710668
C    -1.2947245   -1.5042009    0.7036729
H    -2.1175258   -1.2184102    1.3382094
C    -1.2947245   -1.5042009   -0.7036729
H    -2.1175258   -1.2184102   -1.3382094
C     0.8030822   -2.1371771    0.0000000
H     1.8381200   -2.4383331    0.0000000
C     0.0080248   -1.8771354   -1.1446908
H     0.3280028   -1.9552398   -2.1710668
H     0.2880669    1.2756303   -2.3785798
H     0.5554758    3.5487613   -1.2933463
H     0.5554758    3.5487613    1.2933463
H     0.2880669    1.2756303    2.3785798

25
Energy = -1809.551237772
C    -1.9353909    1.4193196    0.0154002
C    -0.9303934    1.3660484    1.1092652
C    -1.5293859    0.5794801   -0.9300935
C    -0.6384963    0.2088791    1.7847824
```

```
Co     0.1561132   -0.0150174   -0.2305034
C      2.3046879    0.2088739    0.0678268
H      2.7791604    0.2830940    1.0330269
C      2.0329901   -0.9807987   -0.6273310
H      2.2503943   -1.9787953   -0.2849327
C      1.3334082   -0.6435401   -1.8247542
H      0.9784256   -1.3348234   -2.5711329
C      1.8251400    1.3066839   -0.7169707
H      1.8782119    2.3490287   -0.4489027
C      1.2492750    0.7806973   -1.8868740
H      0.7681862    1.3490838   -2.6655486
C     -0.7762215   -1.6757749    0.3507445
H     -1.4937438   -2.0552322   -0.3759295
C     -1.4027345   -1.0901413    1.6097578
H     -0.0287840   -2.4394702    0.5668558
H     -2.0205853    0.3721106   -1.8759182
H      0.1443283    0.2409530    2.5350942
H     -0.3849064    2.2683179    1.3761618
H     -2.7977049    2.0824937    0.0315736
H     -1.2993737   -1.7237974    2.4938881
H     -2.4626006   -0.8776731    1.4645139

25
Energy = -1809.564186268
C     -1.0434343    2.2766408    0.6288743
C     -0.3253541    2.1019739    1.8924528
C     -1.0904179    1.4657948   -0.4376387
C      0.1269721    1.0089349    2.5263664
Co    -0.2396739   -0.2451128   -0.6332909
C      1.2822290   -1.7781895   -1.1710208
H      1.6726428   -2.4575402   -0.4304931
C      0.1147928   -1.9902620   -1.9674418
H     -0.5255573   -2.8565993   -1.9309408
C     -0.0539720   -0.8620074   -2.7977220
H     -0.8568297   -0.7012265   -3.4987233
C      1.8336997   -0.5262271   -1.5248627
H      2.7016081   -0.0652600   -1.0821016
C      0.9956979    0.0527824   -2.5085035
H      1.1213485    1.0285840   -2.9486041
C     -0.9119020   -0.9120111    1.0935869
H     -1.9344590   -0.5670022    1.2441765
C      0.0120543   -0.4575578    2.2159268
H     -0.9126341   -2.0027796    1.0278634
H     -1.6687032    1.8049922   -1.2975464
H      0.6691018    1.1973390    3.4499665
H     -0.1294209    3.0417186    2.4031482
H     -1.5582397    3.2360186    0.5574071
H      1.0267275   -0.8425015    2.0417529
H     -0.3062765   -0.9505021    3.1473681

7
Energy = -188.8006793621
Rh     0.0000000    0.0000000   -1.7745792
C      0.0000000   -0.7000144    0.1980737
H     -0.9254320   -1.2516911    0.3446079
H      0.9254320   -1.2516911    0.3446079
C      0.0000000    0.7000144    0.1980737
H      0.9254320    1.2516911    0.3446079
H     -0.9254320    1.2516911    0.3446079

7
Energy = -188.8334961649
Rh     0.0000000    0.0000000   -1.8725663
C      0.0000000   -0.6901106    0.2244990
H     -0.9229127   -1.2482614    0.3558921
H      0.9229127   -1.2482614    0.3558921
C      0.0000000    0.6901106    0.2244990
H      0.9229127    1.2482614    0.3558921
H     -0.9229127    1.2482614    0.3558921

11
Energy = -303.9576808772
Rh    -0.3587701    1.8099630    0.0000000
C     -1.2193990   -0.0966693    0.0000000
C     -0.3401977   -0.0125748    1.1289780
C     -0.3401977   -0.0125748   -1.1289780
```

```
H    -2.2914196   -0.2149165    0.0000000
C     1.0356043   -0.3068442    0.6789949
H    -0.6545066   -0.0381624    2.1633230
C     1.0356043   -0.3068442   -0.6789949
H    -0.6545066   -0.0381624   -2.1633230
H     1.8938944   -0.3916073    1.3278986
H     1.8938944   -0.3916073   -1.3278986

11
Energy = -303.9822457421
Rh    0.0620696    1.7755941    0.0000000
C    -1.2186520   -0.1166039    0.0000000
C    -0.3804136   -0.1459995    1.1543507
C    -0.3804136   -0.1459995   -1.1543507
H    -2.2974848   -0.1156012    0.0000000
C     0.9758138   -0.1936994    0.7134266
H    -0.7145754   -0.1710529    2.1798188
C     0.9758138   -0.1936994   -0.7134266
H    -0.7145754   -0.1710529   -2.1798188
H     1.8462089   -0.2609428    1.3472909
H     1.8462089   -0.2609428   -1.3472909

17
Energy = -382.6099166774
Rh   -0.2946125    0.5848710    0.0000000
C    -2.2239120    0.2243180    0.7124707
H    -2.3253149   -0.7021391    1.2679927
H    -2.6084160    1.0937220    1.2435175
C    -2.2239120    0.2243180   -0.7124707
H    -2.6084160    1.0937220   -1.2435175
H    -2.3253149   -0.7021391   -1.2679927
C     1.3060447   -0.5079120    1.1761734
C     0.8067343   -1.1952986    0.0000000
C     1.9210388    0.6593652    0.7255287
H     1.1740598   -0.8193127    2.1993762
C     1.3060447   -0.5079120   -1.1761734
H     0.3172340   -2.1582061    0.0000000
C     1.9210388    0.6593652   -0.7255287
H     2.3418216    1.4362754    1.3451268
H     1.1740598   -0.8193127   -2.1993762
H     2.3418216    1.4362754   -1.3451268

17
Energy = -382.6013724368
Rh   -0.4464471    0.5261772    0.0000000
C    -2.6106785    0.3584264    0.0000000
H    -2.9752417    0.8063143    0.9189046
H    -2.9752417    0.8063143   -0.9189046
C    -2.0818616   -0.9259088    0.0000000
H    -2.0270329   -1.5016184   -0.9165088
H    -2.0270329   -1.5016184    0.9165088
C     1.4542555   -0.2267580    1.1525306
C     1.3222614   -1.0467534    0.0000000
C     1.6531763    1.1114017    0.7125210
H     1.4147086   -0.5588214    2.1775538
C     1.4542555   -0.2267580   -1.1525306
H     1.1508541   -2.1116858    0.0000000
C     1.6531763    1.1114017   -0.7125210
H     1.8130701    1.9693540    1.3468019
H     1.4147086   -0.5588214   -2.1775538
H     1.8130701    1.9693540   -1.3468019
```

9.2.5 CAM-B3LYP

```
7
Energy = -1461.119969158
Co    0.0000000    0.0000000   -1.7187963
C     0.0000000   -0.6834587    0.2111080
H    -0.9246067   -1.2414511    0.3241451
H     0.9246067   -1.2414511    0.3241451
C     0.0000000    0.6834587    0.2111080
H     0.9246067    1.2414511    0.3241451
H    -0.9246067    1.2414511    0.3241451
```

```
7
Energy = -1461.202146324
Co     0.0000000     0.0000000    -1.7589085
C      0.0000000    -0.6826701     0.2162087
H     -0.9233512    -1.2419496     0.3316228
H      0.9233512    -1.2419496     0.3316228
C      0.0000000     0.6826701     0.2162087
H      0.9233512     1.2419496     0.3316228
H     -0.9233512     1.2419496     0.3316228

11
Energy = -1576.291146479
Co     0.0432588     1.5292177     0.0000000
C     -1.2362786    -0.1345486     0.0000000
C     -0.3817109    -0.0961537     1.1307871
C     -0.3817109    -0.0961537    -1.1307871
H     -2.3123659    -0.1688126     0.0000000
C      0.9886388    -0.1944213     0.7001570
H     -0.7024961    -0.0664144     2.1610665
C      0.9886388    -0.1944213    -0.7001570
H     -0.7024961    -0.0664144    -2.1610665
H      1.8482610    -0.2559387     1.3472709
H      1.8482610    -0.2559387    -1.3472709

11
Energy = -1576.351358982
Co     0.0560498     1.6010022     0.0000000
C     -1.2134773    -0.0995653     0.0000000
C     -0.3782289    -0.1287399     1.1496582
C     -0.3782289    -0.1287399    -1.1496582
H     -2.2915287    -0.0990599     0.0000000
C      0.9725265    -0.1762335     0.7107406
H     -0.7120417    -0.1527974     2.1744921
C      0.9725265    -0.1762335    -0.7107406
H     -0.7120417    -0.1527974    -2.1744921
H      1.8422223    -0.2434177     1.3442753
H      1.8422223    -0.2434177    -1.3442753

17
Energy = -1654.944196276
Co    -0.2270067     0.4690543     0.0000000
C     -2.0375615     0.2357223     0.7048235
H     -2.1766561    -0.6785563     1.2680469
H     -2.3451662     1.1328897     1.2366607
C     -2.0375615     0.2357223    -0.7048235
H     -2.3451662     1.1328897    -1.2366607
H     -2.1766561    -0.6785563    -1.2680469
C      1.2053667    -0.5274208     1.1609226
C      0.7989321    -1.2532597     0.0000000
C      1.7463820     0.6826341     0.7169072
H      1.0659428    -0.8335592     2.1838112
C      1.2053667    -0.5274208    -1.1609226
H      0.3168488    -2.2176699     0.0000000
C      1.7463820     0.6826341    -0.7169072
H      2.0973051     1.4892278     1.3406491
H      1.0659428    -0.8335592    -2.1838112
H      2.0973051     1.4892278    -1.3406491

17
Energy = -1654.979554775
Co    -0.3966860     0.4415566     0.0000000
C     -2.2026488    -0.1070328     0.6951763
H     -2.1539936    -1.0296909     1.2582194
H     -2.6095853     0.7410228     1.2372072
C     -2.2026488    -0.1070328    -0.6951763
H     -2.6095853     0.7410228    -1.2372072
H     -2.1539936    -1.0296909    -1.2582194
C      1.2894340    -0.9263830     0.7047289
C      1.2894340    -0.9263830    -0.7047289
C      1.4726612     0.4029481     1.1447232
H      1.1620965    -1.7888489     1.3388582
C      1.4726612     0.4029481    -1.1447232
H      1.1620965    -1.7888489    -1.3388582
C      1.5963019     1.2325665     0.0000000
H      1.5413643     0.7255297     2.1712636
H      1.5413643     0.7255297    -2.1712636
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H     1.8017275    2.2907869    0.0000000

19
Energy = -1731.073050974
C     0.6667929    2.4558243   -0.7391057
C     0.6667929    2.4558243    0.7391057
C     0.3174766    1.2948717   -1.2879643
C     0.3174766    1.2948717    1.2879643
Co   -0.3679399    0.0457719    0.0000000
C    -0.0449630   -1.6700157    1.1528522
H     0.2884812   -1.6228826    2.1755640
C    -1.3681686   -1.7133965    0.7156939
H    -2.2437311   -1.7179224    1.3446969
C    -1.3681686   -1.7133965   -0.7156939
H    -2.2437311   -1.7179224   -1.3446969
C     0.7926270   -1.5768828    0.0000000
H     1.8666408   -1.5044788    0.0000000
C    -0.0449630   -1.6700157   -1.1528522
H     0.2884812   -1.6228826   -2.1755640
H     0.2924901    1.1512380   -2.3645729
H     0.9459579    3.3400779   -1.3063465
H     0.9459579    3.3400779    1.3063465
H     0.2924901    1.1512380    2.3645729

19
Energy = -1731.099417393
C     0.4804644    2.6134370   -0.7301662
C     0.4804644    2.6134370    0.7301662
C     0.3241177    1.4092448   -1.2937391
C     0.3241177    1.4092448    1.2937391
Co    0.1861076   -0.0143391    0.0000000
C     0.0069896   -1.8583071    1.1398727
H     0.3260796   -1.9380939    2.1660902
C    -1.3004075   -1.5209701    0.7003169
H    -2.1333918   -1.2672104    1.3349973
C    -1.3004075   -1.5209701   -0.7003169
H    -2.1333918   -1.2672104   -1.3349973
C     0.8040822   -2.1012079    0.0000000
H     1.8439356   -2.3839369    0.0000000
C     0.0069896   -1.8583071   -1.1398727
H     0.3260796   -1.9380939   -2.1660902
H     0.2878726    1.2767256   -2.3705320
H     0.5912127    3.5349160   -1.2966677
H     0.5912127    3.5349160    1.2966677
H     0.2878726    1.2767256    2.3705320

25
Energy = -1809.696485360
C    -1.9327504    1.4040217    0.0183264
C    -0.9410326    1.3650355    1.1200017
C    -1.5095364    0.5754097   -0.9211790
C    -0.6492917    0.2195191    1.7916583
Co    0.1659996   -0.0119234   -0.2301354
C     2.3005578    0.2011705    0.0633017
H     2.7900352    0.2766777    1.0207402
C     2.0231501   -0.9835111   -0.6249391
H     2.2451167   -1.9808790   -0.2846456
C     1.3201615   -0.6475675   -1.8142683
H     0.9645374   -1.3385962   -2.5597746
C     1.8226448    1.2953290   -0.7191368
H     1.8925164    2.3387475   -0.4596662
C     1.2448977    0.7710484   -1.8813351
H     0.7711226    1.3397151   -2.6638545
C    -0.7670403   -1.6451725    0.3363911
H    -1.4884949   -2.0196075   -0.3864716
C    -1.3937874   -1.0819713    1.6001978
H    -0.0315689   -2.4194610    0.5477919
H    -2.0024645    0.3712068   -1.8658214
H     0.1233280    0.2570045    2.5509976
H    -0.4084901    2.2721313    1.3923133
H    -2.8058571    2.0499845    0.0281984
H    -1.2770319   -1.7247795    2.4738845
H    -2.4567214   -0.8835324    1.4674249

25
Energy = -1809.710078142
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C    -1.0142846    2.2627273    0.6261223
C    -0.2781462    2.0848697    1.8799999
C    -1.0701183    1.4528177   -0.4286488
C     0.1369823    0.9891474    2.5157607
Co   -0.2190219   -0.2482541   -0.6382486
C     1.3046626   -1.7341556   -1.1572677
H     1.7292674   -2.3999029   -0.4235718
C     0.1352706   -1.9822363   -1.9305786
H    -0.4791666   -2.8662258   -1.8808710
C    -0.0701288   -0.8744250   -2.7698959
H    -0.8809980   -0.7461453   -3.4681896
C     1.8196811   -0.4805361   -1.5353854
H     2.6904076    0.0011796   -1.1215128
C     0.9562550    0.0647216   -2.5079117
H     1.0593668    1.0326777   -2.9702925
C    -0.9151292   -0.9013973    1.0630874
H    -1.9392268   -0.5554119    1.1825853
C    -0.0365286   -0.4705064    2.2235661
H    -0.9236720   -1.9899601    0.9940444
H    -1.6606960    1.7863775   -1.2796064
H     0.6930152    1.1653846    3.4322308
H    -0.0392864    3.0227889    2.3725248
H    -1.5331789    3.2183295    0.5626570
H     0.9646395   -0.9056134    2.1170469
H    -0.4299659   -0.9262513    3.1423553

7
Energy = -188.7786745617
Rh    0.0000000    0.0000000   -1.7661652
C     0.0000000   -0.6939067    0.1993614
H    -0.9244058   -1.2450004    0.3418606
H     0.9244058   -1.2450004    0.3418606
C     0.0000000    0.6939067    0.1993614
H     0.9244058    1.2450004    0.3418606
H    -0.9244058    1.2450004    0.3418606

7
Energy = -188.8126619809
Rh    0.0000000    0.0000000   -1.8650332
C     0.0000000   -0.6845413    0.2278258
H    -0.9223471   -1.2421580    0.3523454
H     0.9223471   -1.2421580    0.3523454
C     0.0000000    0.6845413    0.2278258
H     0.9223471    1.2421580    0.3523454
H    -0.9223471    1.2421580    0.3523454

11
Energy = -303.9434466112
Rh   -0.0086090    1.7065497    0.0000000
C    -1.2416190   -0.1698880    0.0000000
C    -0.3814613   -0.0717526    1.1212741
C    -0.3814613   -0.0717526   -1.1212741
H    -2.3163882   -0.2145379    0.0000000
C     1.0031203   -0.2354254    0.6889060
H    -0.6976166   -0.0531004    2.1533215
C     1.0031203   -0.2354254   -0.6889060
H    -0.6976166   -0.0531004   -2.1533215
H     1.8592658   -0.3007835    1.3396303
H     1.8592658   -0.3007835   -1.3396303

11
Energy = -303.9706943815
Rh    0.0615617    1.7562319    0.0000000
C    -1.2132066   -0.1156768    0.0000000
C    -0.3787263   -0.1449552    1.1492435
C    -0.3787263   -0.1449552   -1.1492435
H    -2.2909019   -0.1130987    0.0000000
C     0.9714682   -0.1923485    0.7102692
H    -0.7125832   -0.1684247    2.1736522
C     0.9714682   -0.1923485   -0.7102692
H    -0.7125832   -0.1684247   -2.1736522
H     1.8411147   -0.2579998    1.3433933
H     1.8411147   -0.2579998   -1.3433933

17
Energy = -382.5967904848
```

```
Rh   -0.2823646    0.5670651    0.0000000
C    -2.2027238    0.2288079    0.7088069
H    -2.3172975   -0.6936629    1.2645823
H    -2.5756771    1.1033948    1.2358818
C    -2.2027238    0.2288079   -0.7088069
H    -2.5756771    1.1033948   -1.2358818
H    -2.3172975   -0.6936629   -1.2645823
C     1.3002763   -0.5137934    1.1704281
C     0.8144911   -1.2043075    0.0000000
C     1.8922143    0.6606442    0.7222731
H     1.1705775   -0.8251493    2.1927254
C     1.3002763   -0.5137934   -1.1704281
H     0.3318506   -2.1689453    0.0000000
C     1.8922143    0.6606442   -0.7222731
H     2.3006418    1.4428525    1.3416397
H     1.1705775   -0.8251493   -2.1927254
H     2.3006418    1.4428525   -1.3416397

17
Energy = -382.5912734353
Rh   -0.4444953    0.5052412    0.0000000
C    -2.6081747    0.3656049    0.0000000
H    -2.9606900    0.8220176    0.9189784
H    -2.9606900    0.8220176   -0.9189784
C    -2.1042747   -0.9276968    0.0000000
H    -2.0586113   -1.5030208   -0.9166239
H    -2.0586113   -1.5030208    0.9166239
C     1.4658366   -0.2290381    1.1523863
C     1.3456870   -1.0507762    0.0000000
C     1.6448259    1.1117750    0.7124943
H     1.4300328   -0.5611655    2.1773991
C     1.4658366   -0.2290381   -1.1523863
H     1.1915313   -2.1182593    0.0000000
C     1.6448259    1.1117750   -0.7124943
H     1.7884692    1.9723749    1.3467023
H     1.4300328   -0.5611655   -2.1773991
H     1.7884692    1.9723749   -1.3467023
```

9.2.6 M06-L

```
11
E(RM06L) =  -1576.26826075
Co   -0.893770   -0.038639    0.000000
C     0.765156   -1.217632    0.000000
C     0.668048   -0.352309    1.129289
C     0.668048   -0.352309   -1.129289
H     0.924649   -2.283658    0.000000
C     0.668048    1.034636    0.701686
H     0.618335   -0.671780    2.161602
C     0.668048    1.034636   -0.701686
H     0.618335   -0.671780   -2.161602
H     0.673194    1.894167    1.354063
H     0.673194    1.894167   -1.354063

11
E(UM06L) =  -1576.31743238
Co   -0.927344   -0.000214    0.000000
C     0.710623   -1.215981    0.000000
C     0.710591   -0.375665    1.156600
C     0.710591   -0.375665   -1.156600
H     0.744256   -2.294522    0.000000
C     0.710591    0.984069    0.714813
H     0.744166   -0.708933    2.182370
C     0.710591    0.984069   -0.714813
H     0.744166   -0.708933   -2.182370
H     0.743889    1.856600    1.348829
H     0.743889    1.856600   -1.348829

17
E(RM06L) =  -1654.97200498
Co    0.380479    0.241550   -0.000000
C     0.345573    2.054554    0.711216
H    -0.547456    2.311303    1.270305
H     1.266620    2.277738    1.246222
```

```
C     0.345573    2.054554   -0.711216
H     1.266620    2.277738   -1.246222
H    -0.547456    2.311303   -1.270305
C    -0.767870   -0.968351    1.169554
C    -1.430839   -0.458295    0.000000
C     0.345573   -1.691147    0.719974
H    -1.051177   -0.786369    2.193408
C    -0.767870   -0.968351   -1.169554
H    -2.298960    0.184418    0.000000
C     0.345573   -1.691147   -0.719974
H     1.097877   -2.151256    1.342491
H    -1.051177   -0.786369   -2.193408
H     1.097877   -2.151256   -1.342491

17
E(UM06L) =  -1654.99410507
Co    0.384679   -0.003723   -0.345277
C     2.190681   -0.697578    0.144350
H     2.197729   -1.259075    1.070628
H     2.570774   -1.241144   -0.716478
C     2.187300    0.702014    0.139059
H     2.564338    1.241055   -0.725950
H     2.191356    1.270575    1.061030
C    -1.094652   -0.692349    1.155511
C    -1.095922    0.719172    1.138453
C    -1.398973   -1.149596   -0.148208
H    -0.870207   -1.316590    2.006169
C    -1.401103    1.144320   -0.175942
H    -0.872357    1.364112    1.973760
C    -1.601902   -0.012649   -0.982430
H    -1.484692   -2.181669   -0.451188
H    -1.488114    2.168653   -0.503800
H    -1.907738   -0.025395   -2.016451

19
E(RM06L) =  -1731.13771235
C    -2.190428    0.746719   -0.315726
C    -2.435177   -0.696598   -0.182520
C    -1.272038    1.382176    0.469153
C    -1.381143   -1.308048    0.356275
Co   -0.088423    0.069051    0.069439
C     1.443405   -1.250874   -0.390744
H     1.288205   -2.286040   -0.647112
C     1.485520   -0.172692   -1.290950
H     1.365370   -0.243191   -2.360968
C     1.657903    1.034765   -0.550371
H     1.713593    2.029292   -0.962203
C     1.538820   -0.719083    0.931120
H     1.506713   -1.282836    1.848925
C     1.701659    0.694094    0.817632
H     1.777459    1.383113    1.643448
H    -1.143599    2.457977    0.546855
H    -2.754058    1.309015   -1.064752
H    -3.381719   -1.127237   -0.507365
H    -1.275672   -2.367228    0.565101

19
E(UM06L) =  -1731.15033824
C     0.063187    2.657111    0.716600
C     0.063187    2.657111   -0.716600
C    -0.016010    1.416352    1.267748
C    -0.016010    1.416352   -1.267748
Co   -0.252377    0.018676    0.000000
C    -0.198991   -1.760640   -1.145236
H    -0.521846   -1.816736   -2.172730
C     1.125396   -1.492633   -0.703167
H     1.970661   -1.276265   -1.336444
C     1.125396   -1.492633    0.703167
H     1.970661   -1.276265    1.336444
C    -1.013046   -1.948529    0.000000
H    -2.068168   -2.172228    0.000000
C    -0.198991   -1.760640    1.145236
H    -0.521846   -1.816736    2.172730
H     0.048557    1.273416    2.346399
H     0.141447    3.578022    1.292171
H     0.141447    3.578022   -1.292171
```

```
H     0.048557    1.273416   -2.346399

25
E(RM06L) =  -1809.80512699
C     1.747502   -1.663574   -0.258042
C     1.392765   -0.963014    0.993012
C     0.948304   -1.139106   -1.176374
C     1.541069    0.409497    1.122629
Co   -0.111344    0.035352   -0.084471
C    -1.711633    0.397924    1.246391
H    -1.602735    0.739665    2.264114
C    -1.818643    1.217333    0.109633
H    -1.798416    2.295219    0.100241
C    -1.877879    0.373176   -1.038192
H    -1.955322    0.694745   -2.064282
C    -1.751368   -0.964971    0.823828
H    -1.686301   -1.831170    1.462736
C    -1.867415   -0.975497   -0.577525
H    -1.885635   -1.853754   -1.202922
C     1.018890    1.501971   -0.841100
H     1.219531    1.383321   -1.904396
C     2.195594    1.268092    0.072930
H     0.512863    2.448762   -0.658847
H     0.880884   -1.374754   -2.235280
H     1.266954    0.867414    2.067127
H     1.030518   -1.525636    1.851144
H     2.494070   -2.453363   -0.332323
H     2.637510    2.172388    0.496637
H     2.989241    0.711662   -0.426375

25
E(UM06L) =  -1809.79909961
C    -2.048858    1.654293   -0.176693
C    -2.846255    0.652453    0.509524
C    -0.755109    1.608347   -0.527152
C    -2.740355   -0.681286    0.615699
Co    0.386776    0.099338   -0.291739
C     1.807781   -1.217048    0.622799
H     1.586034   -2.255554    0.814670
C     2.347559   -0.689558   -0.588589
H     2.615705   -1.261836   -1.462401
C     2.458358    0.707386   -0.439314
H     2.815264    1.403018   -1.181658
C     1.598477   -0.146617    1.515726
H     1.174645   -0.214328    2.504887
C     1.975933    1.042213    0.852851
H     1.884982    2.040279    1.251714
C    -0.831871   -1.231625   -1.056820
H    -1.323866   -0.768550   -1.912238
C    -1.817320   -1.679934   -0.002117
H    -0.242387   -2.077131   -1.412550
H    -0.327075    2.494292   -0.995124
H    -3.487533   -1.149279    1.251032
H    -3.695384    1.077729    1.038114
H    -2.592591    2.581941   -0.364755
H    -1.286737   -2.191873    0.812754
H    -2.454054   -2.472570   -0.422967

11
E(RM06L) =  -304.153217144
Rh   -0.783656   -0.071087    0.000000
C     1.168791   -1.152374    0.000000
C     0.962456   -0.300037    1.120263
C     0.962456   -0.300037   -1.120263
H     1.355529   -2.212239    0.000000
C     0.962456    1.103436    0.693123
H     0.953353   -0.616889    2.154384
C     0.962456    1.103436   -0.693123
H     0.953353   -0.616889   -2.154384
H     0.945301    1.959189    1.348525
H     0.945301    1.959189   -1.348525

11
E(UM06L) =  -304.176677756
Rh   -0.811609    0.000208    0.000000
C     1.038460   -1.213604    0.000000
```

```
C     1.038525   -0.375253    1.153928
C     1.038525   -0.375253   -1.153928
H     1.073077   -2.291641    0.000000
C     1.038525    0.981397    0.713195
H     1.073349   -0.708405    2.179200
C     1.038525    0.981397   -0.713195
H     1.073349   -0.708405   -2.179200
H     1.073635    1.853492    1.346902
H     1.073635    1.853492   -1.346902

17
E(RM06L) =  -382.852155836
Rh    0.348917    0.246319    0.000000
C     0.234149    2.186537    0.713643
H    -0.668502    2.417912    1.268340
H     1.142383    2.465953    1.243535
C     0.234149    2.186537   -0.713643
H     1.142383    2.465953   -1.243535
H    -0.668502    2.417912   -1.268340
C    -0.867818   -1.164277    1.175850
C    -1.509315   -0.611452   -0.000000
C     0.234149   -1.889423    0.723073
H    -1.164671   -1.003411    2.198922
C    -0.867818   -1.164277   -1.175850
H    -2.411712   -0.016529    0.000000
C     0.234149   -1.889423   -0.723073
H     0.971067   -2.377031    1.342145
H    -1.164671   -1.003411   -2.198922
H     0.971067   -2.377031   -1.342145

17
E(UM06L) =  -382.838479556
Rh    0.397577   -0.200620    0.000000
C     2.496162    0.214211    0.000000
H     2.922299   -0.179137    0.916429
H     2.922299   -0.179137   -0.916429
C     1.809513    1.426387    0.000000
H     1.696974    1.997922   -0.913518
H     1.696974    1.997922    0.913518
C    -1.515598    0.247913    1.152224
C    -1.499654    1.074774    0.000000
C    -1.515598   -1.103678    0.711229
H    -1.521934    0.582590    2.176666
C    -1.515598    0.247913   -1.152224
H    -1.471749    2.152995    0.000000
C    -1.515598   -1.103678   -0.711229
H    -1.537835   -1.975450    1.345672
H    -1.521934    0.582590   -2.176666
H    -1.537835   -1.975450   -1.345672
```

9.2.7 TPSS-D3

```
11
Energy = -1576.447411357
Co    0.0460546    1.4561302    0.0000000
C    -1.2631333   -0.1330687    0.0000000
C    -0.3894560   -0.0913086    1.1360981
C    -0.3894560   -0.0913086   -1.1360981
H    -2.3419761   -0.2053606    0.0000000
C     1.0084277   -0.1922607    0.7050587
H    -0.7063918   -0.0160193    2.1719110
C     1.0084277   -0.1922607   -0.7050587
H    -0.7063918   -0.0160193   -2.1719110
H     1.8669475   -0.2592618    1.3612277
H     1.8669475   -0.2592618   -1.3612277

11
Energy = -1576.492602052
Co    0.0529005    1.5121941    0.0000000
C    -1.2278923   -0.0945501    0.0000000
C    -0.3827526   -0.1242090    1.1638849
C    -0.3827526   -0.1242090   -1.1638849
H    -2.3106745   -0.0841483    0.0000000
C     0.9846347   -0.1721946    0.7193177
```

```
H    -0.7179326   -0.1399797    2.1934061
C     0.9846347   -0.1721946   -0.7193177
H    -0.7179326   -0.1399797   -2.1934061
H     1.8588837   -0.2303646    1.3555878
H     1.8588837   -0.2303646   -1.3555878

17
Energy = -1655.188011324
Co   -0.1871770    0.4777658    0.0000000
C    -1.9905493    0.2125242    0.7167669
H    -2.1352327   -0.7102242    1.2767860
H    -2.3240879    1.1062025    1.2523237
C    -1.9905493    0.2125242   -0.7167669
H    -2.3240879    1.1062025   -1.2523237
H    -2.1352327   -0.7102242   -1.2767860
C     1.1686304   -0.5090846    1.1789977
C     0.7406626   -1.2364663    0.0000000
C     1.7561614    0.6888436    0.7257210
H     1.0224603   -0.8137704    2.2060410
C     1.1686304   -0.5090846   -1.1789977
H     0.2138651   -2.1835405    0.0000000
C     1.7561614    0.6888436   -0.7257210
H     2.1189425    1.4966294    1.3493024
H     1.0224603   -0.8137704   -2.2060410
H     2.1189425    1.4966294   -1.3493024

17
Energy = -1655.199401784
Co   -0.3873915    0.5348670    0.0000000
C    -2.1523379   -0.1213842    0.7059917
H    -2.0611543   -1.0482510    1.2680347
H    -2.6283728    0.6981264    1.2482011
C    -2.1523379   -0.1213842   -0.7059917
H    -2.6283728    0.6981264   -1.2482011
H    -2.0611543   -1.0482510   -1.2680347
C     1.2380096   -0.9248091    0.7111218
C     1.2380096   -0.9248091   -0.7111218
C     1.4666190    0.4085284    1.1556433
H     1.0535035   -1.7804803    1.3472016
C     1.4666190    0.4085284   -1.1556433
H     1.0535035   -1.7804803   -1.3472016
C     1.6175926    1.2440076    0.0000000
H     1.5353084    0.7301733    2.1869115
H     1.5353084    0.7301733   -2.1869115
H     1.8666480    2.2973185    0.0000000

19
Energy = -1731.388182171
C    -0.5132928    2.0090369    1.0800565
C     0.9540176    2.1525202    0.9315240
C    -1.2713249    1.4695380    0.0673627
C     1.4183512    1.2911249    0.0144639
Co   -0.0815251    0.1088176   -0.0729754
C     1.0724431   -1.6207538   -0.2642007
H     2.1223769   -1.6806618   -0.0141936
C    -0.0092234   -1.8888437    0.6082737
H     0.0777953   -2.1796948    1.6473290
C    -1.2385174   -1.6509694   -0.0933550
H    -2.2342630   -1.7526443    0.3156443
C     0.5245270   -1.1603318   -1.5108212
H     1.0859563   -0.8437001   -2.3789058
C    -0.9088712   -1.2071992   -1.4017074
H    -1.6070381   -0.9012691   -2.1689752
H    -2.3589485    1.4824612    0.0057626
H    -0.9871654    2.3186314    2.0187439
H     1.5045117    2.8866944    1.5238808
H     2.4501907    1.1672434   -0.3079071

19
Energy = -1731.398020299
C     0.4059026    2.5768158   -0.7200273
C     0.4059026    2.5768158    0.7200273
C     0.3228126    1.3197831   -1.2664138
C     0.3228126    1.3197831    1.2664138
Co    0.3506139   -0.0884006    0.0000000
C     0.0300779   -1.8494873    1.1534447
```

```
H     0.3440475   -1.9533238    2.1834768
C    -1.2399535   -1.3656042    0.7096224
H    -2.0414829   -1.0127033    1.3439546
C    -1.2399535   -1.3656042   -0.7096224
H    -2.0414829   -1.0127033   -1.3439546
C     0.8086230   -2.1634047    0.0000000
H     1.8208078   -2.5464522    0.0000000
C     0.0300779   -1.8494873   -1.1534447
H     0.3440475   -1.9533238   -2.1834768
H     0.2392143    1.1840121   -2.3487923
H     0.4493590    3.4996364   -1.3021369
H     0.4493590    3.4996364    1.3021369
H     0.2392143    1.1840121    2.3487923

25
Energy = -1810.091393008
C    -1.9053627    1.4255674    0.0289187
C    -0.8294523    1.3475437    1.0565240
C    -1.5169208    0.5705264   -0.9181956
C    -0.5474396    0.1522857    1.7282156
Co    0.1814744    0.0088140   -0.2093402
C     2.2612188    0.2661732    0.1126007
H     2.7303098    0.3767019    1.0815000
C     2.0038366   -0.9584178   -0.5486232
H     2.2391441   -1.9452590   -0.1741469
C     1.3107577   -0.6647962   -1.7705516
H     0.9624366   -1.3846623   -2.4986316
C     1.7731962    1.3376029   -0.7109671
H     1.8155514    2.3925002   -0.4766234
C     1.1978442    0.7634990   -1.8701526
H     0.7125579    1.3043396   -2.6711058
C    -0.8050111   -1.6681774    0.2974745
H    -1.5300292   -1.9887160   -0.4549974
C    -1.4012595   -1.0972540    1.5778145
H    -0.0651341   -2.4528323    0.4778849
H    -2.0077814    0.3113630   -1.8561207
H     0.2345834    0.1587436    2.4853124
H    -0.2679632    2.2424062    1.3305977
H    -2.7768967    2.0813522    0.0848222
H    -1.3167680   -1.7552643    2.4506094
H    -2.4528925   -0.8240396    1.4471813

25
Energy = -1810.069658587
C    -1.0156309    2.2638122    0.5855793
C    -0.2909557    2.0760732    1.8371114
C    -1.0526450    1.4497419   -0.4975057
C     0.1677375    0.9679628    2.4628475
Co   -0.2209215   -0.2409583   -0.6445688
C     1.2662039   -1.7235452   -1.0836156
H     1.6660250   -2.3859245   -0.3272111
C     0.0957821   -1.9641766   -1.8779666
H    -0.5368217   -2.8402169   -1.8255356
C    -0.0871428   -0.8470807   -2.7362558
H    -0.8959427   -0.7076071   -3.4409334
C     1.8005273   -0.4616161   -1.4581340
H     2.6626254    0.0233091   -1.0200131
C     0.9525605    0.0888790   -2.4596392
H     1.0626357    1.0649863   -2.9127240
C    -0.9180455   -0.9467738    1.0428705
H    -1.9377592   -0.5790956    1.1941094
C     0.0211823   -0.5016213    2.1649528
H    -0.9390336   -2.0415482    0.9899471
H    -1.6185296    1.8067803   -1.3643049
H     0.7245575    1.1531789    3.3829575
H    -0.0890446    3.0117915    2.3612451
H    -1.5421389    3.2221988    0.5261850
H     1.0306309   -0.9117031    1.9925389
H    -0.3058565   -0.9768468    3.1080633

11
Energy = -304.1313096923
Rh   -0.3726772    1.7734791    0.0000000
C    -1.2331373   -0.0884072    0.0000000
C    -0.3377984    0.0020680    1.1327760
C    -0.3377984    0.0020680   -1.1327760
```

```
H    -2.3055645   -0.2377693    0.0000000
C     1.0415661   -0.3099293    0.6810542
H    -0.6494764   -0.0139052    2.1725783
C     1.0415661   -0.3099293   -0.6810542
H    -0.6494764   -0.0139052   -2.1725783
H     1.9013982   -0.4018848    1.3335524
H     1.9013982   -0.4018848   -1.3335524

11
Energy = -304.1539676548
Rh    0.0595115    1.7010630    0.0000000
C    -1.2270339   -0.1079188    0.0000000
C    -0.3828128   -0.1375684    1.1626347
C    -0.3828128   -0.1375684   -1.1626347
H    -2.3096467   -0.1085905    0.0000000
C     0.9831097   -0.1855528    0.7185409
H    -0.7182219   -0.1644140    2.1916189
C     0.9831097   -0.1855528   -0.7185409
H    -0.7182219   -0.1644140   -2.1916189
H     1.8565096   -0.2547416    1.3544949
H     1.8565096   -0.2547416   -1.3544949

17
Energy = -382.8670141291
Rh   -0.2623052    0.5558590    0.0000000
C    -2.1849883    0.2248363    0.7194783
H    -2.3096368   -0.7033354    1.2746795
H    -2.5653345    1.1023262    1.2484925
C    -2.1849883    0.2248363   -0.7194783
H    -2.5653345    1.1023262   -1.2484925
H    -2.3096368   -0.7033354   -1.2746795
C     1.2840490   -0.5093079    1.1843440
C     0.7978099   -1.2108913    0.0000000
C     1.8949838    0.6688703    0.7286098
H     1.1565794   -0.8235000    2.2110827
C     1.2840490   -0.5093079   -1.1843440
H     0.3021036   -2.1749097    0.0000000
C     1.8949838    0.6688703   -0.7286098
H     2.3055432    1.4550814    1.3497802
H     1.1565794   -0.8235000   -2.2110827
H     2.3055432    1.4550814   -1.3497802

17
Energy = -382.8525182120
Rh   -0.4073289    0.5096413    0.0000000
C    -2.5530312    0.3671804    0.0000000
H    -2.9268635    0.8099803    0.9218205
H    -2.9268635    0.8099803   -0.9218205
C    -2.0166993   -0.9293419    0.0000000
H    -1.9747999   -1.5089328   -0.9192995
H    -1.9747999   -1.5089328    0.9192995
C     1.4174902   -0.2270873    1.1609418
C     1.2717660   -1.0479275    0.0000000
C     1.6306270    1.1162206    0.7165228
H     1.3744474   -0.5603205    2.1890670
C     1.4174902   -0.2270873   -1.1609418
H     1.0803643   -2.1130696    0.0000000
C     1.6306270    1.1162206   -0.7165228
H     1.7915634    1.9768984    1.3529139
H     1.3744474   -0.5603205   -2.1890670
H     1.7915634    1.9768984   -1.3529139
```

9.2.8 PBE-D3

```
11
Energy = -1575.875765294
Co    0.0452126    1.4589777    0.0000000
C    -1.2649739   -0.1391803    0.0000000
C    -0.3904274   -0.0895069    1.1366242
C    -0.3904274   -0.0895069   -1.1366242
H    -2.3487501   -0.2099859    0.0000000
C     1.0107588   -0.1939527    0.7052780
H    -0.7090648   -0.0098904    2.1768200
C     1.0107588   -0.1939527   -0.7052780
```

```
H    -0.7090648   -0.0098904   -2.1768200
H     1.8729892   -0.2615558    1.3645839
H     1.8729892   -0.2615558   -1.3645839

11
Energy = -1575.917656601
Co    0.0528270    1.5123009    0.0000000
C    -1.2291918   -0.0958909    0.0000000
C    -0.3831837   -0.1255863    1.1650806
C    -0.3831837   -0.1255863   -1.1650806
H    -2.3168081   -0.0825389    0.0000000
C     0.9856122   -0.1736194    0.7200513
H    -0.7198026   -0.1385403    2.1992961
C     0.9856122   -0.1736194   -0.7200513
H    -0.7198026   -0.1385403   -2.1992961
H     1.8639606   -0.2291895    1.3592128
H     1.8639606   -0.2291895   -1.3592128

17
Energy = -1654.484785067
Co   -0.1967553    0.4580502    0.0000000
C    -2.0021333    0.2145749    0.7160808
H    -2.1644079   -0.7069411    1.2823161
H    -2.3087122    1.1211080    1.2558517
C    -2.0021333    0.2145749   -0.7160808
H    -2.3087122    1.1211080   -1.2558517
H    -2.1644079   -0.7069411   -1.2823161
C     1.1778369   -0.5126837    1.1812017
C     0.7543283   -1.2438876    0.0000000
C     1.7543702    0.6914221    0.7265945
H     1.0371349   -0.8210400    2.2131307
C     1.1778369   -0.5126837   -1.1812017
H     0.2364062   -2.2018299    0.0000000
C     1.7543702    0.6914221   -0.7265945
H     2.1089217    1.5073933    1.3528020
H     1.0371349   -0.8210400   -2.2131307
H     2.1089217    1.5073933   -1.3528020

17
Energy = -1654.493220771
Co   -0.3457560    0.5116576    0.0000000
C    -2.1099691   -0.1351544    0.7050237
H    -2.0388335   -1.0657852    1.2724450
H    -2.5617831    0.7020670    1.2510239
C    -2.1099691   -0.1351544   -0.7050237
H    -2.5617831    0.7020670   -1.2510239
H    -2.0388335   -1.0657852   -1.2724450
C     1.1977093   -0.9160536    0.7117756
C     1.1977093   -0.9160536   -0.7117756
C     1.4436174    0.4157638    1.1566346
H     1.0013013   -1.7733289    1.3504673
C     1.4436174    0.4157638   -1.1566346
H     1.0013013   -1.7733289   -1.3504673
C     1.6064689    1.2504500    0.0000000
H     1.5084339    0.7374338    2.1933713
H     1.5084339    0.7374338   -2.1933713
H     1.8583346    2.3080075    0.0000000

19
Energy = -1730.575292054
C    -0.5099581    2.0263824    1.0861452
C     0.9535974    2.1720716    0.9173764
C    -1.2782953    1.4628777    0.0938159
C     1.4107723    1.3005762    0.0029355
Co   -0.0813011    0.1101293   -0.0587332
C     1.0723238   -1.6364477   -0.2550321
H     2.1246089   -1.7068580    0.0042545
C    -0.0192966   -1.9142464    0.6044448
H     0.0585185   -2.2228516    1.6444233
C    -1.2426027   -1.6643008   -0.1038721
H    -2.2464158   -1.7724731    0.2969915
C     0.5363275   -1.1541197   -1.5000558
H     1.1081324   -0.8301057   -2.3649957
C    -0.9009671   -1.1963427   -1.4029542
H    -1.5949898   -0.8828301   -2.1780303
H    -2.3696045    1.4722348    0.0253764
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H    -0.9761923    2.3476605    2.0307565
H     1.5153255    2.9150690    1.4969999
H     2.4400169    1.1735743   -0.3398465

19
Energy = -1730.583320883
C     0.4212726    2.5854562   -0.7180834
C     0.4212726    2.5854562    0.7180834
C     0.3009088    1.3235486   -1.2577294
C     0.3009088    1.3235486    1.2577294
Co    0.3418510   -0.0786319    0.0000000
C     0.0333859   -1.8523140    1.1556510
H     0.3493337   -1.9573477    2.1902005
C    -1.2387921   -1.3739068    0.7113624
H    -2.0485971   -1.0274778    1.3474514
C    -1.2387921   -1.3739068   -0.7113624
H    -2.0485971   -1.0274778   -1.3474514
C     0.8157734   -2.1563991    0.0000000
H     1.8356400   -2.5333601    0.0000000
C     0.0333859   -1.8523140   -1.1556510
H     0.3493337   -1.9573477   -2.1902005
H     0.1970963    1.1793658   -2.3419458
H     0.4887598    3.5068712   -1.3087479
H     0.4887598    3.5068712    1.3087479
H     0.1970963    1.1793658    2.3419458

25
Energy = -1809.148204760
C    -1.9235221    1.4148561    0.0197454
C    -0.8494464    1.3477599    1.0475869
C    -1.5161162    0.5638175   -0.9259756
C    -0.5544501    0.1577294    1.7298635
Co    0.1791338    0.0131343   -0.2055381
C     2.2782848    0.2547251    0.1104002
H     2.7576634    0.3554796    1.0809530
C     2.0051456   -0.9650166   -0.5573175
H     2.2376195   -1.9606290   -0.1894904
C     1.3107190   -0.6577436   -1.7766224
H     0.9556819   -1.3731654   -2.5133777
C     1.7969012    1.3357420   -0.7055842
H     1.8519227    2.3939477   -0.4651657
C     1.2091654    0.7738789   -1.8664021
H     0.7284905    1.3276881   -2.6681760
C    -0.8217607   -1.6579890    0.3037965
H    -1.5597493   -1.9671464   -0.4473073
C    -1.3962069   -1.0988614    1.5956885
H    -0.0785541   -2.4500332    0.4622650
H    -1.9905329    0.2918119   -1.8737004
H     0.2266702    0.1832017    2.4946054
H    -0.2985420    2.2550354    1.3227407
H    -2.8057129    2.0649919    0.0656514
H    -1.2823389   -1.7624746    2.4664245
H    -2.4604658   -0.8407403    1.4949363

25
Energy = -1809.127059195
C    -1.0198574    2.2587341    0.5817936
C    -0.2990340    2.0817827    1.8337748
C    -1.0521535    1.4378296   -0.4997882
C     0.1667621    0.9754557    2.4640920
Co   -0.2234145   -0.2441300   -0.6372856
C     1.2610482   -1.7385914   -1.0964444
H     1.6616379   -2.4158056   -0.3463024
C     0.0853688   -1.9605347   -1.8885631
H    -0.5561721   -2.8368474   -1.8466213
C    -0.0918602   -0.8294835   -2.7350936
H    -0.9042528   -0.6763537   -3.4404974
C     1.8043421   -0.4743828   -1.4577783
H     2.6758536    0.0004717   -1.0148534
C     0.9587012    0.0943722   -2.4529304
H     1.0780894    1.0781594   -2.8990950
C    -0.9054444   -0.9486911    1.0514456
H    -1.9342069   -0.5902290    1.1981165
C     0.0252355   -0.4915730    2.1705116
H    -0.9184342   -2.0477957    0.9999535
H    -1.6142255    1.7894383   -1.3766015
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```
H     0.7241879    1.1679099    3.3881676
H    -0.1049992    3.0236930    2.3598815
H    -1.5566268    3.2165690    0.5130350
H     1.0422271   -0.9029014    2.0117283
H    -0.3027723   -0.9670961    3.1193549

11
Energy = -303.8905890317
Rh   -0.4347451    1.7884764    0.0000000
C    -1.2294188   -0.0820322    0.0000000
C    -0.3297448    0.0172173    1.1321516
C    -0.3297448    0.0172173   -1.1321516
H    -2.3041160   -0.2536563    0.0000000
C     1.0476399   -0.3179706    0.6808263
H    -0.6433457    0.0018694    2.1767073
C     1.0476399   -0.3179706   -0.6808263
H    -0.6433457    0.0018694   -2.1767073
H     1.9095905   -0.4275101    1.3360292
H     1.9095905   -0.4275101   -1.3360292

11
Energy = -303.9103918147
Rh    0.0593656    1.6956370    0.0000000
C    -1.2285797   -0.1083044    0.0000000
C    -0.3833063   -0.1379928    1.1640862
C    -0.3833063   -0.1379928   -1.1640862
H    -2.3159557   -0.1068631    0.0000000
C     0.9843318   -0.1860329    0.7194390
H    -0.7201634   -0.1628191    2.1976663
C     0.9843318   -0.1860329   -0.7194390
H    -0.7201634   -0.1628191   -2.1976663
H     1.8617227   -0.2533900    1.3582274
H     1.8617227   -0.2533900   -1.3582274

17
Energy = -382.4948289835
Rh   -0.2692017    0.5426454    0.0000000
C    -2.1888664    0.2241908    0.7192507
H    -2.3264588   -0.7045323    1.2798271
H    -2.5543294    1.1119446    1.2518976
C    -2.1888664    0.2241908   -0.7192507
H    -2.5543294    1.1119446   -1.2518976
H    -2.3264588   -0.7045323   -1.2798271
C     1.2878011   -0.5105614    1.1859760
C     0.8032286   -1.2140725    0.0000000
C     1.8955348    0.6707184    0.7292172
H     1.1622147   -0.8266354    2.2174369
C     1.2878011   -0.5105614   -1.1859760
H     0.3111117   -2.1857935    0.0000000
C     1.8955348    0.6707184   -0.7292172
H     2.3015346    1.4634856    1.3534257
H     1.1622147   -0.8266354   -2.2174369
H     2.3015346    1.4634856   -1.3534257

17
Energy = -382.4794340961
Rh   -0.4100725    0.4944675    0.0000000
C    -2.5415274    0.3750739    0.0000000
H    -2.9138529    0.8236597    0.9259043
H    -2.9138529    0.8236597   -0.9259043
C    -2.0236243   -0.9317284    0.0000000
H    -1.9947638   -1.5156130   -0.9230808
H    -1.9947638   -1.5156130    0.9230808
C     1.4237445   -0.2287678    1.1623039
C     1.2845396   -1.0515616    0.0000000
C     1.6239887    1.1180337    0.7171068
H     1.3814009   -0.5634179    2.1950167
C     1.4237445   -0.2287678   -1.1623039
H     1.1009000   -2.1229456    0.0000000
C     1.6239887    1.1180337   -0.7171068
H     1.7743749    1.9844526    1.3564648
H     1.3814009   -0.5634179   -2.1950167
H     1.7743749    1.9844526   -1.3564648
```

9.2.9 BP86-D3

```
11
Energy = -1576.610283922
Co     0.0448757     1.4647762     0.0000000
C     -1.2641305    -0.1401496     0.0000000
C     -0.3905060    -0.0904950     1.1371183
C     -0.3905060    -0.0904950    -1.1371183
H     -2.3473355    -0.2041673     0.0000000
C      1.0105959    -0.1953027     0.7050278
H     -0.7095967    -0.0146555     2.1768056
C      1.0105959    -0.1953027    -0.7050278
H     -0.7095967    -0.0146555    -2.1768056
H      1.8728019    -0.2597764     1.3632466
H      1.8728019    -0.2597764    -1.3632466

11
Energy = -1576.652671245
Co     0.0530264     1.5165602     0.0000000
C     -1.2292288    -0.0975181     0.0000000
C     -0.3832374    -0.1272120     1.1650513
C     -0.3832374    -0.1272120    -1.1650513
H     -2.3159678    -0.0818137     0.0000000
C      0.9855294    -0.1752458     0.7200355
H     -0.7195165    -0.1377750     2.1985149
C      0.9855294    -0.1752458    -0.7200355
H     -0.7195165    -0.1377750    -2.1985149
H      1.8633095    -0.2283814     1.3587472
H      1.8633095    -0.2283814    -1.3587472

17
Energy = -1655.338318634
Co    -0.1954151     0.4671440     0.0000000
C     -2.0033195     0.2151132     0.7162796
H     -2.1565998    -0.7093816     1.2802947
H     -2.3247892     1.1156551     1.2574253
C     -2.0033195     0.2151132    -0.7162796
H     -2.3247892     1.1156551    -1.2574253
H     -2.1565998    -0.7093816    -1.2802947
C      1.1790760    -0.5116556     1.1812806
C      0.7507105    -1.2406795     0.0000000
C      1.7613475     0.6893003     0.7269161
H      1.0340031    -0.8178904     2.2123355
C      1.1790760    -0.5116556    -1.1812806
H      0.2278265    -2.1951972     0.0000000
C      1.7613475     0.6893003    -0.7269161
H      2.1187209     1.5032254     1.3526500
H      1.0340031    -0.8178904    -2.2123355
H      2.1187209     1.5032254    -1.3526500

17
Energy = -1655.347475390
Co    -0.3842141     0.5445935     0.0000000
C     -2.1504667    -0.1239174     0.7054837
H     -2.0555143    -1.0539524     1.2708077
H     -2.6293181     0.6972451     1.2526279
C     -2.1504667    -0.1239174    -0.7054837
H     -2.6293181     0.6972451    -1.2526279
H     -2.0555143    -1.0539524    -1.2708077
C      1.2368968    -0.9250423     0.7121322
C      1.2368968    -0.9250423    -0.7121322
C      1.4687979     0.4090738     1.1571867
H      1.0411305    -1.7817111     1.3500655
C      1.4687979     0.4090738    -1.1571867
H      1.0411305    -1.7817111    -1.3500655
C      1.6210014     1.2454499     0.0000000
H      1.5338909     0.7321104     2.1924071
H      1.5338909     0.7321104    -2.1924071
H      1.8723784     2.3023443     0.0000000

19
Energy = -1731.526711939
C     -0.5103449     2.0284060     1.0875308
C      0.9544377     2.1747850     0.9183660
C     -1.2782015     1.4643398     0.0948244
C      1.4116523     1.3012978     0.0061981
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Co   -0.0817121    0.1118439   -0.0602859
C     1.0720605   -1.6378569   -0.2567129
H     2.1236368   -1.7034286    0.0027072
C    -0.0190030   -1.9142758    0.6036369
H     0.0588511   -2.2183922    1.6439305
C    -1.2427165   -1.6656820   -0.1053354
H    -2.2455137   -1.7691483    0.2965846
C     0.5356205   -1.1575617   -1.5025487
H     1.1075619   -0.8342728   -2.3667511
C    -0.9016904   -1.2009307   -1.4054403
H    -1.5958159   -0.8874290   -2.1793092
H    -2.3693275    1.4735119    0.0274333
H    -0.9759587    2.3443675    2.0331550
H     1.5157144    2.9182062    1.4964163
H     2.4407489    1.1722197   -0.3343997

19
Energy = -1731.535473300
C     0.4169046    2.5837562   -0.7183448
C     0.4169046    2.5837562    0.7183448
C     0.3047744    1.3210726   -1.2595495
C     0.3047744    1.3210726    1.2595495
Co    0.3476891   -0.0797079    0.0000000
C     0.0329283   -1.8545847    1.1556370
H     0.3493372   -1.9564770    2.1892763
C    -1.2372925   -1.3702559    0.7114185
H    -2.0423896   -1.0158451    1.3473151
C    -1.2372925   -1.3702559   -0.7114185
H    -2.0423896   -1.0158451   -1.3473151
C     0.8138194   -2.1624056    0.0000000
H     1.8321354   -2.5409304    0.0000000
C     0.0329283   -1.8545847   -1.1556370
H     0.3493372   -1.9564770   -2.1892763
H     0.2005975    1.1780664   -2.3434279
H     0.4783182    3.5057895   -1.3076208
H     0.4783182    3.5057895    1.3076208
H     0.2005975    1.1780664    2.3434279

25
Energy = -1810.218472136
C    -1.9159421    1.4249061    0.0248653
C    -0.8449460    1.3474733    1.0574229
C    -1.5169531    0.5753350   -0.9255311
C    -0.5520208    0.1538242    1.7318937
Co    0.1753404    0.0094016   -0.2092136
C     2.2722244    0.2646465    0.1106776
H     2.7407987    0.3741371    1.0843871
C     2.0102705   -0.9606720   -0.5506121
H     2.2447336   -1.9517712   -0.1748707
C     1.3168147   -0.6650519   -1.7737117
H     0.9662980   -1.3866527   -2.5052150
C     1.7879279    1.3382893   -0.7139602
H     1.8297831    2.3966645   -0.4768321
C     1.2077701    0.7655003   -1.8730236
H     0.7231576    1.3103657   -2.6772886
C    -0.8214347   -1.6663900    0.2982080
H    -1.5617165   -1.9759844   -0.4500460
C    -1.3946964   -1.1037678    1.5913230
H    -0.0814687   -2.4611543    0.4566087
H    -1.9946958    0.3145071   -1.8737033
H     0.2315837    0.1727008    2.4934883
H    -0.2885401    2.2502595    1.3339546
H    -2.7918083    2.0822392    0.0729953
H    -1.2856760   -1.7673674    2.4619560
H    -2.4568040   -0.8414384    1.4862271

25
Energy = -1810.198110694
C    -1.0213572    2.2635327    0.5839550
C    -0.3267084    2.0822934    1.8510256
C    -1.0340377    1.4491780   -0.5042846
C     0.1497051    0.9777536    2.4772216
Co   -0.2184559   -0.2388552   -0.6390275
C     1.2506516   -1.7473494   -1.0924269
H     1.6408535   -2.4207696   -0.3349337
C     0.0734424   -1.9636712   -1.8843436
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H    -0.5771707   -2.8316202   -1.8341793
C    -0.0940406   -0.8359632   -2.7371250
H    -0.9069630   -0.6775770   -3.4391801
C     1.8038446   -0.4889051   -1.4592230
H     2.6755852   -0.0173461   -1.0156904
C     0.9633378    0.0811531   -2.4586672
H     1.0872132    1.0630244   -2.9053133
C    -0.9005985   -0.9454248    1.0491219
H    -1.9252921   -0.5823815    1.2123886
C     0.0499861   -0.4881230    2.1539840
H    -0.9176015   -2.0443989    0.9994452
H    -1.5748898    1.8131487   -1.3893931
H     0.6840932    1.1690311    3.4144255
H    -0.1637161    3.0208157    2.3925651
H    -1.5561926    3.2215951    0.5097350
H     1.0733571   -0.8619530    1.9515543
H    -0.2350457   -0.9971877    3.0983658

11
Energy = -304.2521155304
Rh   -0.4470989    1.8009246    0.0000000
C    -1.2278974   -0.0777845    0.0000000
C    -0.3284975    0.0196449    1.1328352
C    -0.3284975    0.0196449   -1.1328352
H    -2.3012375   -0.2557465    0.0000000
C     1.0487094   -0.3211620    0.6806050
H    -0.6418639   -0.0011482    2.1768920
C     1.0487094   -0.3211620   -0.6806050
H    -0.6418639   -0.0011482   -2.1768920
H     1.9097689   -0.4310315    1.3356488
H     1.9097689   -0.4310315   -1.3356488

11
Energy = -304.2718437578
Rh    0.0598020    1.7087090    0.0000000
C    -1.2285233   -0.1081332    0.0000000
C    -0.3832825   -0.1378447    1.1640397
C    -0.3832825   -0.1378447   -1.1640397
H    -2.3154631   -0.1096444    0.0000000
C     0.9842977   -0.1858815    0.7194094
H    -0.7200788   -0.1655976    2.1971059
C     0.9842977   -0.1858815   -0.7194094
H    -0.7200788   -0.1655976   -2.1971059
H     1.8611558   -0.2561419    1.3578766
H     1.8611558   -0.2561419   -1.3578766

17
Energy = -382.9726507975
Rh   -0.2744796    0.5553177    0.0000000
C    -2.1954069    0.2227244    0.7192923
H    -2.3225677   -0.7080434    1.2786746
H    -2.5718852    1.1050568    1.2527795
C    -2.1954069    0.2227244   -0.7192923
H    -2.5718852    1.1050568   -1.2527795
H    -2.3225677   -0.7080434   -1.2786746
C     1.2889162   -0.5073400    1.1861815
C     0.7971035   -1.2070339    0.0000000
C     1.9049492    0.6689688    0.7296248
H     1.1635472   -0.8238097    2.2170896
C     1.2889162   -0.5073400   -1.1861815
H     0.3022721   -2.1767741    0.0000000
C     1.9049492    0.6689688   -0.7296248
H     2.3199992    1.4566883    1.3534440
H     1.1635472   -0.8238097   -2.2170896
H     2.3199992    1.4566883   -1.3534440

17
Energy = -382.9586335126
Rh   -0.4160422    0.5090540    0.0000000
C    -2.5533721    0.3713036    0.0000000
H    -2.9320175    0.8152531    0.9252383
H    -2.9320175    0.8152531   -0.9252383
C    -2.0228524   -0.9300724    0.0000000
H    -1.9870221   -1.5138884   -0.9225828
H    -1.9870221   -1.5138884    0.9225828
C     1.4239866   -0.2281934    1.1621979
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C     1.2807637   -1.0503338    0.0000000
C     1.6309595    1.1178671    0.7171715
H     1.3825085   -0.5630035    2.1944189
C     1.4239866   -0.2281934   -1.1621979
H     1.0922011   -2.1203358    0.0000000
C     1.6309595    1.1178671   -0.7171715
H     1.7912361    1.9821573    1.3562792
H     1.3825085   -0.5630035   -2.1944189
H     1.7912361    1.9821573   -1.3562792
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