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Supporting Information for

Conformational Isomerization in $\mathrm{Co(acac)_2}$ via Spin-State Switch: A Computational Study

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TABLE S1: Optimized energy and Gibbs free energy of the ^{2}SQP state with respect to the ^{4}TD state. The $\langle S^2 \rangle$ value for the HS and LS spin states, and $\Delta E_{\mathrm{el+ZPE}}$ (^{2}SQP$-^4$TD) of $\mathrm{Co(acac)_2}$ complex with different functionals (arranged with increasing %of Hartree-Fock exchange). All DFT calculations employ def2-TZVP basis set and D3 dispersion correction. B2PLYP functional energy is the single-point energy calculation on the B3LYP-D3 optimized energy, DLPNO-CCSD(T) energy is the single-point energy calculation on the B3LYP-D3 optimized energy. All energy in kcal/mol. The T_1 diagnostic of DLPNO-CCSD(T) are given in the parentheses.

		Relative Optimized Energy		$\langle S^2 \rangle$		Relative Gibbs Free Energy		$\Delta E_{\mathrm{el+ZPE}}$
Functional	%HF-Exchange	^{4}TD	^{2}SQP	^{4}TD	^{2}SQP	^{4}TD	^{2}SQP	(^{2}SQP$-^4$TD)
BP86-D3	0	0.0	–5.3	3.76	0.76	0.0	–2.4	–4.2
BLYP-D3	0	0.0	–4.2	3.76	0.76	0.0	–1.4	–3.2
TPSSh-D3	10	0.0	7.0	3.76	0.77	0.0	9.4	7.7
B3LYP*-D3	15	0.0	10.3	3.76	0.76	0.0	3.3	11.6
B3PW91-D3	20	0.0	11.1	3.76	0.81	0.0	13.6	12.1
B3LYP-D3	20	0.0	8.6	3.76	0.76	0.0	10.8	9.6
PBE0-D3	25	0.0	12.7	3.76	0.76	0.0	15.2	13.7
M06-D3	27	0.0	4.7	3.77	0.76	0.0	8.13	6.2
M05-D3	28	0.0	13.3	3.77	0.88	0.0	15.8	14.1
CAM-B3LYP-D3	19-65	0.0	11.9	3.76	0.76	0.0	14.9	13.3
B2PLYP-D3	53	0.0	33.9					
DLPNO-CCSD(T)	-	0.0 ($T_1 = 0.014$)	16.9 ($T_1 = 0.014$)					

TABLE S2: The relative optimized energy (kcal/mol) of HS and LS state geometries of complex $\mathrm{Co(acac)_2}$ with different orders of dispersion corrections in different spin-states with respect to corresponding ^{4}TD energy by using B3LYP and CAM-B3LYP functional and def2tzvp basis set.

	$E(^2\text{SQP}) - E(^4\text{TD})$	RMSD (Å)	
	in kcal/mol	^{4}TD	^{2}SQP
B3LYP-D3	8.6	0	0
B3LYP	10.7	0.004	0.017
B3LYP-D3BJ	8.5	0.009	0.014
CAM-B3LYP-D3	11.9	0	0
CAM-B3LYP	12.3	0.003	0.003
CAM-B3LYP-D3BJ	11.9	0.005	0.003

TABLE S3: DFT optimized structural parameters (Co – O bond length in Å, O – Co – O angle in °) and shape-deviation parameter (δ, obtained from shape program[1]) for $\mathrm{Co(acac)_2}$ complex in HS and LS states with different functionals together with their experimental values of tetrameric $\mathrm{Co(acac)_2}$ complex [2]. All calculations employ def2-TZVP basis set and D3-dispersion correction.

	BP86-D3	BLYP-D3	TPSSh-D3	B3LYP*-D3	B3PW91-D3	B3LYP-D3	PBE0-D3	M06-D3	M05-D3	CAM-B3LYP-D3	Expt [2]
High Spin Geometry (^{4}TD)											
$Co-O_1$	1.93	1.95	1.93	1.95	1.94	1.95	1.94	1.94	1.95	1.94	
$Co-O_2$	1.93	1.95	1.93	1.95	1.94	1.95	1.94	1.94	1.95	1.94	1.93 to 2.13
$Co-O_3$	1.93	1.95	1.93	1.95	1.94	1.95	1.94	1.94	1.95	1.94	
$Co-O_4$	1.93	1.95	1.93	1.95	1.94	1.95	1.94	1.94	1.95	1.94	
O_1-Co-O_2	98.1	96.5	96.3	94.9	95.8	94.9	95.7	95.8	94.9	94.5	
O_2-Co-O_3	115.5	116.3	116.4	117.2	116.7	117.2	116.8	116.5	117.1	117.4	68.6 to 104.7
O_3-Co-O_4	98.1	96.5	96.4	94.9	95.8	94.9	95.7	95.8	94.9	94.5	
O_1-Co-O_4	115.5	116.3	116.4	117.2	116.7	117.2	116.8	116.8	117.1	117.5	
δ	1.0	1.3	1.3	1.6	1.4	1.6	1.4	1.4	1.6	1.7	
Low Spin Geometry (^{2}SQP)											
$Co-O_1$	1.85	1.87	1.85	1.87	1.86	1.89	1.88	1.88	1.88	1.86	
$Co-O_2$	1.85	1.87	1.85	1.87	1.86	1.89	1.88	1.88	1.88	1.86	
$Co-O_3$	1.85	1.87	1.85	1.87	1.86	1.89	1.88	1.88	1.88	1.86	
$Co-O_4$	1.85	1.87	1.85	1.87	1.86	1.89	1.88	1.88	1.88	1.86	NA
O_1-Co-O_2	95	93.9	93.9	93.1	93.4	93.4	93.9	93.8	92.7	92.8	
O_2-Co-O_3	85	86.0	86.1	86.9	86.6	86.6	86.1	86.2	87.3	87.2	
O_3-Co-O_4	95	93.9	93.9	93.1	93.4	93.4	93.9	93.8	92.7	92.8	
O_1-Co-O_4	85.4	86.0	86.1	86.9	86.6	86.6	86.1	86.2	87.4	87.2	
δ	0.16	0.12	0.12	0.07	0.09	0.09	0.11	0.12	0.07	0.06	

TABLE S4: Geometrical parameters (bond length in Å, bond angle °) of ^{4}TD and ^{2}SQP geometries using different basis sets and B3LYP functional with D3 dispersion correction.

Structures	Co–O_1	Co–O_2	Co–O_3	Co–O_4	O_1–Co–O_2	O_2–Co–O_3	O_3–Co–O_4	O_4–Co–O_1
6-311G(d,p)								
^{4}TD	1.94	1.94	1.94	1.94	95.5	116.9	95.5	116.9
^{2}SQP	1.87	1.87	1.87	1.87	93.3	86.7	93.3	86.7
def2-SVP								
^{4}TD	1.95	1.95	1.95	1.95	94.7	117.3	94.7	117.3
^{2}SQP	1.89	1.89	1.89	1.89	93.2	86.8	93.2	86.8
def2-TZVP								
^{4}TD	1.95	1.95	1.95	1.95	94.9	117.2	94.9	117.2
^{2}SQP	1.89	1.89	1.89	1.89	93.4	86.6	93.4	86.6
def2-TZVPP								
^{4}TD	1.95	1.95	1.95	1.95	94.9	117.2	94.9	117.2
^{2}SQP	1.89	1.89	1.89	1.89	93.3	86.7	93.3	86.7

TABLE S5: The relative energy (kcal/mol) of $\mathrm{Co(acac)_2}$ complex in all possible spin-states with respect to corresponding ^{4}TD geometry by employing different basis sets and B3LYP functional with D3 dispersion correction.

Basis-sets	^{4}TD	^{2}SQP
6-311G(d,p)	0.0	7.6
def2-SVP	0.0	11.9
def2-TZVP	0.0	8.6
def2-TZVPP	0.0	8.9

TABLE S6: The energy difference between ^{4}TD and ^{2}SQP conformers by using B3LYP* and B2PLYP functionals with and without D3 dispersion correction and def2-TZVP basis set. These energies are in the kcal/mol.

method	E(^{2}SQP-^{4}TD)	RMSD(Å)
B3LYP*/def2TZVP (opt.)	10.7	0.039(^{4}TD), 0.016(^{2}SQP)
B3LYP*-D3/def2TZVP (opt.)	10.3	0.036 (^{4}TD),0.013 (^{2}SQP)
B3LYP*-D3/def2TZVP (single point)	9.9	
B2PLYP/def2TZVP (single point)	31.5	
B2PLYP-D3/def2TZVP (single point)	33.9	

TABLE S7: The ΔE_{el}, $\Delta\ E_{\mathrm{el+ZPE}}$ and $\Delta\ G_{\mathrm{LS-HS}}$ for ^{4}TD and ^{2}SQP conformers by using B3LYP functional with D3 dispersion correction and def2-TZVP basis set. These calculations were performed in both the gas phase and in non-coordinating solvents. All energy differences are in kcal/mol.

	ΔE_{el} (^{2}SQP-^{4}TD)	$\Delta\ E_{\mathrm{el+ZPE}}$ (^{2}SQP-^{4}TD)	ΔG (^{2}SQP-^{4}TD)
Gas phase	8.6	9.6	10.8
benzene (PCM)	7.6	8.8	10.5
toluene (PCM)	9.7	10.7	12.3

TABLE S8: The relative energy (kcal/mol) of HS and LS state geometries of complex $\mathrm{Co(acac)_2}$ in different spin-states with respect to corresponding ^{4}TD energy by using different functionals and DKH-def2-TZVP and ZORA-def2-TZVP basis sets.

	def2-TZVP	DKH-def2-TZVP	ZORA-def2-TZVP
	ΔE(^{2}SQP-^{4}TD)	ΔE (^{2}SQP-^{4}TD)	ΔE (^{2}SQP-^{4}TD)
PBE0	15.8	14.6	14.5
TPSSh	6.9	5.4	5.3
B3LYP	10.9	9.5	9.4

TABLE S9: The lowest spin-free energy of the HS and LS geometries of $\mathrm{Co(acac)_2}$ complex with CASSCF, NEVPT2, and QD-NEVPT2 methods using CAS(7,5), CAS(7,10), CAS(9,11), and CAS(11,12) with one quartet and three doublet roots.

		ΔE (kcal/mol)		
Active-space	Complex	CASSCF	NEVPT2	QD-NEVPT2
CAS(7,5)	^{4}TD	0.0	0.0	0.0
	^{2}SQP	38.4	16.0	18.4
CAS(7,10)	^{4}TD	0.0	0.0	0.0
	^{2}SQP	35.8	26.4	26.2
CAS(9,11)	^{4}TD	0.0	0.0	0.0
	^{2}SQP	28.1	19.7	17.4
CAS(11,12)	^{4}TD	0.0	0.0	0.0
	^{2}SQP	29.1	20.2	19.0

TABLE S10: Energy of d-orbitals (in eV) of $Co(acac)_2$ in different spin-states. All energies are with reference to the barycentre.

Complex	d_{yz}	d_{xz}	d_{z^2}	$d_{x^2-y^2}$	d_{xy}
^{4}TD	0.015036	0.015046	-0.007854	-0.015194	-0.007034
^{2}SQP	-0.018634	-0.021824	-0.021064	0.066356	-0.004834
^{4}MECP	-0.01528	-0.01796	-0.01741	0.05304	-0.00239
^{2}MECP	-0.01565	-0.01874	-0.01798	0.05503	-0.00266

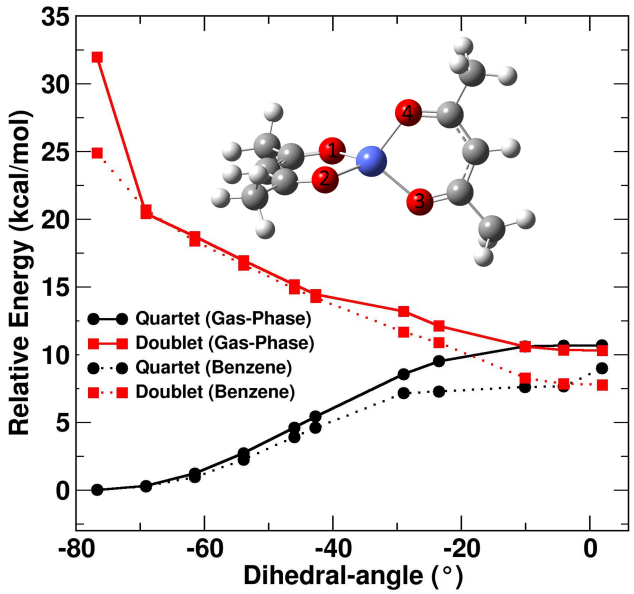


FIG. S1: The one-dimensional potential energy scan of the ^{4}TD and ^{2}SQP states along the rotation of the dihedral angle (1-2-3-4 highlighted in the inset) with B3LYP-D3/def2-TZVP method in the gas-phase and benzene solvent.

TABLE S11: The $\Delta\ E_{\mathrm{el(LS-HS)}}$, $\Delta\ E_{\mathrm{el+ZPE(LS-HS)}}$ and $\Delta\ G_{\mathrm{LS-HS}}$ for ^{4}TD and ^{2}SQP conformers by using B3LYP functional with D3 dispersion correction and def2-TZVP basis set. All energy differences are in kcal/mol.

Complex	ΔE_{el}	$\Delta E_{\mathrm{el+ZPE}}$	$\Delta G_{\mathrm{LS-HS}}$
^{4}TD	0.0	0.0	0.0
^{2}SQP	8.6	9.6	10.8

TABLE S12: Geometrical parameters of all the structures generated along quartet and doublet potential energy surface with B3LYP-D3/def2-TZVP. The Co – O bond distances are in Å and the O – Co – O angles are in °.

Structures	Co – O_1	Co – O_2	Co – O_3	Co – O_4	O_1 – Co – O_2	O_2 – Co – O_3	O_3 – Co – O_4	O_4 – Co – O_1
^{4}TD	1.95	1.95	1.95	1.95	94.9	117.2	94.9	117.2
TS1	1.99	1.99	1.99	1.99	89.5	90.6	89.5	90.6
^{4}TD′	1.95	1.95	1.95	1.95	94.9	117.2	94.9	117.2
MECP	1.94	1.94	1.94	1.94	91.4	89.0	91.4	88.4
^{2}SQP	1.89	1.89	1.89	1.89	93.4	86.6	93.4	86.6
TS2	1.96	1.96	1.92	1.91	92.5	111.3	94.6	123.9
^{2}SQP′	1.89	1.89	1.89	1.89	93.4	86.6	93.4	86.6

TABLE S13: The relative energy gap (ΔE_{el} and $\Delta E_{\mathrm{el+ZPE}}$), and the number of vibrational modes with imaginary frequency ($n_{Q_{\mathrm{imaginary}}}$) for all the structures along the ^{4}TD to ^{2}SQP interconversion process at B3LYP-D3/def2-TZVP. All energy differences are in kcal/mol. Since MECP structure is not a geometric minimum but a geometry where the two spin states have the same energy, no Hessian calculation was done at the MECP.

Complex	ΔE_{el}	$\Delta E_{\mathrm{el+ZPE}}$	$n_{Q_{\mathrm{imaginary}}}$
^{4}TD	0.0	0.0	0
TS1	10.7	10.2	1
^{4}TD′	0.0	0.0	0
MECP	10.3		
^{2}SQP	8.6	9.6	0
TS2	13.2	12.1	1
^{2}SQP′	8.6	9.6	0

TABLE S14: Imaginary frequencies, activation energy barriers (E_a) of TS-1 and TS-2 calculated using various functionals and basis sets, along with deviations in different transition state structures relative to the B3LYP/def2-TZVP level transition state geometry.

Method	Imaginary frequencies (cm^{-1})	E_a (kcal/mol)	RMSD (Å)
TS-1			
B3LYP-D3/def2-TZVP	-21	10.6	0.0
B3LYP-D3/def2-SVP	-29	11.0	0.010
CAM-B3LYP-D3/def2-SVP	-31	11.0	0.018
B3LYP-D3/6-311g(d,p)+6-31g(d,p)	-30	9.0	0.072
TS-2			
B3LYP-D3/def2-TZVP	-123	13.2	0.0
B3LYP-D3/def2-SVP	-106	10.5	0.214
CAM-B3LYP-D3/def2-SVP	-100	8.2	0.211
B3LYP-D3/6-311g(d,p)+6-31g(d,p)	-130	17.9	0.051

TABLE S15: The configuration state functions (CSF) of the lowest spin-free state of $\mathrm{Co(acac)_2}$ complex in the HS and LS state conformers with CSF weight $> 5\%$ (given in the parenthesis) from different active-space calculations by using 10 quartet and 40 doublet states. The ground, first, and second excited states have dominant electronic configurations. The occupancy of the electron is given by 2, u/d (1 electron), 0.

Complex	Ground state	1st excited state	2nd excited state	3rd excited state
CAS(7,5)				
^{4}TD	22111 (100)	12211 (100)	21121 (83)	21112 (83)
^{2}SQP	21220 (94)	22120 (90)	12220 (89)	22210 (48)
CAS(7,10)				
^{4}TD	2211100000 (97)	1221100000 (97)	2112100000 (81)	2111200000 (81)
^{2}SQP	2122000000 (92)	2212000000 (88)	1222000000 (87)	2221000000 (54)

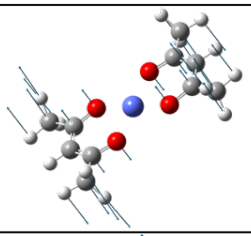
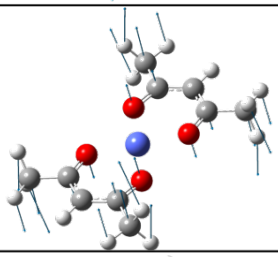
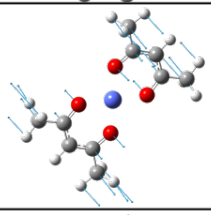
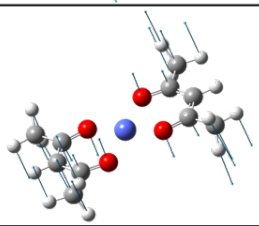
	Mode1
B3LYP-D3/def2-TZVP	
B3LYP-D3/def2-SVP	
CAM-B3LYP/def2-SVP	
B3LYP-D3/6-311g(d,p)+6-31g(d,p)	

FIG. S2: The normal mode of vibration with imaginary frequency in TS-1 obtained from different levels of theory.

TABLE S16: Composition of the spin-orbit coupled states generated from NEVPT2 spin-free energy levels of ^{4}TD, and ^{2}SQP conformers of $\mathrm{Co(acac)_2}$ complex by using different set of active spaces.

Complex	KD1	KD2	KD3	KD4
		CAS(7,5)		
^{4}TD	$0.95\|Q_0\rangle+0.04\|Q_1\rangle$	$0.95\|Q_0\rangle+0.04\|Q_1\rangle$	$0.99\|Q_0\rangle$	$0.99\ \|Q_0\rangle$
^{2}SQP	$0.63\|D_0\rangle+0.36\|D_1\rangle$	$0.63\|D_0\rangle+0.36\|D_1\rangle$	$0.27\|D_0\rangle+0.57\|D_1\rangle+0.16\|D_2\rangle$	$0.27\|D_0\rangle+0.57\|D_1\rangle+0.16\|D_2\rangle$
		CAS(7,10)		
^{4}TD	$0.95\|Q_0\rangle+0.04\|Q_1\rangle$	$0.95\|Q_0\rangle+0.04\|Q_1\rangle$	$0.99\|Q_0\rangle$	$0.99\|Q_0\rangle$
^{2}SQP	$0.71\|D_0\rangle+0.28\|D_1\rangle$	$0.71\|D_0\rangle+0.28\|D_1\rangle$	$0.19\|D_0\rangle+0.62\|D_1\rangle+0.19\|D_2\rangle$	$0.19\|D_0\rangle+0.62\|D_1\rangle+0.19\|D_2\rangle$

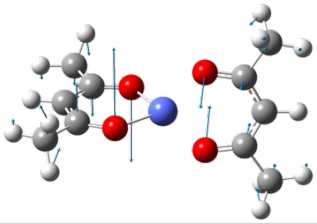
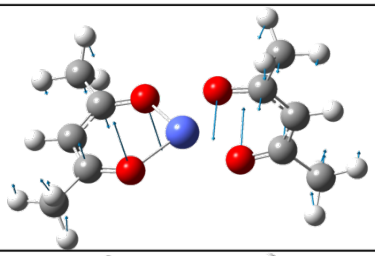
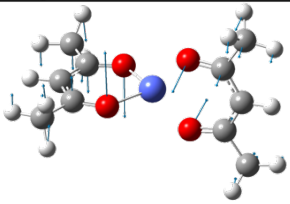
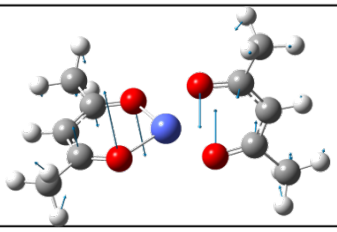
	Mode1
B3LYP-D3/def2-TZVP	
B3LYP-D3/def2-SVP	
CAM-B3LYP/def2-SVP	
B3LYP-D3/6-311g(d,p)+6-31g(d,p)	

FIG. S3: The normal mode of vibration with imaginary frequency in TS2 obtained from different levels of theory.

TABLE S17: Zero-field splitting parameters (D, E, and E/D) and the effective anisotropic barrier U_{eff} with different active spaces in ^{4}TD geometry using 10 quartet roots. D, E, and U_{eff} are in cm^{-1}.

Complex	Active-space	CASSCF				NEVPT2			
		D	E	E/D	U_{eff}	D	E	E/D	U_{eff}
^{4}TD	CAS(7,5)	-34.5	-0.003	0.0001	68.9	-30.6	-0.003	0.0001	61.2
	CAS(7,10)	-31.2	-0.003	0.0001	62.3	-28.8	-0.003	0.0001	57.6

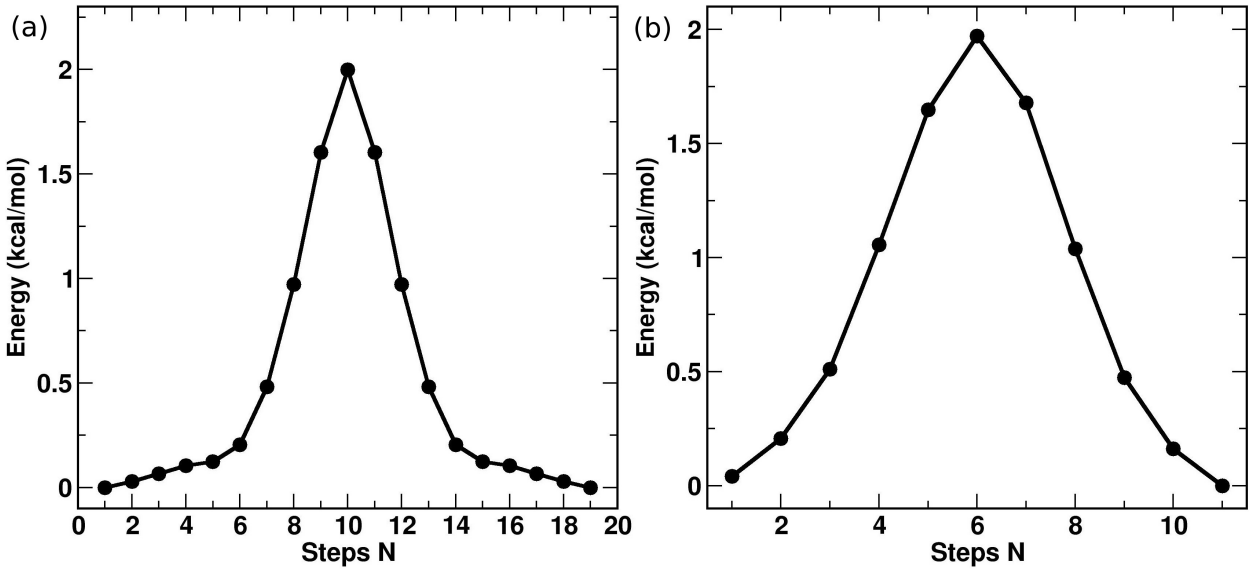


FIG. S4: (a) The IRC plot (with B3LYP-D3/def2-TZVP method) for transition states (a) TS1 and (b) TS2.

TABLE S18: Computed g-tensors and g_z-angle (the angle between the g_z component of the lowest and the n^{th} Kramers doublet) for the lowest two spin-orbit states of ^{4}TD and ^{2}SQP conformers of $\mathrm{Co(acac)_2}$ complex with SA-CASSCF(7,5) + NEVPT2 methods using 10 quartet and 40 doublet roots, respectively.

Complex	KD	CASSCF+Spin-orbit				NEVPT2+Spin-orbit			
		g_x	g_y	g_z	g_z-angle (in °)	g_x	g_y	g_z	g_z-angle (in °)
CAS(7,5)									
^{4}TD	1	0.0	0.0	7.8	180	0.0	0.0	7.6	180
	2	4.4	4.4	2.7	90	4.3	4.3	2.6	90
^{2}SQP	1	3.5	2.8	1.9	180	0.8	1.1	5.4	180
	2	0.4	0.5	3.8	90	1.3	1.3	2.3	90
CAS(7,10)									
^{4}TD	1	0.0	0.0	7.7	180	0.0	0.0	7.6	180
	2	4.4	4.4	2.6	90	4.3	4.3	2.6	90
^{2}SQP	1	1.7	2.6	4.0	180	1.1	1.6	5.2	180
	2	0.03	0.09	3.7	90	0.9	1.05	2.9	90

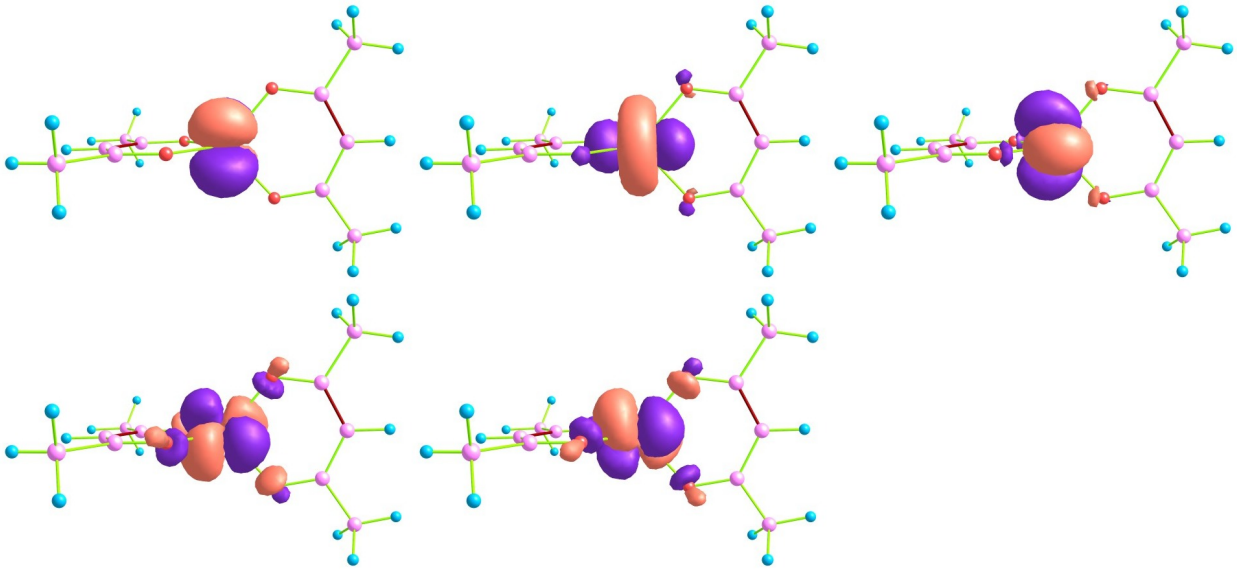


FIG. S5: CAS(7,5) active-space orbitals for ^{4}TD conformer of $\mathrm{Co(acac)_2}$.

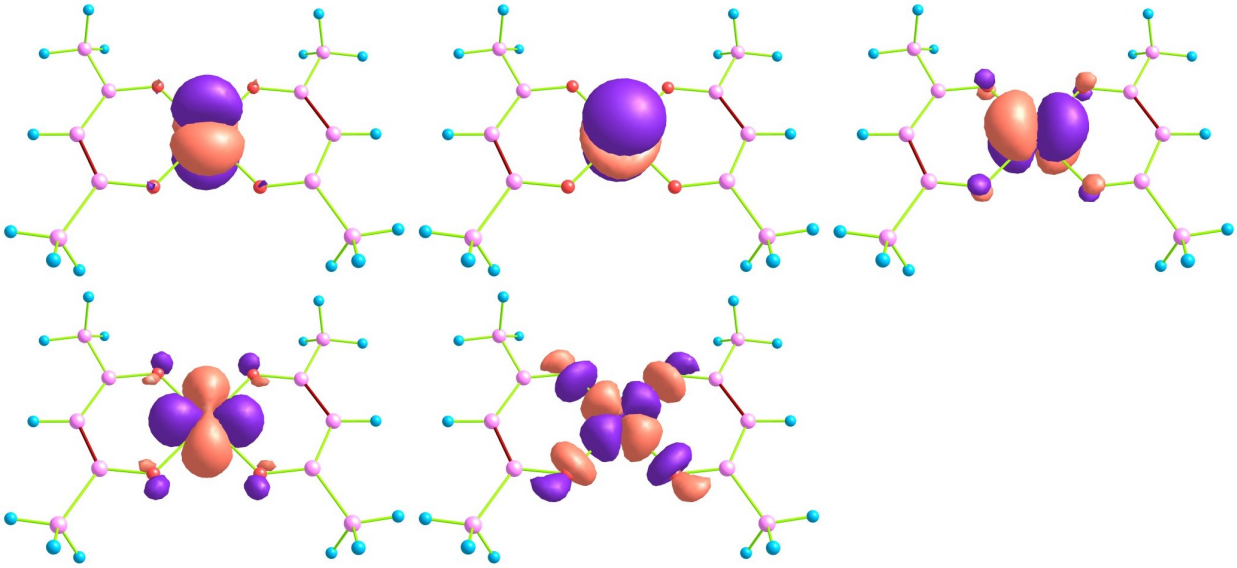


FIG. S6: CAS(7,5) active-space orbitals for ^{2}SQP conformer of $\mathrm{Co(acac)_2}$.

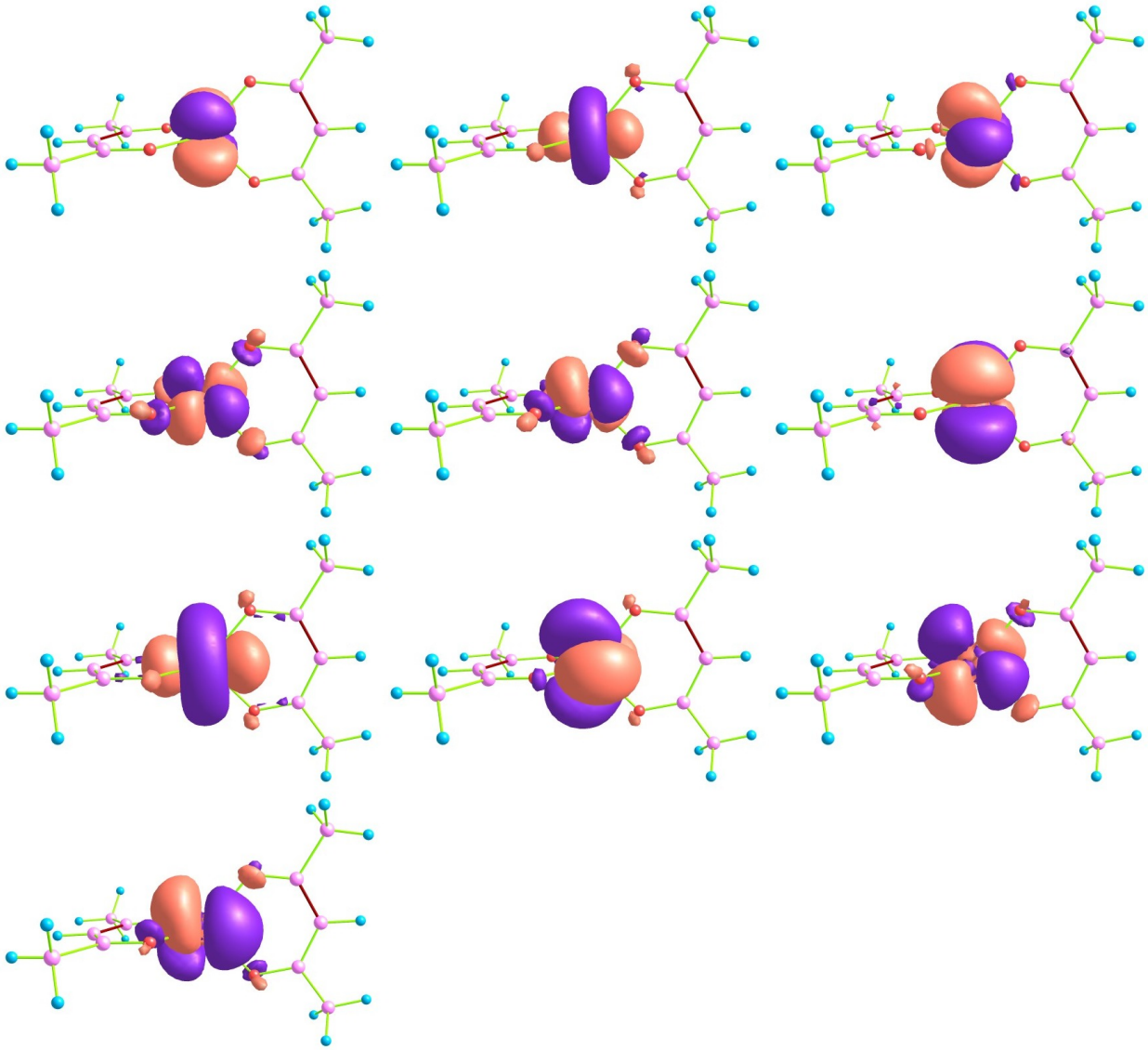


FIG. S7: CAS(7,10) active-space orbitals for ^{4}TD conformer of $\mathrm{Co(acac)_2}$.

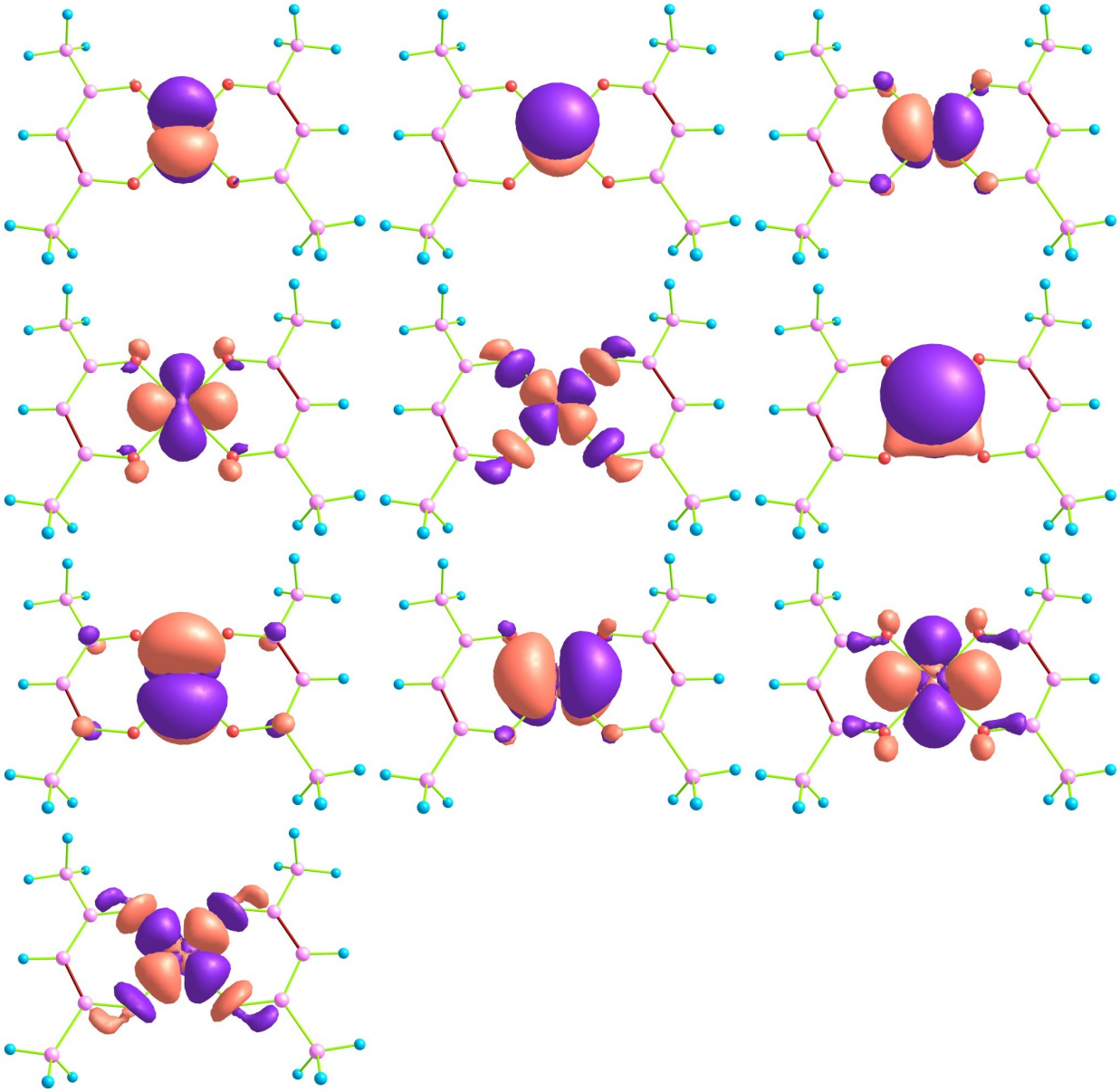


FIG. S8: CAS(7,10) active-space orbitals for ^{2}SQP conformer of $\mathrm{Co(acac)_2}$.

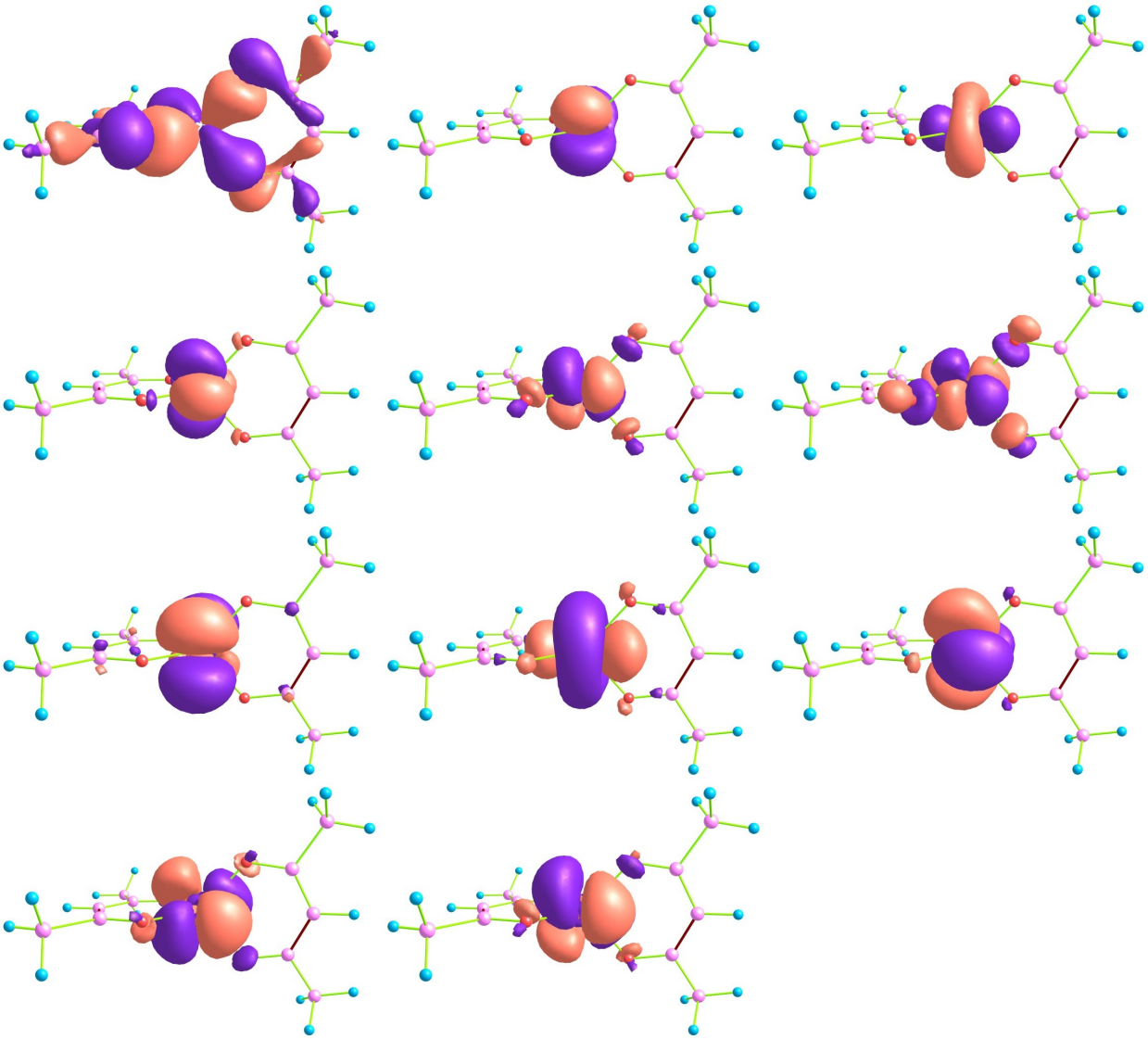


FIG. S9: CAS(9,11) active-space orbitals for ^{4}TD conformer of $\mathrm{Co(acac)_2}$.

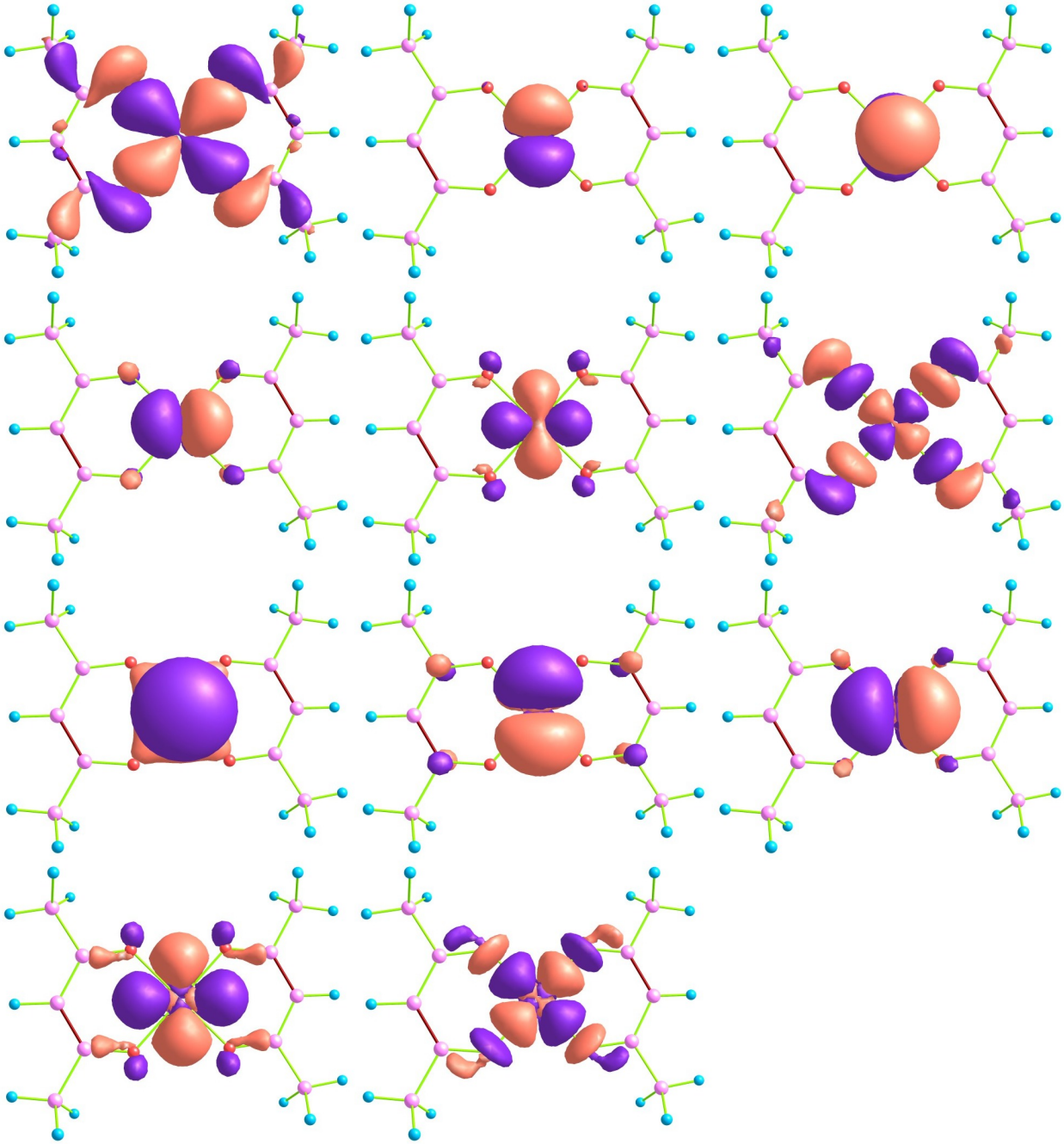


FIG. S10: CAS(9,11) active-space orbitals for ^{2}SQP conformer of $\mathrm{Co(acac)_2}$.

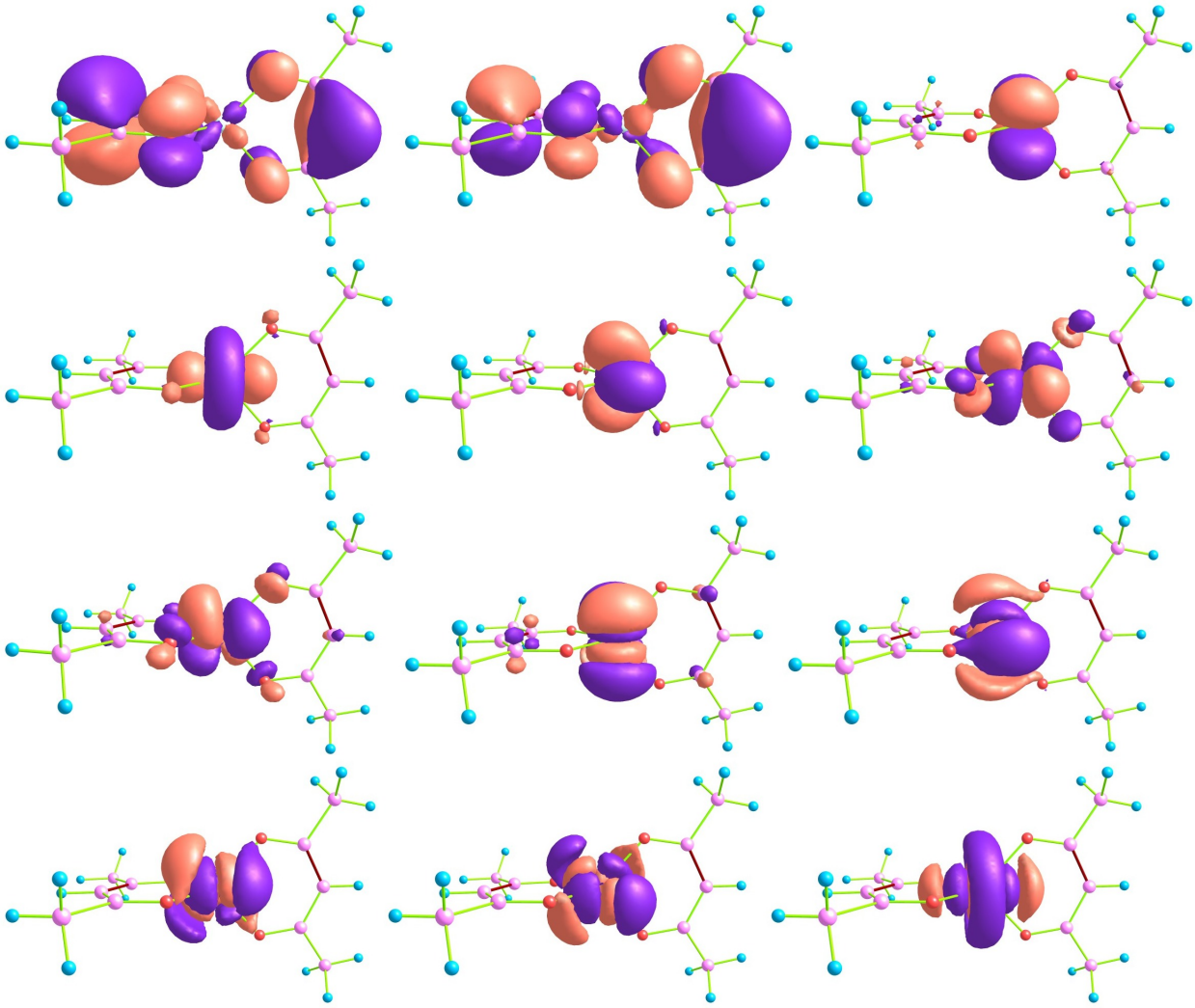


FIG. S11: CAS(11,12) active-space orbitals for ^{4}TD conformer of $\mathrm{Co(acac)_2}$.

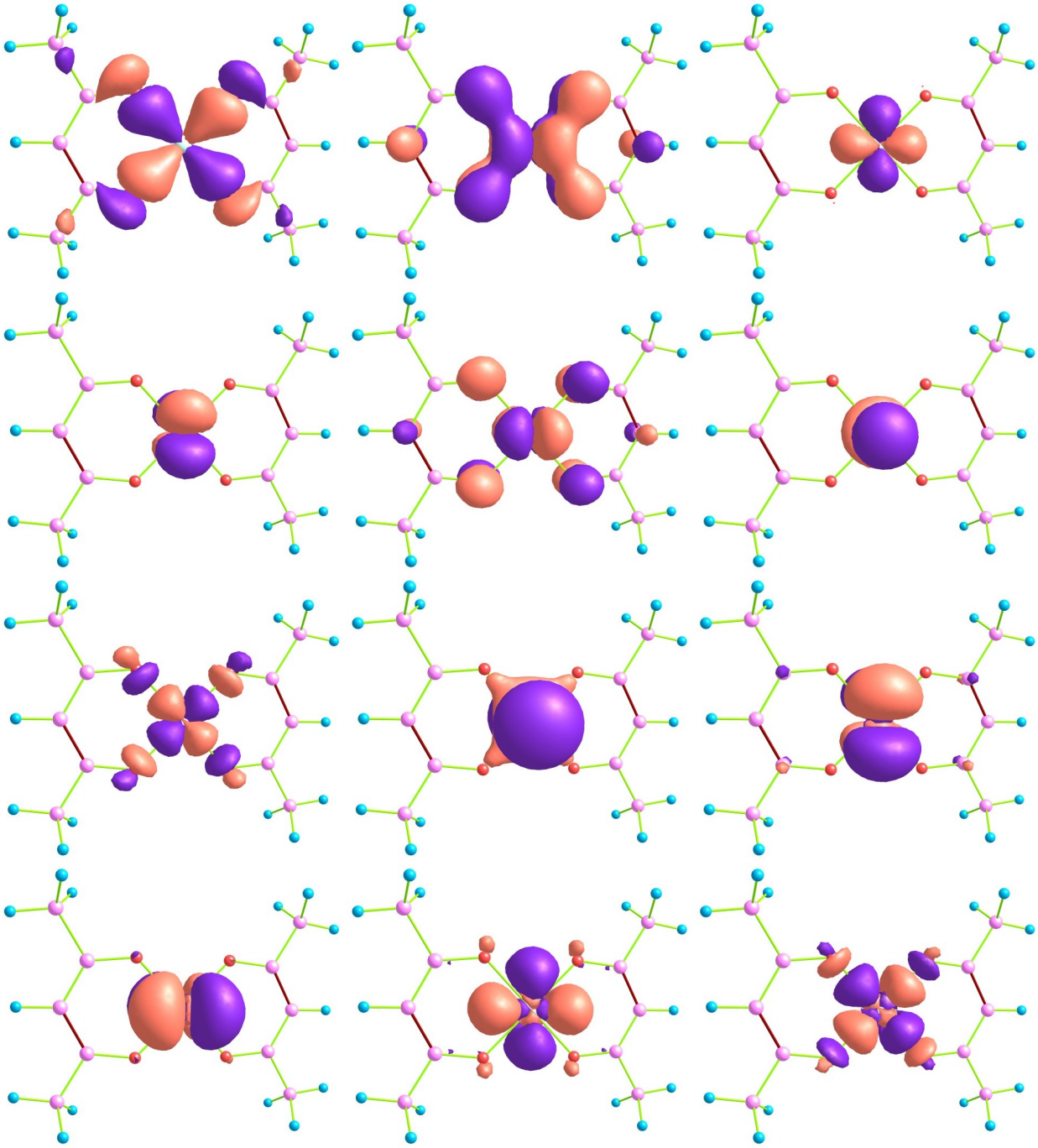


FIG. S12: CAS(11,12) active-space orbitals for ^{2}SQP conformer of $\mathrm{Co(acac)_2}$.

The minimum energy crossing point (MECP) is the point where the two non-interacting spin-states are degenerate. It is a non-stationary point in either of the two (HS or LS) 3N-6 dimension potential energy surfaces. The energies E_i on the two PESs and their energy gradients with respect to the nuclear coordinates ($\partial E_i/\partial q$) are combined to yield two effective gradients, f and g. These vectors f and g are orthogonal and approach zero at MECP. At MECP, the energy gradients on the HS and LS surfaces are parallel. Near the MECP, f is orthogonal to the surface crossing hyperline, and g is parallel and points towards the minimum. These gradients are defined as follows, [3]

$$f = (E_1 - E_2)\left[\left(\frac{\partial E_1}{\partial q}\right) - \left(\frac{\partial E_2}{\partial q}\right)\right] = (E_1 - E_2)x_1 \tag{S1}$$

$$g = \left(\frac{\partial E_1}{\partial q}\right) - \left(\frac{x_1}{|x_1|}\right)\left[\left(\frac{\partial E_1}{\partial q}\right)\cdot\left(\frac{x_1}{|x_1|}\right)\right] \tag{S2}$$

Locating MECP between different types of non-interacting surfaces is described in literature [3–7]. In practical terms, the MECP search starts with an initial guess of the geometry, where the potential energies of the two spin states and gradients on both surfaces are calculated. These are then combined to generate the effective gradients. Standard geometry optimization can then be used to search for points where this gradient goes to 0, which are the MECPs.

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[1] J. Cirera, E. Ruiz, and S. Alvarez, Organometallics **24**, 1556–1562 (2005).

[2] F. A. Cotton and R. C. Elder, Inorg. Chem. **4**, 1145 (1965).

[3] J. N. Harvey, M. Aschi, H. Schwarz, and W. Koch, Theor. Chem. Acc. **99**, 95 (1998).

[4] N. Koga and K. Morokuma, Chem. Phys. Lett. **119**, 371–374 (1985).

[5] A. Farazdel and M. Dupuis, J. Comput. Chem. **12**, 276–282 (1991).

[6] D. R. Yarkony, J. Phys. Chem. **97**, 4407–4412 (1993).

[7] M. J. Bearpark, M. A. Robb, and H. Bernhard Schlegel, Chem. Phys. Lett. **223**, 269–274 (1994).

#Format of .xyz files are
number of atoms in a complex
Method, Lowest_frequency(in cm-1)
x1 y1 z1
x2 y2 z2
…. ….
In Method, “b3lyp/def2tzvp” means the geometry is optimized with B3lyp functional and def2-TZVP basis set. “b3lyp-D3/def2tzvp” means the geometry is optimized using the B3lyp functional and def2-TZVP basis set, with D3 dispersion correction. “b3lyp-D3/def2tzvp, benzene” B3lyp functional and def2-TZVP basis set, with D3 dispersion correction in benzene solvent.

Section 1: ^{4}TD Geometries

29
B3LYP-D3/6-311G(d,p), Lowest_Frequency_28.9

O	8.15822800	0.31873500	10.44957800
O	10.69957100	1.63735700	10.68806000
C	8.78930000	2.40722400	9.48245300
H	8.42648000	3.21794100	8.86612700
C	10.95164600	3.69747400	9.58648400
H	11.84979700	3.35378000	9.06645200
H	11.28169600	4.19146200	10.50422900
H	10.42191100	4.41459600	8.95930300
C	7.89960900	1.34954600	9.74629000
C	6.50469200	1.39041500	9.16956800
H	5.78255800	1.33927400	9.98879200
H	6.35218600	0.50150600	8.55166500
H	6.31398600	2.28301900	8.57364200
C	10.11199400	2.49742200	9.95382300
O	10.77037900	-1.66384600	10.88507900
O	9.83882000	-0.29381800	13.23223700
C	10.94431200	-2.40706100	13.14622100
H	11.30721900	-3.21726200	13.76317200
C	10.19071900	-1.34514600	15.30394000
H	10.68786100	-0.46113000	15.71210100
H	9.13227300	-1.26771900	15.56644800
H	10.61255000	-2.24094300	15.75984300
C	11.13328500	-2.52001800	11.75647700
C	11.82069600	-3.74249000	11.19691600
H	11.14801900	-4.23187200	10.48753800
H	12.70323500	-3.42492000	10.63521400
H	12.11788300	-4.45583800	11.96571600
C	10.32234700	-1.32732200	13.79980200
Co	9.86670200	-0.00039600	11.31376000

29
B3LYP-D3BJ/def2-TVZP, Lowest_Frequency_33.6

O	8.15023200	0.32106200	10.44604700
O	10.70260300	1.64501500	10.68546500
C	8.79155200	2.40223900	9.48583500
H	8.42956800	3.21144300	8.87005900
C	10.93574400	3.70182800	9.57726400
H	11.83307300	3.36903300	9.05209400
H	11.26449400	4.20674400	10.48760900
H	10.39019000	4.40454400	8.95107500
C	7.89899300	1.35218100	9.74469300
C	6.51127200	1.40695800	9.16247300
H	5.78206100	1.36344800	9.97371100
H	6.35114400	0.52565200	8.53844900
H	6.34109200	2.30420900	8.57126200
C	10.11045000	2.49927000	9.95209400
O	10.77406700	-1.67126000	10.88381100
O	9.83874000	-0.29571400	13.24130000
C	10.94215300	-2.40221800	13.14258300
H	11.30465500	-3.21114900	13.75841100
C	10.19973400	-1.36215100	15.30172300
H	10.69886200	-0.48585100	15.71972400
H	9.14496700	-1.29208100	15.57430300
H	10.62650200	-2.26316900	15.73714200
C	11.13394200	-2.52175700	11.75866400
C	11.82128800	-3.74646900	11.21517300
H	11.15454700	-4.24647800	10.51006200
H	12.70805300	-3.43979500	10.65717500
H	12.11020400	-4.44537500	11.99722800
C	10.32349800	-1.32997000	13.80125700
Co	9.86627500	-0.00021900	11.31423900

29
B3LYP-D3/def2-SVP, Lowest_Frequency_34.8

O	8.15392200	0.33235100	10.43961600
O	10.69368800	1.65045000	10.67667100
C	8.78231600	2.42306500	9.47041000
H	8.41614700	3.24033200	8.84925800
C	10.95095300	3.71383400	9.57664900
H	11.86010300	3.36737900	9.05933300
H	11.28334200	4.21167400	10.50183500
H	10.42226500	4.43738200	8.94202400
C	7.89077300	1.36119000	9.73616300
C	6.49361600	1.40031900	9.16030600
H	5.76625600	1.34572100	9.98627600
H	6.33805800	0.50192100	8.54150600
H	6.29662300	2.29741500	8.55847700
C	10.10947200	2.51273400	9.94335400
O	10.77761600	-1.67645700	10.89582100
O	9.84597700	-0.30720900	13.24129000
C	10.95104900	-2.42314700	13.15807200
H	11.31603100	-3.24029200	13.78008300
C	10.19383800	-1.35533900	15.31835300
H	10.69302900	-0.46326500	15.72979800
H	9.12734600	-1.27150400	15.58252500
H	10.61569900	-2.25681300	15.78220800
C	11.14098600	-2.53520800	11.76364000
C	11.82853600	-3.75869800	11.20190300
H	11.15165300	-4.24976400	10.48431400
H	12.71579300	-3.43864300	10.63218300
H	12.12981300	-4.48024500	11.97286700
C	10.32711600	-1.33903600	13.81264200
Co	9.86793800	-0.00017600	11.31335200

29
B3LYP-D3/def2-TZVP, benzene, Lowest_Frequency_28.8

O	8.15047400	0.32611900	10.43300100

O	10.68888100	1.66430100	10.69630600
C	8.78564000	2.41331900	9.47606500
H	8.42446600	3.22045700	8.85654500
C	10.92221700	3.73074500	9.60536300
H	11.83260700	3.40525600	9.09798800
H	11.22844000	4.23253000	10.52559500
H	10.38741200	4.43517000	8.97148000
C	7.89864600	1.35460100	9.72415300
C	6.51801500	1.39025600	9.12215100
H	5.77889800	1.32959300	9.92346900
H	6.38346300	0.50835900	8.49243600
H	6.33760300	2.28590700	8.53113000
C	10.09879200	2.51976600	9.95957200
O	10.75908600	-1.68745800	10.89018100
O	9.87451300	-0.28967300	13.25089400
C	10.94601300	-2.41466700	13.15104800
H	11.30456300	-3.22638300	13.76608800
C	10.24039300	-1.34861800	15.31482000
H	10.75628500	-0.47560600	15.71973000
H	9.18864200	-1.25942500	15.59450100
H	10.65624500	-2.25125300	15.75794900
C	11.12010900	-2.54122900	11.76426900
C	11.78709600	-3.77429600	11.21228500
H	11.10953300	-4.25904300	10.50657300
H	12.67590100	-3.47606100	10.65236200
H	12.07067600	-4.48417400	11.98669200
C	10.35030600	-1.32965800	13.81227100
Co	9.86503800	0.00113400	11.31601200

29

B3LYP-D3/def2-TZVP, toluene, Lowest_Frequency_29.2

O	8.150368	0.325882	10.432311
O	10.688014	1.665458	10.697903
C	8.785470	2.413407	9.475904
H	8.424442	3.220357	8.856053
C	10.920841	3.732479	9.607803
H	11.832225	3.407903	9.101623
H	11.225321	4.234507	10.528491
H	10.386245	4.436464	8.973272
C	7.898794	1.354201	9.723011
C	6.518928	1.389067	9.119270
H	5.778761	1.327626	9.919561
H	6.385846	0.507319	8.489019
H	6.338681	2.284776	8.528302
C	10.098041	2.520745	9.960786
O	10.757942	-1.688352	10.890020
O	9.876893	-0.288724	13.251237
C	10.946056	-2.414892	13.151066
H	11.304329	-3.226759	13.766068
C	10.243623	-1.347494	15.315177
H	10.760735	-0.474880	15.719398
H	9.192216	-1.257271	15.595849
H	10.659033	-2.250401	15.758147
C	11.118902	-2.542159	11.764203
C	11.784361	-3.776046	11.212271
H	11.106101	-4.260242	10.506848
H	12.673391	-3.478926	10.652098
H	12.067377	-4.486049	11.986760
C	10.352117	-1.329065	13.812538
Co	9.864900	0.001039	11.315938

29

B3LYP-D3/def2-TZVP, Lowest_Frequency_33.2

O	8.15163700	0.32964200	10.44152300
O	10.69559400	1.64930500	10.68008700
C	8.78695800	2.41250500	9.47808000
H	8.42480600	3.22197500	8.86216500
C	10.94087500	3.70594300	9.57689200
H	11.83794400	3.36615600	9.05544800
H	11.26997500	4.20355800	10.49130300
H	10.40601500	4.41725200	8.95043500
C	7.89638100	1.35980200	9.73921500
C	6.50512600	1.40509700	9.16115700
H	5.78108800	1.35709000	9.97696800
H	6.35016500	0.51948500	8.54167200
H	6.32199800	2.29849200	8.56719200
C	10.10656200	2.50629800	9.94644700
O	10.77555000	-1.67542500	10.89257300
O	9.84325800	-0.30435700	13.24227900
C	10.94669500	-2.41247600	13.15037200
H	11.30922200	-3.22168900	13.76640300
C	10.19810700	-1.36018800	15.30777300
H	10.69550900	-0.47954700	15.71905000
H	9.14174300	-1.28586700	15.57357100
H	10.62158200	-2.25703300	15.75590600
C	11.13701100	-2.52875200	11.76481100
C	11.82385900	-3.75069900	11.21084200
H	11.15379200	-4.24336800	10.50348600
H	12.70733200	-3.43701000	10.65122400
H	12.11777300	-4.45841600	11.98365100
C	10.32701000	-1.33759400	13.80621800
Co	9.86638600	-0.00021100	11.31418600

29

B3LYP-D3/def2-TZVPP, Lowest_Frequency_33.4

O	8.15241700	0.32853400	10.44234800
O	10.69594700	1.64808000	10.68093900
C	8.78744700	2.41142600	9.47894100
H	8.42550600	3.22037500	8.86347700
C	10.94139500	3.70505800	9.57776300
H	11.83795800	3.36563300	9.05686200
H	11.27056000	4.20216300	10.49148600
H	10.40755300	4.41635800	8.95181400
C	7.89681000	1.35871400	9.73996200
C	6.50551800	1.40396000	9.16189200
H	5.78192900	1.35565300	9.97702900
H	6.35053100	0.51889900	8.54301600
H	6.32173000	2.29645800	8.56824700
C	10.10708100	2.50535100	9.94726400
O	10.77496900	-1.67422400	10.89184200
O	9.84287900	-0.30327000	13.24117300
C	10.94620500	-2.41138300	13.14952900
H	11.30846200	-3.22005800	13.76516800
C	10.19765300	-1.35903400	15.30706100

H	10.69445300	-0.47891200	15.71808500
H	9.14209500	-1.28447200	15.57275900
H	10.62059000	-2.25494400	15.75563300
C	11.13655800	-2.52781100	11.76396400
C	11.82335800	-3.74982400	11.20998100
H	11.15390600	-4.24204300	10.50294700
H	12.70606100	-3.43648300	10.65049000
H	12.11735700	-4.45750700	11.98166500
C	10.32656700	-1.33650100	13.80546900
Co	9.86646000	-0.00022800	11.31412100

29

B3LYP/def2-TZVP, Lowest_Frequency_33.8

O	8.14909100	0.32941600	10.44071900
O	10.69734600	1.65131700	10.67968200
C	8.78746800	2.41138200	9.47889300
H	8.42530100	3.22089600	8.86287800
C	10.93642000	3.71033200	9.57253600
H	11.83422200	3.37732400	9.04775600
H	11.26594800	4.21482400	10.48315300
H	10.39367000	4.41548000	8.94619900
C	7.89490700	1.35990000	9.73858300
C	6.50472100	1.41159100	9.15720600
H	5.77542100	1.36729700	9.96868000
H	6.34439900	0.52966500	8.53364100
H	6.33097300	2.30790900	8.56514800
C	10.10741700	2.50760400	9.94602000
O	10.77672300	-1.67739400	10.89126100
O	9.84284600	-0.30406500	13.24496700
C	10.94621000	-2.41136600	13.14953100
H	11.30877400	-3.22066100	13.76560100
C	10.20127600	-1.36678300	15.31006700
H	10.69991000	-0.48987400	15.72807400
H	9.14626900	-1.29593500	15.58258100
H	10.62715700	-2.26682300	15.74900000
C	11.13776200	-2.53004400	11.76426700
C	11.82555000	-3.75500800	11.21682300
H	11.15888500	-4.25456400	10.51090700
H	12.71218500	-3.44816100	10.65819500
H	12.11582700	-4.45643300	11.99647000
C	10.32689300	-1.33768400	13.80784800
Co	9.86638000	-0.00017500	11.31424000

29

B3LYP*-D3/def2-TZVP, Lowest_Frequency_85.7

O	8.120556	0.350471	10.416858
O	10.700313	1.689324	10.658682
C	8.762268	2.467832	9.435966
H	8.392286	3.294328	8.807032
C	10.957635	3.780031	9.540506
H	11.873809	3.427923	9.009191
H	11.292465	4.284597	10.478022
H	10.412233	4.508042	8.900001
C	7.860117	1.392992	9.705346
C	6.441278	1.436373	9.117453
H	5.705056	1.385681	9.954740
H	6.287264	0.528832	8.486351
H	6.252220	2.349012	8.509951
C	10.105177	2.558094	9.915731
O	10.796255	-1.715155	10.899001
O	9.850676	-0.324665	13.281963
C	10.971357	-2.467843	13.192457
H	11.341187	-3.294337	13.821484
C	10.206699	-1.391051	15.385217
H	10.715593	-0.488936	15.800985
H	9.125729	-1.313194	15.651818
H	10.638691	-2.307438	15.844923
C	11.162534	-2.580602	11.780909
C	11.861968	-3.825366	11.213492
H	11.173631	-4.324617	10.490601
H	12.763196	-3.500022	10.641138
H	12.163150	-4.549872	12.002220
C	10.339680	-1.370505	13.854695
Co	9.866958	0.000040	11.314197

29

B3LYP*/def2-TZVP, Lowest_Frequency_33.8

O	8.149003	0.329437	10.440697
O	10.697382	1.651417	10.679684
C	8.787460	2.411406	9.478868
H	8.425295	3.220916	8.862837
C	10.936379	3.710398	9.572496
H	11.834139	3.377388	9.047638
H	11.265990	4.214839	10.483115
H	10.393588	4.415580	8.946225
C	7.894882	1.359930	9.738550
C	6.504716	1.411640	9.157135
H	5.775401	1.367313	9.968599
H	6.344421	0.529715	8.533554
H	6.330972	2.307971	8.565087
C	10.107408	2.507658	9.946004
O	10.776730	-1.677482	10.891238
O	9.842850	-0.304069	13.245073
C	10.946226	-2.411387	13.149557
H	11.308799	-3.220685	13.765626
C	10.201330	-1.366842	15.310116
H	10.699915	-0.489897	15.728116
H	9.146315	-1.296045	15.582632
H	10.627263	-2.266866	15.749042
C	11.137762	-2.530091	11.764288
C	11.825546	-3.755070	11.216876
H	11.158896	-4.254589	10.510915
H	12.712210	-3.448224	10.658286
H	12.115776	-4.456516	11.996528
C	10.326918	-1.337709	13.807897
Co	9.866378	-0.000167	11.314253

29

B3PW91-D3/def2-TZVP, Lowest_Frequency_34.3

O	8.15676100	0.31374200	10.45283300
O	10.70380000	1.63506200	10.69193600
C	8.79532600	2.39382000	9.49226100
H	8.43283900	3.20416100	8.87559500
C	10.94193500	3.68599700	9.58910600

H	11.83971100	3.34711300	9.06697600
H	11.27157000	4.18481000	10.50341900
H	10.40497900	4.39636800	8.96240400
C	7.90519400	1.34273400	9.75257900
C	6.51899800	1.39173700	9.17419500
H	5.79361000	1.34409800	9.98966800
H	6.36302800	0.50608400	8.55391900
H	6.33795700	2.28627500	8.58028400
C	10.11341400	2.48825500	9.95982900
O	10.76911500	-1.66121400	10.87965500
O	9.83584400	-0.28845300	13.23230800
C	10.93842300	-2.39375500	13.13618400
H	11.30147900	-3.20381700	13.75288200
C	10.19317800	-1.34696400	15.28928300
H	10.69068600	-0.46619700	15.70182300
H	9.13646800	-1.27313700	15.55642400
H	10.61766000	-2.24493300	15.73556800
C	11.12870400	-2.51067400	11.75234200
C	11.81392700	-3.73062700	11.20402400
H	11.14402200	-4.22466200	10.49649800
H	12.69814000	-3.41787100	10.64383200
H	12.10735900	-4.43723600	11.97881700
C	10.31956400	-1.32054300	13.79202000
Co	9.86626300	-0.00020300	11.31426300

29

BLYP-D3/def2-TZVP, Lowest_Frequency_33.8

O	8.14148700	0.30611500	10.45138100
O	10.71869800	1.64287900	10.69327100
C	8.78882600	2.40823800	9.48127500
H	8.42444900	3.22290900	8.86131900
C	10.95915700	3.71613600	9.57811800
H	11.86160400	3.37797600	9.05107200
H	11.29119900	4.22009900	10.49587500
H	10.41992600	4.43139400	8.94824900
C	7.88808700	1.35170200	9.74064800
C	6.48618000	1.39629700	9.15863400
H	5.75480500	1.34998500	9.97684500
H	6.32736500	0.50744100	8.53314500
H	6.30314100	2.29557700	8.56122900
C	10.11749100	2.50804700	9.94985800
O	10.77451900	-1.66947200	10.86588500
O	9.83019300	-0.28056200	13.24633100
C	10.94480700	-2.40821900	13.14718600
H	11.30986400	-3.22256700	13.76716400
C	10.19180400	-1.35094300	15.32558500
H	10.69289500	-0.46705900	15.74294400
H	9.12991100	-1.27806200	15.59685400
H	10.61822800	-2.25371600	15.77532400
C	11.13896500	-2.53075400	11.75356700
C	11.83106200	-3.76129300	11.19423900
H	11.15923300	-4.26047300	10.48292800
H	12.72185300	-3.44936100	10.63233400
H	12.12606600	-4.47280500	11.97258500
C	10.32202600	-1.32931200	13.81275900
Co	9.86610900	-0.00022800	11.31432300

29

BP86-D3/def2-TZVP, Lowest_frequency_34.7

O	8.15252100	0.27976100	10.47070900
O	10.73097900	1.61722600	10.71286300
C	8.80194400	2.37896000	9.50363200
H	8.43656000	3.19588700	8.88216600
C	10.96340200	3.68360100	9.59918400
H	11.86842500	3.34642600	9.07154200
H	11.29596100	4.18998400	10.51795100
H	10.42012800	4.39753300	8.96775800
C	7.90205000	1.32416600	9.76207900
C	6.50726900	1.37228900	9.18086900
H	5.77333700	1.32617700	9.99963300
H	6.34669200	0.48226600	8.55379200
H	6.32767500	2.27447400	8.58308000
C	10.12879600	2.47920300	9.97119600
O	10.76299800	-1.64422600	10.84551200
O	9.81834900	-0.25438700	13.22705200
C	10.93182300	-2.37886300	13.12485900
H	11.29796000	-3.19528000	13.74655300
C	10.18233500	-1.32691800	15.29620700
H	10.68401700	-0.44176800	15.71571400
H	9.11878000	-1.25421300	15.56954000
H	10.61071400	-2.23259200	15.74318900
C	11.12583500	-2.50202900	11.73331500
C	11.81515000	-3.72869800	11.18044300
H	11.14278300	-4.23030500	10.46809100
H	12.70774100	-3.41776100	10.61673100
H	12.10958800	-4.43880900	11.96312600
C	10.30998700	-1.30178800	13.79001600
Co	9.86615600	-0.00034700	11.31412600

29

CAM-B3LYP-D3BJ/def2-TZVP, Lowest_Frequency_33.5

O	8.16207800	0.32891500	10.44609500
O	10.68952900	1.64004900	10.68329800
C	8.79168100	2.40201600	9.48599800
H	8.42996000	3.21062600	8.87064000
C	10.93439300	3.68923900	9.58436800
H	11.83004100	3.35113500	9.06253500
H	11.26172100	4.18807100	10.49695900
H	10.39456900	4.39515800	8.95859000
C	7.90601200	1.35279700	9.74700500
C	6.52142100	1.39999300	9.17024500
H	5.79746300	1.35364500	9.98421100
H	6.36638000	0.51679900	8.54997500
H	6.34528200	2.29447400	8.57846200
C	10.10563200	2.49386800	9.95344500
O	10.77007100	-1.66600300	10.89636800
O	9.84407600	-0.30375200	13.23093500
C	10.94211800	-2.40194500	13.14241800
H	11.30437700	-3.21030000	13.75779600
C	10.19762600	-1.35533200	15.28907900
H	10.69528300	-0.47693700	15.70086200
H	9.14285300	-1.28308700	15.55560600
H	10.62264100	-2.25324100	15.73004500
C	11.13063600	-2.51620100	11.76226600

C	11.81455100	-3.73376800	11.21293300
H	11.14510100	-4.22779900	10.50826000
H	12.69748700	-3.42173300	10.65448200
H	12.10596400	-4.43585100	11.98977700
C	10.32472600	-1.33066300	13.79401700
Co	9.86628100	-0.00020400	11.31425900

29

CAM-B3LYP-D3/def2-TZVP, Lowest_Frequency_33.1

O	8.16347700	0.33359500	10.44387800
O	10.68531400	1.64184400	10.68051000
C	8.78918000	2.40760600	9.48177500
H	8.42736600	3.21636900	8.86634200
C	10.93748800	3.69027100	9.58498000
H	11.83277600	3.34703100	9.06587000
H	11.26481200	4.18377600	10.50047300
H	10.40477200	4.40179800	8.95904100
C	7.90513500	1.35687900	9.74428100
C	6.51875900	1.39799100	9.17039100
H	5.79872600	1.34851400	9.98765800
H	6.36762800	0.51181200	8.55340400
H	6.33409400	2.28987200	8.57683900
C	10.10322800	2.49718500	9.95054400
O	10.77057300	-1.66773200	10.90141800
O	9.84660200	-0.30847700	13.23078500
C	10.94459300	-2.40753000	13.14666100
H	11.30686900	-3.21604000	13.76215400
C	10.19630800	-1.35327000	15.29135100
H	10.69279400	-0.47186600	15.69810900
H	9.14046600	-1.27807800	15.55282100
H	10.61912800	-2.24836100	15.74067500
C	11.13203100	-2.51949800	11.76578300
C	11.81539700	-3.73486200	11.20992400
H	11.14344800	-4.22357200	10.50390700
H	12.69582100	-3.41765700	10.65040000
H	12.11016800	-4.44267300	11.98061800
C	10.32665800	-1.33475300	13.79611100
Co	9.86634000	-0.00020400	11.31422500

29

CAM-B3LYP/def2-TZVP, Lowest_Frequency_33.7

O	8.16172500	0.33362400	10.44318400
O	10.68640200	1.64336400	10.68007200
C	8.78947400	2.40695900	9.48224700
H	8.42767000	3.21568800	8.86681400
C	10.93411800	3.69371100	9.58163500
H	11.83000300	3.35566400	9.05996400
H	11.26171400	4.19253000	10.49425700
H	10.39540900	4.40054600	8.95575500
C	7.90403200	1.35710100	9.74371500
C	6.51837000	1.40295300	9.16735300
H	5.79429800	1.35636600	9.98133600
H	6.36312900	0.51957600	8.54721700
H	6.34082500	2.29705600	8.57523200
C	10.10376100	2.49826700	9.95011600
O	10.77145600	-1.66923500	10.90068800
O	9.84643100	-0.30847100	13.23269200
C	10.94430700	-2.40689600	13.14617000
H	11.30656300	-3.21539400	13.76164000
C	10.19872300	-1.35829700	15.29317600
H	10.69623200	-0.47975800	15.70509600
H	9.14389000	-1.28574200	15.55979100
H	10.62333500	-2.25584100	15.73552100
C	11.13263300	-2.52057800	11.76551600
C	11.81672900	-3.73824800	11.21447400
H	11.14738500	-4.23221900	10.50950200
H	12.69966500	-3.42628600	10.65578600
H	12.10867000	-4.44131400	11.99037100
C	10.32664700	-1.33497200	13.79736700
Co	9.86635700	-0.00018500	11.31424100

29

M05-D3/def2-TZVP, Lowest_Frequency_31.8

O	8.15471400	0.32891000	10.44540400
O	10.69869900	1.65042700	10.67992700
C	8.79033100	2.40621900	9.48241300
H	8.42711700	3.21489900	8.86595900
C	10.93519600	3.69776400	9.57537500
H	11.83097400	3.36122000	9.05146200
H	11.26832400	4.19772600	10.48594700
H	10.39736700	4.40681600	8.95075000
C	7.90163800	1.35255100	9.74722400
C	6.51543300	1.40371400	9.17052500
H	5.79115400	1.36087800	9.98524200
H	6.35457100	0.51742500	8.55514200
H	6.33460100	2.29464500	8.57410200
C	10.11029200	2.49953600	9.95026300
O	10.77942900	-1.67190900	10.89145900
O	9.84402300	-0.30201500	13.24145800
C	10.94281900	-2.40684600	13.14540400
H	11.30295900	-3.21735700	13.76125600
C	10.19400400	-1.36213900	15.29604000
H	10.69113400	-0.48501300	15.71273600
H	9.13885200	-1.28621800	15.56251600
H	10.61459100	-2.26048600	15.74129100
C	11.13524700	-2.51991900	11.75970900
C	11.82082600	-3.74041400	11.21464700
H	11.15536500	-4.23331300	10.50449500
H	12.70638100	-3.43035500	10.65803300
H	12.11048800	-4.44761400	11.98804300
C	10.32265400	-1.33101800	13.79962200
Co	9.87077000	0.00185600	11.31448400

29

M06-D3/def2-TZVP, Lowest_Frequency_31.2

O	8.15187000	0.31449700	10.45161100
O	10.69839800	1.62491600	10.69130700
C	8.79674800	2.38791100	9.49719500
H	8.43629500	3.20108500	8.88096100
C	10.93686400	3.66868600	9.59333600
H	11.83482900	3.33311800	9.07057700
H	11.27000000	4.16952100	10.50460000
H	10.39811400	4.37794700	8.96745500
C	7.90628600	1.34162200	9.75583400

C	6.52718500	1.39966400	9.17817800
H	5.79803100	1.35682200	9.98981400
H	6.36219400	0.51625600	8.55803300
H	6.35462900	2.29559300	8.58440300
C	10.11181700	2.47654300	9.96364200
O	10.76197000	-1.66343400	10.87997500
O	9.82774700	-0.29342400	13.22724300
C	10.93890400	-2.38656600	13.13185100
H	11.30807000	-3.19420000	13.75021300
C	10.19437500	-1.34694100	15.27535800
H	10.68484000	-0.46437200	15.69095500
H	9.13933400	-1.28047900	15.54869800
H	10.62653600	-2.24275400	15.71785400
C	11.12607900	-2.50444100	11.75136300
C	11.81489900	-3.71790800	11.21099000
H	11.15194700	-4.21972600	10.50328000
H	12.69863600	-3.40665800	10.65026700
H	12.10967100	-4.41897000	11.98987900
C	10.31631600	-1.31814700	13.78427500
Co	9.85736900	-0.00619100	11.31178200

29

PBE0-D3/def2-TZVP, Lowest_Frequency_33.8

O	8.15693400	0.31578500	10.45173900
O	10.70222400	1.63628500	10.69074600
C	8.79571700	2.39299100	9.49286600
H	8.43317700	3.20345500	8.87602600
C	10.93621700	3.68471500	9.58765000
H	11.83449900	3.34781200	9.06485900
H	11.26613800	4.18552000	10.50091600
H	10.39477600	4.39163700	8.96093500
C	7.90636500	1.34266200	9.75305100
C	6.52357300	1.39565400	9.17359900
H	5.79652700	1.34879600	9.98780000
H	6.36594300	0.51087000	8.55229000
H	6.34779600	2.29191000	8.58073000
C	10.11274700	2.48729600	9.96017700
O	10.76949500	-1.66227700	10.88167000
O	9.83689700	-0.29047600	13.23279400
C	10.93809600	-2.39290500	13.13556500
H	11.30123700	-3.20313500	13.75235900
C	10.19568500	-1.35108200	15.28560500
H	10.69329900	-0.47118200	15.70018100
H	9.13931000	-1.27804300	15.55477000
H	10.62161700	-2.25089500	15.72672600
C	11.12812700	-2.50962100	11.75277300
C	11.81253600	-3.72919200	11.20971000
H	11.14349700	-4.22530200	10.50262700
H	12.69739500	-3.41846800	10.64917600
H	12.10415600	-4.43220100	11.98842900
C	10.31970100	-1.32049600	13.79082200
Co	9.86627300	-0.00014500	11.31433900

29

TPSSh-D3/def2-TZVP, Lowest_Frequency_29.7

O	8.15859800	0.30481900	10.45870700
O	10.70902900	1.62814500	10.69846500
C	8.79579800	2.39281700	9.49288500
H	8.43302700	3.20383700	8.87553500
C	10.95412100	3.68439200	9.59518300
H	11.85110100	3.33891200	9.07518600
H	11.28147900	4.17807700	10.51356500
H	10.42174600	4.39894400	8.96743600
C	7.90506900	1.33952900	9.75418000
C	6.51272100	1.38019200	9.17804500
H	5.79208800	1.33147600	9.99819300
H	6.36224700	0.49098900	8.56080700
H	6.32597400	2.27331500	8.58178200
C	10.11575700	2.48654200	9.96194400
O	10.76600300	-1.65411400	10.87197900
O	9.83166300	-0.27948800	13.22800600
C	10.93804500	-2.39277400	13.13546200
H	11.30149800	-3.20359200	13.75267600
C	10.18709400	-1.33539300	15.29299900
H	10.68512700	-0.45153700	15.69930200
H	9.12851300	-1.25985000	15.55379800
H	10.61050700	-2.23218500	15.74528500
C	11.12795400	-2.50888300	11.74925900
C	11.81412500	-3.72910700	11.19030300
H	11.13970300	-4.21771800	10.48268800
H	12.69633100	-3.40973500	10.62990700
H	12.11031400	-4.44016200	11.96150200
C	10.31811100	-1.31737200	13.79142400
Co	9.86620900	-0.00010400	11.31442500

Section 2: ^{2}SQP geometries

29

B3LYP-D3/6-311g(d,p), Lowest_Frequency_38.6

Co	9.86689500	-0.00000100	11.31417000
C	8.76712300	2.39027400	9.44556500
O	8.28197400	0.99562600	11.30312000
O	10.60877800	0.96135100	9.88983300
H	8.39478200	3.18374800	8.81334700
C	10.91455500	2.46698300	8.11733800
H	11.19988700	1.66392300	7.43292100
H	11.83667200	2.85979400	8.55366600
H	10.41160400	3.25787700	7.56058300
C	7.95963000	1.92371500	10.49189100
C	6.60081600	2.53053600	10.73743400
H	6.57206700	2.93881600	11.75108300
H	5.84493700	1.74259600	10.68713300
H	6.35503400	3.31659200	10.02318400
C	10.05752300	1.89285100	9.21768000
O	11.45181600	-0.99562800	11.32522000
O	9.12501200	-0.96135300	12.73850700
C	10.96666700	-2.39027600	13.18277500
H	11.33900800	-3.18375100	13.81499300
C	8.81923400	-2.46698500	14.51100200
H	8.53390300	-1.66392500	15.19541900
H	7.89711700	-2.85979600	14.07467400
H	9.32218600	-3.25787900	15.06775700
C	11.77416000	-1.92371700	12.13644900
C	13.13297400	-2.53053800	11.89090500

H	13.16172200	-2.93881800	10.87725700
H	13.88885300	-1.74259800	11.94120700
H	13.37875600	-3.31659400	12.60515600
C	9.67626700	-1.89285300	13.41066000

29

B3LYP-D3BJ/def2-TZVP, Lowest_Frequency_36.7

O	8.24723500	0.97270600	11.29306000
O	10.59922000	0.95017500	9.85432100
C	8.77729300	2.41981000	9.49487800
H	8.41370900	3.23437700	8.88781900
C	10.86849000	2.48148400	8.10068200
H	11.10300100	1.69249400	7.38377300
H	11.81673600	2.84529500	8.50053700
H	10.35584500	3.29370700	7.58950200
C	7.94876500	1.92396200	10.50568200
C	6.58518800	2.52307600	10.72148900
H	6.51544300	2.89813900	11.74418100
H	5.82899500	1.74353500	10.61227300
H	6.37443700	3.33147600	10.02443900
C	10.04735900	1.90374200	9.22175000
O	11.48639500	-0.97290400	11.33506200
O	9.13446400	-0.95036600	12.77386700
C	10.95648400	-2.41984100	13.13342600
H	11.32013600	-3.23432700	13.74055500
C	8.86527600	-2.48159000	14.52759400
H	8.63063200	-1.69255500	15.24440900
H	7.91709700	-2.84557100	14.12773400
H	9.37800200	-3.29369600	15.03887900
C	11.78497400	-1.92400100	12.12259000
C	13.14869200	-2.52287700	11.90700800
H	13.21901000	-2.89716500	10.88407700
H	13.90476300	-1.74335300	12.01722700
H	13.35915500	-3.33175200	12.60359600
C	9.68638300	-1.90385500	13.40650400
Co	9.86677600	-0.00015600	11.31401000

29

B3LYP-D3/def2-SVP, Lowest_Frequency_35.4

O	8.26296100	0.99714200	11.29280800
O	10.60771100	0.96117000	9.86689200
C	8.77169500	2.41261600	9.45238000
H	8.40129900	3.22123900	8.82294000
C	10.90861700	2.47674400	8.09799200
H	11.18626900	1.66810000	7.40315000
H	11.84750200	2.86209700	8.52713400
H	10.40395300	3.27931900	7.54379000
C	7.95065900	1.93440200	10.49081800
C	6.58739700	2.54165500	10.72400400
H	6.53995200	2.93187000	11.75331100
H	5.82459500	1.75007500	10.64976400
H	6.34954000	3.34689600	10.01621900
C	10.06045400	1.90219700	9.20800200
O	11.47082700	-0.99714500	11.33553000
O	9.12607800	-0.96117300	12.76144700
C	10.96209400	-2.41262000	13.17595900
H	11.33249100	-3.22124000	13.80540000
C	8.82517300	-2.47674500	14.53034800
H	8.54752200	-1.66810000	15.22518900
H	7.88628700	-2.86210000	14.10120800
H	9.32983700	-3.27932000	15.08455200
C	11.78312900	-1.93440600	12.13752000
C	13.14639300	-2.54165600	11.90433700
H	13.19384100	-2.93187200	10.87503100
H	13.90919300	-1.75007400	11.97857700
H	13.38425100	-3.34689600	12.61212400
C	9.67333400	-1.90220100	13.42033600
Co	9.86689400	-0.00000200	11.31416900

29

B3LYP-D3/def2-TZVP, benzene, Lowest_Frequency_37.9

Co	9.86689500	-0.00000100	11.31417000
C	8.78253500	2.41590200	9.46984700
O	8.25553900	0.99993100	11.29693400
O	10.61047400	0.95523200	9.85282500
H	8.41846500	3.22201500	8.85133900
C	10.88978900	2.48063800	8.09424400
H	11.15067700	1.68530500	7.39346800
H	11.82426100	2.86486300	8.50809600
H	10.37703500	3.27872700	7.56098900
C	7.95557100	1.93929100	10.49298400
C	6.59382100	2.54530100	10.70685700
H	6.52702800	2.92512000	11.72814200
H	5.83618300	1.76604200	10.60251100
H	6.38102200	3.35081900	10.00677800
C	10.05829900	1.90365000	9.20913100
O	11.47825000	-0.99993300	11.33140600
O	9.12331500	-0.95523300	12.77551500
C	10.95125500	-2.41590400	13.15849300
H	11.31532500	-3.22201700	13.77700100
C	8.84400100	-2.48064000	14.53409700
H	8.58311400	-1.68530600	15.23487300
H	7.90952900	-2.86486400	14.12024400
H	9.35675500	-3.27872800	15.06735100
C	11.77821900	-1.93929300	12.13535600
C	13.13996800	-2.54530300	11.92148200
H	13.20676200	-2.92512200	10.90019700
H	13.89760600	-1.76604400	12.02582800
H	13.35276800	-3.35082200	12.62156100
C	9.67549100	-1.90365100	13.41920900

29

B3lYP-D3/def2-TZVP, toluene, Lowest_Frequency_27.7

Co	9.866895	-0.000001	11.314170
C	8.783206	2.419142	9.469949
O	8.271952	0.989598	11.289518
O	10.601457	0.954058	9.860909
H	8.419891	3.226420	8.852586
C	10.897618	2.472278	8.098050
H	11.153920	1.674682	7.398223
H	11.833722	2.851186	8.512864
H	10.390058	3.272878	7.563643
C	7.962824	1.937860	10.487754
C	6.600145	2.532094	10.715121

H	6.541225	2.910400	11.737596
H	5.847892	1.746579	10.618748
H	6.374372	3.336471	10.017831
C	10.060809	1.901915	9.211612
O	11.461837	-0.989600	11.338821
O	9.132333	-0.954060	12.767431
C	10.950584	-2.419144	13.158391
H	11.313898	-3.226422	13.775754
C	8.836172	-2.472280	14.530290
H	8.579870	-1.674684	15.230118
H	7.900068	-2.851188	14.115477
H	9.343732	-3.272880	15.064697
C	11.770966	-1.937862	12.140585
C	13.133645	-2.532096	11.913219
H	13.192564	-2.910403	10.890744
H	13.885897	-1.746581	12.009591
H	13.359417	-3.336474	12.610509
C	9.672981	-1.901916	13.416728

29

B3LYP-D3/def2-TZVPP, Lowest_Frequency_36.7

O	8.25631400	0.99401700	11.29277200
O	10.61124300	0.95987300	9.86262100
C	8.78006100	2.41176600	9.46695900
H	8.41523200	3.21648600	8.84706500
C	10.89599600	2.47778100	8.10168000
H	11.14994000	1.68185200	7.39899200
H	11.83393900	2.85059700	8.51767100
H	10.39061900	3.28220300	7.57047600
C	7.95565300	1.93360700	10.49139000
C	6.59510500	2.54044800	10.71385700
H	6.54056800	2.92927400	11.73250300
H	5.83772300	1.75904500	10.62712800
H	6.37330100	3.33968700	10.00909100
C	10.05873700	1.90307700	9.21412500
O	11.47747500	-0.99402000	11.33556700
O	9.12254600	-0.95987600	12.76571800
C	10.95372900	-2.41176900	13.16138000
H	11.31855800	-3.21648800	13.78127500
C	8.83779400	-2.47778300	14.52666000
H	8.58385100	-1.68185300	15.22934800
H	7.89985100	-2.85059900	14.11067000
H	9.34317100	-3.28220400	15.05786500
C	11.77813500	-1.93361000	12.13694800
C	13.13868400	-2.54045000	11.91448300
H	13.19322300	-2.92927700	10.89583800
H	13.89606600	-1.75904600	12.00121200
H	13.36049000	-3.33968800	12.61925000
C	9.67505200	-1.90308100	13.41421400
Co	9.86689500	-0.00000100	11.31417000

29

B3LYP-D3/def2-TZVPP, Lowest_Frequency_36.7

Co	9.86689500	-0.00000100	11.31417000
C	8.77411300	2.40102700	9.45680300
O	8.26309200	0.99882100	11.29731800
O	10.61244000	0.96432600	9.87046700
H	8.40583400	3.19875600	8.83119200
C	10.89871000	2.47760100	8.10507000
H	11.16375200	1.68180300	7.40758100
H	11.83022300	2.85835000	8.52622300
H	10.39232800	3.27604200	7.56747800
C	7.95581300	1.93151900	10.48974600
C	6.59750000	2.54103700	10.71757500
H	6.55095500	2.93807700	11.73260000
H	5.83945200	1.76007400	10.64361800
H	6.37037900	3.33407200	10.00874200
C	10.05757100	1.90063700	9.21322600
O	11.47069800	-0.99882300	11.33102200
O	9.12134900	-0.96432800	12.75787200
C	10.95967700	-2.40102900	13.17153600
H	11.32795600	-3.19875800	13.79714800
C	8.83508000	-2.47760300	14.52327000
H	8.57003800	-1.68180400	15.22075900
H	7.90356700	-2.85835200	14.10211800
H	9.34146200	-3.27604400	15.06086200
C	11.77797600	-1.93152200	12.13859300
C	13.13629000	-2.54103800	11.91076500
H	13.18283600	-2.93807900	10.89574000
H	13.89433700	-1.76007500	11.98472300
H	13.36341100	-3.33407300	12.61959900
C	9.67621800	-1.90064000	13.41511300

29

B3LYP*-D3/def2-TZVP, Lowest_Frequency_87.2

Co	9.866895	-0.000001	11.314170
C	8.762504	2.464313	9.436179
O	8.244851	1.005518	11.276985
O	10.602979	0.970937	9.844869
H	8.392471	3.290069	8.806972
C	10.920886	2.504905	8.049840
H	11.170290	1.683467	7.336853
H	11.882521	2.873066	8.479981
H	10.415284	3.332191	7.503918
C	7.928889	1.964228	10.475833
C	6.538861	2.569537	10.711498
H	6.485766	2.953488	11.757960
H	5.773623	1.762977	10.615721
H	6.305015	3.392283	9.999832
C	10.058311	1.932921	9.182495
O	11.488939	-1.005520	11.351354
O	9.130811	-0.970940	12.783471
C	10.971286	-2.464315	13.192162
H	11.341319	-3.290071	13.821368
C	8.812904	-2.504907	14.578500
H	8.563498	-1.683469	15.291486
H	7.851269	-2.873069	14.148358
H	9.318506	-3.332192	15.124423
C	11.804901	-1.964230	12.152507
C	13.194929	-2.569539	11.916842
H	13.248024	-2.953491	10.870380
H	13.960167	-1.762979	12.012619
H	13.428774	-3.392285	12.628508
C	9.675479	-1.932923	13.445845

29
B3LYP*/def2-TZVP, Lowest_Frequency_32.2

Co	9.866895	-0.000001	11.314170
C	8.784620	2.414864	9.473809
O	8.275282	0.980364	11.284381
O	10.594954	0.946350	9.875578
H	8.422155	3.223570	8.857522
C	10.901636	2.460417	8.108240
H	11.147733	1.664162	7.402933
H	11.843873	2.826987	8.520372
H	10.401055	3.268857	7.578798
C	7.962286	1.927869	10.492916
C	6.598573	2.523855	10.721902
H	6.538466	2.906341	11.742757
H	5.842251	1.742228	10.626697
H	6.376554	3.327425	10.022302
C	10.057280	1.897089	9.220472
O	11.458508	-0.980366	11.343959
O	9.138835	-0.946352	12.752762
C	10.949169	-2.414866	13.154531
H	11.311635	-3.223572	13.770818
C	8.832154	-2.460419	14.520100
H	8.586057	-1.664164	15.225407
H	7.889917	-2.826989	14.107968
H	9.332735	-3.268859	15.049542
C	11.771504	-1.927872	12.135424
C	13.135216	-2.523857	11.906438
H	13.195324	-2.906343	10.885583
H	13.891539	-1.742230	12.001644
H	13.357235	-3.327427	12.606038
C	9.676509	-1.897091	13.407868

29
B3PW91-D3/def2-TZVP, Lowest_Frequency_27.5

Co	9.86689500	-0.00000100	11.31417000
C	8.78781900	2.40779800	9.47912500
O	8.28005000	0.97276000	11.28935500
O	10.59846100	0.94300300	9.87673400
H	8.42488000	3.21727600	8.86234600
C	10.90352800	2.45052400	8.11719200
H	11.14887600	1.65077500	7.41489800
H	11.84582200	2.81401600	8.53307200
H	10.40610900	3.26005000	7.58504000
C	7.97105700	1.92065300	10.49494800
C	6.61143500	2.51056500	10.72766800
H	6.55714200	2.88636800	11.75194500
H	5.86085500	1.72229900	10.63508200
H	6.37984600	3.31615500	10.03245300
C	10.06276500	1.88780000	9.22661900
O	11.45374000	-0.97276200	11.33898500
O	9.13532900	-0.94300500	12.75160600
C	10.94597100	-2.40780000	13.14921500
H	11.30891000	-3.21727800	13.76599400
C	8.83026200	-2.45052600	14.51114800
H	8.58491400	-1.65077700	15.21344200
H	7.88796800	-2.81401700	14.09526800
H	9.32768100	-3.26005200	15.04330000
C	11.76273300	-1.92065500	12.13339200
C	13.12235400	-2.51056700	11.90067200
H	13.17664700	-2.88637100	10.87639400
H	13.87293500	-1.72230100	11.99325800
H	13.35394400	-3.31615700	12.59588700
C	9.67102500	-1.88780200	13.40172200

29
BLYP-D3/def2-TZVP, Lowest_Frequency_28.6

Co	9.86689500	-0.00000100	11.31417000
C	8.78102100	2.42277000	9.46768000
O	8.26883900	0.97327700	11.29569600
O	10.60784600	0.93903500	9.87522100
H	8.41622300	3.23667400	8.84739600
C	10.92200400	2.46149300	8.09450800
H	11.16928500	1.65738500	7.38831000
H	11.86959000	2.82720300	8.51257800
H	10.42733900	3.27609300	7.55501900
C	7.95164900	1.93484600	10.49216600
C	6.57701500	2.52551100	10.73360200
H	6.51982700	2.90753300	11.76183100
H	5.81923300	1.73598400	10.63953700
H	6.34332000	3.33525000	10.03430300
C	10.06169400	1.90387800	9.21063000
O	11.46495100	-0.97327900	11.33264400
O	9.12594300	-0.93903700	12.75311800
C	10.95276900	-2.42277200	13.16066000
H	11.31756600	-3.23667600	13.78094400
C	8.81178600	-2.46149500	14.53383200
H	8.56450400	-1.65738700	15.24003000
H	7.86420000	-2.82720500	14.11576200
H	9.30645100	-3.27609500	15.07332100
C	11.78214000	-1.93484800	12.13617400
C	13.15677500	-2.52551300	11.89473800
H	13.21396300	-2.90753500	10.86650900
H	13.91455700	-1.73598600	11.98880300
H	13.39047000	-3.33525200	12.59403700
C	9.67209600	-1.90388000	13.41771000

29
BP86-D3/def2-TZVP, Lowest_Frequency_28.4

Co	9.86689500	-0.00000100	11.31417000
C	8.78807000	2.40709600	9.47966500
O	8.28294100	0.95754500	11.30355400
O	10.60794500	0.92344100	9.89149900
H	8.42231900	3.22307100	8.85777400
C	10.92505800	2.43941600	8.11572700
H	11.17289800	1.63289200	7.40919300
H	11.87475400	2.80406000	8.53545600
H	10.43050300	3.25588600	7.57484500
C	7.96298700	1.91741000	10.50340000
C	6.59395900	2.50321800	10.74637500
H	6.53723700	2.88426300	11.77723300
H	5.83560300	1.71125500	10.65273800
H	6.35898400	3.31479200	10.04645400
C	10.06605400	1.88652400	9.22607100

O	11.45084900	-0.95754800	11.32478500
O	9.12584500	-0.92344400	12.73684000
C	10.94572000	-2.40709800	13.14867500
H	11.31147100	-3.22307300	13.77056600
C	8.80873200	-2.43941800	14.51261300
H	8.56089200	-1.63289400	15.21914700
H	7.85903600	-2.80406200	14.09288400
H	9.30328700	-3.25588800	15.05349500
C	11.77080300	-1.91741300	12.12494000
C	13.13983100	-2.50322000	11.88196500
H	13.19655300	-2.88426500	10.85110700
H	13.89818700	-1.71125700	11.97560100
H	13.37480600	-3.31479400	12.58188600
C	9.66773500	-1.88652600	13.40226900

29

CAM-B3LYP-D3BJ/def2-TZVP, Lowest_Frequency_33.9

Co	9.86689500	-0.00000200	11.31416900
C	8.78902900	2.40516700	9.48127800
O	8.28690200	0.97495300	11.28319700
O	10.58842400	0.94114100	9.88535500
H	8.42696400	3.21298300	8.86564100
C	10.89903700	2.44456200	8.12545900
H	11.14026900	1.64553100	7.42409100
H	11.84035700	2.80434900	8.54131500
H	10.40253900	3.25416000	7.59652700
C	7.97290900	1.91730200	10.49742800
C	6.61476200	2.50778900	10.72781500
H	6.55799000	2.88268800	11.74992000
H	5.86405500	1.72337800	10.62936500
H	6.39159100	3.31311200	10.03256300
C	10.05616200	1.88664100	9.23207300
O	11.44688700	-0.97495700	11.34514200
O	9.14536600	-0.94114400	12.74298400
C	10.94476100	-2.40517000	13.14706100
H	11.30682600	-3.21298500	13.76270000
C	8.83475200	-2.44456400	14.50288100
H	8.59352200	-1.64553200	15.20424900
H	7.89343300	-2.80435100	14.08702600
H	9.33125100	-3.25416100	15.03181400
C	11.76088000	-1.91730600	12.13091000
C	13.11902800	-2.50779000	11.90052600
H	13.17580200	-2.88269000	10.87842100
H	13.86973400	-1.72337800	11.99897500
H	13.34220000	-3.31311200	12.59577800
C	9.67762700	-1.88664400	13.39626600

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CAM-B3LYP-D3/def2-TZVP,Lowest_Frequency_33.8

Co	9.86689500	-0.00000100	11.31417000
C	8.78747000	2.40833500	9.47863200
O	8.28651800	0.97673600	11.28119600
O	10.58687000	0.94294600	9.88408000
H	8.42535200	3.21627000	8.86289200
C	10.90171500	2.44416800	8.12509900
H	11.14562700	1.64142000	7.42894600
H	11.84123100	2.80344300	8.54552200
H	10.40978600	3.25278600	7.58999600
C	7.97207200	1.91949000	10.49557600
C	6.61317700	2.50742100	10.72999500
H	6.56139200	2.88204600	11.75249700
H	5.86582700	1.71920300	10.63674400
H	6.38225800	3.31171100	10.03574600
C	10.05495800	1.88884300	9.23046000
O	11.44727300	-0.97673800	11.34714500
O	9.14692000	-0.94294700	12.74426000
C	10.94632000	-2.40833700	13.14970800
H	11.30843700	-3.21627300	13.76544700
C	8.83207400	-2.44417100	14.50324000
H	8.58816400	-1.64142300	15.19939400
H	7.89255700	-2.80344400	14.08281700
H	9.32400200	-3.25279000	15.03834200
C	11.76171800	-1.91949100	12.13276400
C	13.12061300	-2.50742300	11.89834600
H	13.17239900	-2.88204500	10.87584300
H	13.86796300	-1.71920400	11.99159900
H	13.35153200	-3.31171400	12.59259300
C	9.67883100	-1.88884600	13.39788000

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CAM-B3LYP/def2-TZVP, Lowest_Frequency_33.8

Co	9.86689500	-0.00000100	11.31417000
C	8.78774300	2.40763200	9.47910500
O	8.28595300	0.97699000	11.28120500
O	10.58713900	0.94319100	9.88358200
H	8.42562100	3.21554600	8.86337100
C	10.89893100	2.44766500	8.12298900
H	11.14290000	1.64883300	7.42221800
H	11.83930100	2.81015900	8.53894700
H	10.40169600	3.25590300	7.59247700
C	7.97137500	1.91972300	10.49566000
C	6.61265900	2.51088500	10.72650300
H	6.55659600	2.88884000	11.74764800
H	5.86126700	1.72663900	10.63115300
H	6.38824800	3.31459500	10.02963900
C	10.05535400	1.88906400	9.22987800
O	11.44783700	-0.97699100	11.34713600
O	9.14665200	-0.94319200	12.74475800
C	10.94604600	-2.40763400	13.14923500
H	11.30816800	-3.21554900	13.76496900
C	8.83485800	-2.44766800	14.50535000
H	8.59089000	-1.64883700	15.20612200
H	7.89448700	-2.81016100	14.08939100
H	9.33209300	-3.25590700	15.03586100
C	11.76241500	-1.91972500	12.13268100
C	13.12113100	-2.51088600	11.90183800
H	13.17719500	-2.88883900	10.88069100
H	13.87252300	-1.72664000	11.99719000
H	13.34554100	-3.31459800	12.59870100
C	9.67843600	-1.88906700	13.39846200

29

M05-D3/def2-TZVP, Lowest_Frequency_30.7

Co	9.86689500	-0.00000100	11.31417000

C	8.78486600	2.42332700	9.47411100
O	8.25502800	0.96788100	11.25811800
O	10.58043000	0.93356500	9.84554800
H	8.42838900	3.24181600	8.86737400
C	10.89140000	2.46104700	8.10758700
H	11.12491800	1.66946900	7.39438400
H	11.83949300	2.80615100	8.52210600
H	10.40334700	3.28258900	7.58860700
C	7.95867800	1.92351500	10.48464400
C	6.60275800	2.52454400	10.71268200
H	6.54086100	2.88374800	11.74075600
H	5.84510500	1.74791500	10.60042500
H	6.38541100	3.34266100	10.03012000
C	10.05130100	1.89260300	9.21342300
O	11.47876200	-0.96788300	11.37022200
O	9.15336000	-0.93356800	12.78279200
C	10.94892400	-2.42332900	13.15422900
H	11.30540100	-3.24181800	13.76096600
C	8.84239000	-2.46104900	14.52075300
H	8.60887000	-1.66947100	15.23395500
H	7.89429800	-2.80615400	14.10623300
H	9.33044300	-3.28259000	15.03973300
C	11.77511100	-1.92351700	12.14369600
C	13.13103200	-2.52454500	11.91565800
H	13.19293000	-2.88374900	10.88758400
H	13.88868500	-1.74791700	12.02791500
H	13.34837800	-3.34266300	12.59822000
C	9.68248900	-1.89260500	13.41491700

29

M06-D3/def2-TZVP, Lowest_Frequency_35.9

Co	9.86689500	-0.00000100	11.31417000
C	8.80789000	2.42542300	9.51178200
O	8.25383600	0.95691200	11.27380900
O	10.59505700	0.92273400	9.85220700
H	8.45541200	3.25322500	8.91145700
C	10.88125200	2.44520200	8.11366600
H	11.09462000	1.65270000	7.39373500
H	11.84216500	2.78357600	8.50606400
H	10.38614600	3.27117500	7.60578100
C	7.97044300	1.91658100	10.50244000
C	6.61251700	2.50820900	10.70655800
H	6.52573900	2.86258500	11.73550900
H	5.85817300	1.73001800	10.57507700
H	6.40764400	3.32960500	10.02198700
C	10.06185300	1.88588400	9.23230600
O	11.47995500	-0.95691300	11.35453200
O	9.13873300	-0.92273600	12.77613400
C	10.92589900	-2.42542500	13.11655800
H	11.27837800	-3.25322800	13.71688300
C	8.85253700	-2.44520500	14.51467400
H	8.63917000	-1.65270200	15.23460500
H	7.89162500	-2.78357700	14.12227500
H	9.34764300	-3.27117700	15.02255800
C	11.76334700	-1.91658200	12.12590000
C	13.12127300	-2.50821100	11.92178200
H	13.20805100	-2.86258700	10.89283100
H	13.87561700	-1.73002000	12.05326300
H	13.32614500	-3.32960800	12.60635200
C	9.67193700	-1.88588600	13.39603400

29

PBE0-D3/def2-TZVP, Lowest_Frequency_37.7

Co	9.86686400	-0.00005400	11.31411900
C	8.79015800	2.40249100	9.48320400
O	8.26365200	0.97804200	11.29387200
O	10.60860300	0.94350100	9.86955800
H	8.42732600	3.21217300	8.86627100
C	10.89134900	2.45816800	8.11648300
H	11.13785600	1.66214600	7.41010600
H	11.83452600	2.82508600	8.52778400
H	10.38490400	3.26648800	7.59107900
C	7.96606600	1.91797100	10.50081200
C	6.61072300	2.52154400	10.71677900
H	6.54954500	2.90436600	11.73810000
H	5.85316100	1.74027500	10.62142900
H	6.39505300	3.32487800	10.01389000
C	10.06228000	1.88704700	9.22749500
O	11.47015800	-0.97801100	11.33450100
O	9.12508800	-0.94366800	12.75862200
C	10.94364400	-2.40247200	13.14515700
H	11.30650400	-3.21210800	13.76213400
C	8.84234000	-2.45833700	14.51169600
H	8.59569300	-1.66232800	15.21804000
H	7.89923600	-2.82535400	14.10031800
H	9.34882000	-3.26659800	15.03715700
C	11.76776900	-1.91789800	12.12760100
C	13.12318000	-2.52135700	11.91174400
H	13.18446900	-2.90418800	10.89043300
H	13.88066800	-1.74002100	12.00714000
H	13.33886700	-3.32466200	12.61466100
C	9.67144900	-1.88715000	13.40074800

29

TPSSh-D3/def2-TZVP, Lowest_Frequency_25.4

O	8.28934500	0.96274400	11.29642300
O	10.60008000	0.93095500	9.89170000
C	8.79084400	2.40791500	9.48379900
H	8.42803700	3.21887100	8.86722300
C	10.92079400	2.43695700	8.12551400
H	11.16396700	1.63026700	7.42968400
H	11.86188300	2.79539200	8.54971600
H	10.43218100	3.24835100	7.58593600
C	7.97319600	1.91725900	10.50255600
C	6.60773300	2.49971200	10.74800700
H	6.55954000	2.87048500	11.77483400
H	5.86159700	1.70691900	10.65349700
H	6.36978900	3.30842900	10.05692700
C	10.06362600	1.88575000	9.23308500
O	11.44504700	-0.96174000	11.33289800
O	9.13392000	-0.93065300	12.73698100
C	10.94323000	-2.40740000	13.14499100
H	11.30585200	-3.21868100	13.76124900
C	8.81176400	-2.43905200	14.50083000

H	8.56842900	-1.63356800	15.19800600
H	7.87083500	-2.79629300	14.07528300
H	9.29966100	-3.25165100	15.03924100
C	11.76124400	-1.91614400	12.12683300
C	13.12695300	-2.49819000	11.88179000
H	13.17520600	-2.86987400	10.85528800
H	13.87274200	-1.70498600	11.97551000
H	13.36530100	-3.30621100	12.57354400
C	9.66996100	-1.88609600	13.39492600
Co	9.86719500	0.00050300	11.31466100

Section 3: Transition State 1 Geometries

29

B3LYP-D3/6-311g(d,p)+6-31g(d,p), Lowest_Frequency -30

O	8.263047	1.130786	11.340156
O	10.652686	1.095654	9.888476
C	8.757307	2.467295	9.428335
H	8.368286	3.233701	8.769435
C	10.870542	2.552519	8.050145
H	11.163678	1.734265	7.384314
H	11.794734	2.984207	8.448119
H	10.333589	3.311592	7.477509
C	7.940738	2.019514	10.482517
C	6.562757	2.615836	10.667013
H	6.499467	3.062269	11.664792
H	5.819358	1.812801	10.631097
H	6.318255	3.370432	9.916531
C	10.059224	1.988397	9.195559
O	11.470816	-1.130700	11.288267
O	9.081052	-1.095765	12.739745
C	10.976480	-2.467295	13.200010
H	11.365496	-3.233694	13.858920
C	8.863128	-2.552709	14.578006
H	8.569874	-1.734498	15.243836
H	7.939001	-2.984448	14.179933
H	9.400080	-3.311764	15.150666
C	11.793113	-2.019426	12.145910
C	13.171152	-2.615646	11.961522
H	13.234562	-3.062046	10.963735
H	13.914492	-1.812560	11.997528
H	13.415639	-3.370247	12.712003
C	9.674512	-1.988495	13.432686
Co	9.866885	-0.000007	11.314169

29

B3LYP-D3/def2-SVP, Lowest_Frequency -29

O	8.207552	1.074354	11.230682
O	10.579818	1.039404	9.789367
C	8.745450	2.504315	9.407941
H	8.379580	3.321181	8.785990
C	10.860049	2.570480	8.022669
H	11.113000	1.767102	7.312165
H	11.813039	2.937048	8.436991
H	10.355146	3.386454	7.488225
C	7.908768	2.019296	10.433604
C	6.543484	2.633684	10.644602
H	6.479756	3.015352	11.676343
H	5.779411	1.845119	10.551997
H	6.319380	3.445362	9.939392
C	10.030539	1.988177	9.144631
O	11.526238	-1.074357	11.397657
O	9.153972	-1.039406	12.838974
C	10.988340	-2.504317	13.220399
H	11.354210	-3.321184	13.842350
C	8.873741	-2.570481	14.605673
H	8.620796	-1.767104	15.316179
H	7.920749	-2.937044	14.191352
H	9.378642	-3.386458	15.140113
C	11.825022	-2.019298	12.194736
C	13.190305	-2.633688	11.983737
H	13.254030	-3.015361	10.951998
H	13.954378	-1.845122	12.076336
H	13.414411	-3.445363	12.688950
C	9.703251	-1.988178	13.483710
Co	9.866895	-0.000001	11.314170

29

B3LYP-D3/def2-TZVP, Lowest_Frequency -21

O	8.210558	1.077820	11.236325
O	10.581525	1.033878	9.790105
C	8.755301	2.498753	9.418891
H	8.395124	3.309688	8.803810
C	10.853511	2.564898	8.029184
H	11.095584	1.771379	7.319424
H	11.798613	2.930271	8.435841
H	10.346097	3.374808	7.507967
C	7.919820	2.023445	10.438147
C	6.562716	2.645227	10.647363
H	6.502740	3.030231	11.667264
H	5.799390	1.870449	10.551992
H	6.353080	3.449029	9.943775
C	10.030420	1.984055	9.150456
O	11.525218	-1.071142	11.395653
O	9.147032	-1.044311	12.831322
C	10.978992	-2.501352	13.205441
H	11.340370	-3.312793	13.819150
C	8.874596	-2.583725	14.584828
H	8.624616	-1.794145	15.296226
H	7.933559	-2.952813	14.172145
H	9.383864	-3.392745	15.105615
C	11.816914	-2.018092	12.191813
C	13.178006	-2.632519	11.986734
H	13.244388	-3.013970	10.965879
H	13.937067	-1.854332	12.087952
H	13.388458	-3.437541	12.688682
C	9.700041	-1.994285	13.469812
Co	9.865183	-0.000659	11.314607

29

CAM-B3LYP-D3/def2-SVP, Lowest_Frequency -31

O	8.219220	1.068713	11.228836
O	10.572827	1.034182	9.799035
C	8.749486	2.495399	9.414756

H	8.384021	3.311545	8.793482
C	10.858010	2.556442	8.038465
H	11.108974	1.751694	7.331543
H	11.808653	2.920685	8.455537
H	10.354213	3.371459	7.504448
C	7.918582	2.009670	10.437354
C	6.558190	2.619381	10.650280
H	6.497962	2.998432	11.681317
H	5.798132	1.829424	10.557428
H	6.333974	3.430285	9.946436
C	10.029215	1.978766	9.155211
O	11.514568	-1.068718	11.399501
O	9.160964	-1.034181	12.829308
C	10.984304	-2.495401	13.213584
H	11.349768	-3.311547	13.834858
C	8.875784	-2.556439	14.589881
H	8.624836	-1.751691	15.296810
H	7.925132	-2.920667	14.172814
H	9.379575	-3.371465	15.123889
C	11.815206	-2.009675	12.190984
C	13.175596	-2.619389	11.978054
H	13.235815	-2.998454	10.947022
H	13.935655	-1.829431	12.070889
H	13.399818	-3.430284	12.681907
C	9.704576	-1.978766	13.473131
Co	9.866895	-0.000001	11.314170

Section 4: Transition State 2 Geometries

29

B3lYP-D3/6-311g(d,p)+6-31g(d,p), Lowest_Frequency -130

O	7.952058	0.314815	10.381596
O	10.530584	1.407715	10.760765
C	8.754979	2.382964	9.498361
H	8.482606	3.239847	8.894868
C	11.018495	3.477691	9.752731
H	11.910712	3.077892	9.260136
H	11.345420	3.912926	10.702579
H	10.581676	4.259793	9.128741
C	7.787009	1.386995	9.695535
C	6.417621	1.532179	9.074011
H	5.660811	1.508816	9.864942
H	6.226385	0.672514	8.423417
H	6.308194	2.452553	8.497163
C	10.059049	2.343332	10.033395
O	10.616285	-1.708871	10.868241
O	9.704716	-0.364881	13.191926
C	11.022451	-2.354598	13.130364
H	11.512850	-3.094726	13.750816
C	10.282913	-1.274367	15.288295
H	10.715347	-0.329047	15.632283
H	9.238495	-1.285622	15.616913
H	10.816418	-2.105197	15.754694
C	11.127900	-2.496551	11.734062
C	11.903232	-3.662136	11.159288
H	11.245395	-4.241241	10.502939
H	12.716867	-3.276860	10.535959
H	12.317661	-4.320198	11.925860
C	10.326688	-1.315500	13.776184
Co	9.557136	-0.140269	11.274860

29

B3LYP-D3/def2-SVP, Lowest_Frequency -106

O	8.297116	0.349193	10.490931
O	10.742154	1.738609	10.648155
C	8.794450	2.443982	9.469926
H	8.382326	3.237089	8.846476
C	10.928160	3.797056	9.524871
H	11.835476	3.469465	8.992241
H	11.265111	4.310692	10.439675
H	10.368576	4.501254	8.895063
C	7.959990	1.346433	9.778473
C	6.546799	1.304811	9.245081
H	5.847222	1.230032	10.093023
H	6.418344	0.389408	8.645456
H	6.289576	2.180740	8.634917
C	10.122561	2.580583	9.914356
O	10.827174	-1.634883	10.914866
O	9.913770	-0.288654	13.229257
C	10.908379	-2.453309	13.151944
H	11.213609	-3.300983	13.765479
C	10.147677	-1.372493	15.306406
H	10.673566	-0.507840	15.742431
H	9.078767	-1.245078	15.542087
H	10.516294	-2.296706	15.771341
C	11.130648	-2.536051	11.760967
C	11.776990	-3.773110	11.179089
H	11.095074	-4.215132	10.434811
H	12.689651	-3.477835	10.636714
H	12.029883	-4.527693	11.935965
C	10.323934	-1.347262	13.804756
Co	10.016675	0.097649	11.316171

29

B3LYP-D3/def2-TZVP, Lowest_Frequency -123

O	7.997033	0.342351	10.377255
O	10.548362	1.480991	10.721906
C	8.751384	2.405586	9.474486
H	8.458797	3.249341	8.868037
C	10.987931	3.543205	9.695603
H	11.879136	3.155521	9.198404
H	11.312923	3.991086	10.636618
H	10.528412	4.306806	9.071010
C	7.805203	1.399098	9.686633
C	6.432900	1.513892	9.078218
H	5.687149	1.484590	9.875122
H	6.254163	0.647565	8.438234
H	6.306031	2.425316	8.497258
C	10.056559	2.397083	9.994754
O	10.666418	-1.715580	10.899826
O	9.754214	-0.369873	13.212470
C	11.019110	-2.379243	13.152900
H	11.478934	-3.133892	13.773382
C	10.272104	-1.307249	15.303269

H 10.716062 -0.376041 15.660853
H 9.224663 -1.303161 15.611418
H 10.781377 -2.151108 15.765288
C 11.142676 -2.518561 11.762807
C 11.892826 -3.697190 11.195665
H 11.228090 -4.256317 10.534156
H 12.719867 -3.329871 10.584758
H 12.279937 -4.362421 11.965422
C 10.340112 -1.334805 13.797229
Co 9.617580 -0.107152 11.277947

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CAM-B3LYP-D3/def2-SVP, Lowest_Frequency -100
O 8.302772 0.351112 10.492303
O 10.731900 1.727871 10.650590
C 8.796632 2.436603 9.474919
H 8.386172 3.229590 8.851969
C 10.924732 3.778576 9.534350
H 11.829968 3.447328 9.004028
H 11.259618 4.288038 10.450165
H 10.367217 4.482760 8.905075
C 7.965959 1.342522 9.783073
C 6.558462 1.301120 9.251610
H 5.861976 1.226592 10.099901
H 6.432786 0.386282 8.653676
H 6.302956 2.176363 8.642204
C 10.119032 2.568349 9.920119
O 10.824516 -1.626563 10.921665
O 9.917865 -0.290175 13.219373
C 10.908821 -2.445361 13.147517
H 11.214340 -3.291977 13.760478
C 10.146877 -1.365797 15.289955
H 10.671207 -0.500780 15.722695
H 9.078538 -1.239105 15.520400
H 10.515381 -2.288597 15.754415
C 11.127618 -2.525177 11.761453
C 11.769407 -3.756766 11.178842
H 11.084730 -4.194959 10.437423
H 12.679034 -3.459206 10.636180
H 12.022636 -4.510228 11.934652
C 10.325235 -1.342638 13.794698
Co 10.013562 0.094189 11.317201