

SUPPORTING INFORMATION

Substituent Effects on Excited State Proton Transfer in 2'- Hydroxylchalcone

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SECTION S1. VERTICAL EXCITATIONS

Table S1: Vertical excitation energies (in eV), excitation assignment, and labelling of orbitals, for the first three singlet excitations for systems **1-5** at ADC(2)/def2-TZVP and CC2/def2-TZVP levels of theory.

1						
	ADC(2)/def2-TZVP			RI-CC2/def2-TZVP		
	ΔE (f)	Character	Orbitals	ΔE (f)	Character	Orbitals
S_1	3.36 (0.869)	$\pi\pi^*$	H-L (82%)	3.43 (1.135)	$\pi\pi^*$	H-L (88%)
S_2	3.44 (0.090)	$n\pi^*$	H-5-L (76%)	3.67 (0.009)	$n\pi^*$	H-5-L (84%)
S_3	3.77 (0.008)	$\pi\pi^*$	H-1-L (78%)	3.84 (0.003)	$\pi\pi^*$	H-1-L (78%)
2						
	ADC(2)/def2-TZVP			RI-CC2/def2-TZVP		
	ΔE (f)	Character	Orbitals	ΔE (f)	Character	Orbitals
S_1	3.38 (0.806)	$\pi\pi^*$	H-L (74%)	3.45 (1.167)	$\pi\pi^*$	H-L (88%)
S_2	3.46 (0.196)	$n\pi^*$	H-5-L (67%)	3.68 (0.023)	$n\pi^*$	H-5-L (83%)
S_3	3.77 (0.007)	$\pi\pi^*$	H-1-L (77%)	3.85 (0.005)	$\pi\pi^*$	H-1-L (76%)
3						
	ADC(2)/def2-TZVP			RI-CC2/def2-TZVP		
	ΔE (f)	Character	Orbitals	ΔE (f)	Character	Orbitals
S_1	3.40 (1.063)	$\pi\pi^*$	H-L (90%)	3.47 (1.286)	$\pi\pi^*$	H-L (90%)
S_2	3.51 (0.013)	$n\pi^*$	H-5-L (82%)	3.75 (0.002)	$n\pi^*$	H-5 - L (85%)
S_3	3.86 (0.038)	$\pi\pi^*$	H-1-L (79%)	3.96 (0.034)	$\pi\pi^*$	H-1-L (78%)
4						
	ADC(2)/def2-TZVP			RI-CC2/def2-TZVP		
	ΔE (f)	Character	Orbitals	ΔE (f)	Character	Orbitals
S_1	3.36 (0.857)	$\pi\pi^*$	H-L (79%)	3.42 (1.105)	$\pi\pi^*$	H-L (84%)
S_2	3.42 (0.096)	$n\pi^*$	H-5-L (74%)	3.65 (0.005)	$n\pi^*$	H-5-L (83%)
S_3	3.65 (0.008)	$\pi\pi^*$	H-1-L (78%)	3.72 (0.028)	$\pi\pi^*$	H-1-L (75%)
5						
	ADC(2)/def2-TZVP			RI-CC2/def2-TZVP		
	ΔE (f)	Character	Orbitals	ΔE (f)	Character	Orbitals
S_1	3.20 (0.522)	$\pi\pi^*$	H-L (57%)	3.26 (0.633)	$\pi\pi^*$	H-L (59%)
S_2	3.39 (0.066)	$n\pi^*$	H-5-L (61%)	3.54 (0.390)	$\pi\pi^*$	H-1-L (52%)
S_3	3.50 (0.358)	$\pi\pi^*$	H-1-L (38%)	3.66 (0.094)	$n\pi^*$	H-5-L (73%)

Table S2: Vertical excitation energies (in eV) for the first three singlet excitations for dimers of systems **1** at ADC(2)/def2-SV(P) and ADC(2)/def2-TZVP levels of theory.

Dimers Compound 1						
	Dimer 1			Dimer 2		
	ADC(2)/def2-SV(P)			ADC(2)/def2-SV(P)		
	ΔE (eV)	f	Orbitals	ΔE (eV)	f	Orbitals
S_1	3.18	0.030	H-L (36%)	3.34	0.036	H-L (90%)
S_2	3.35	1.640	H-1-L+1 (32%)	3.36	0.423	H-1-L (82%)
S_3	3.57	0.007	H-10-L (51%)	3.48	1.322	H-L+1 (77%)
	ADC(2)/def2-TZVP			ADC(2)/def2-TZVP		
	ΔE (eV)	f	Orbitals	ΔE (eV)	f	Orbitals
	ΔE (eV)	f	Orbitals	ΔE (eV)	f	Orbitals
S_1	2.99	0.032	H-L (45%)	3.11	0.022	H-L (91%)
S_2	3.16	1.551	H-1-L+1 (42%)	3.19	0.282	H-1-L (78%)
S_3	3.45	0.004	H-10-L (63%)	3.28	1.405	H-L+1 (76%)

Two edge-face dimer configurations were cut from the crystal structure of **1** (CCDC code 94199¹) and optimized at ω B97X-D/6-31G(d) level of theory with the Gaussian 09 program package.² Ten non-H atoms of each monomer (9xC,1xN in fragment B (Figure 1, main text)) were frozen to maintain the edge-face packing mode. The geometry of each dimer is given in Section 8 (pages 50-51). Vertical excitations were calculated as for the monomers at ADC(2)/def2-SV(P) and ADC(2)/def2-TZVP with the Turbomole package as per the monomers in the main text.

SECTION S2: RELATIVE ENERGIES OF STATES

Table S3: Relative S_0 and S_1 energies of important geometries of compounds **1-5** at ADC/def2-SV(P), ADC/def2-TZVP and CC2/def2-TZVP levels of theory. In each case, the dihedral angle and energies of the most stable conformation is reported

1															
	ADC/def2-SV(P)					ADC/def2-TZVP					CC2/def2-TZVP				
	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI
S_0	0.00	1.31	2.86	1.99	2.31	0.00	1.37	2.82	1.85	2.32	0.00	1.26	2.94	1.61	2.44
S_1	3.53	2.64	2.89	2.30	2.33	3.36	2.63	2.84	2.29	2.33	3.43	2.89	3.01	2.43	2.45
Angle (°)	-11.0	-45.7	-59.20	-49.0	-57.6	-7.5	-44.3	-61.8	-44.3	-56.9	-11.0	-43.7	-123.8	-49.8	-78.3
2															
	ADC/def2-SV(P)					ADC/def2-TZVP					CC2/def2-TZVP				
	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI
S_0	0.00	1.40	2.93	2.05	2.37	0.00	1.40	2.81	1.82	2.29	0.00	1.30	3.22	1.54	2.65
S_1	3.53	2.72	2.93	2.37	2.39	3.38	2.64	2.83	2.28	2.32	3.45	2.89	3.26	2.43	2.69
Angle (°)	10.2	46.2	59.1	-42.2	-50.4	6.9	46.4	61.9	-42.2	-49.8	6.9	46.2	72.4	-46.4	-70.0
3															
	ADC/def2-SV(P)					ADC/def2-TZVP					CC2/def2-TZVP				
	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI
S_0	0.00	1.46	2.95	2.13	2.47	0.00	1.50	2.81	1.95	2.39	0.00	1.45	3.24	1.88	2.64
S_1	3.59	2.75	2.97	2.47	2.49	3.40	2.66	2.83	2.38	2.41	3.47	2.91	3.28	2.54	2.65
Angle (°)	-8.0	-48.8	-59.4	53.0	58.2	-4.9	-51.1	-63.4	49.4	57.8	-4.9	-53.8	-71.7	57.8	76.1
4															
	ADC/def2-SV(P)					ADC/def2-TZVP					CC2/def2-TZVP				
	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI
S_0	0.00	-	2.95	2.08	2.27	0.00	-	2.83	1.86	2.17	0.00	-	3.20	1.48	2.38
S_1	3.53	-	2.97	2.28	2.29	3.36	-	2.85	2.17	2.19	3.42	-	3.27	2.34	2.39
Angle (°)	10.5	-	-58.0	47.7	48.6	10.5	-	-59.0	47.7	46.2	10.5	-	-72.2	44.7	86.9
5															
	ADC/def2-SV(P)					ADC/def2-TZVP					CC2/def2-TZVP				
	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI	K*	K*-CI	ΔE_v	E*	E*-CI ¹	K*	K*-CI ^A
S_0	0.00	-	2.95	2.24	2.11	0.00	-	2.82	2.00	2.00	0.00	-	3.04	1.32	2.29
S_1	3.42	-	2.98	2.12	2.12	3.20	-	2.84	2.00	2.00	3.26	-	3.12	2.24	2.38
Angle (°)	-11.7	-	-55.3	52.4	48.3	-8.7	-	-57.3	47.3	47.3	-8.7	-	-78.4	-41.2	-64.3

^A Smallest S_1/S_0 gap found with CIOpt

SECTION S3: ABSORPTION SPECTRA

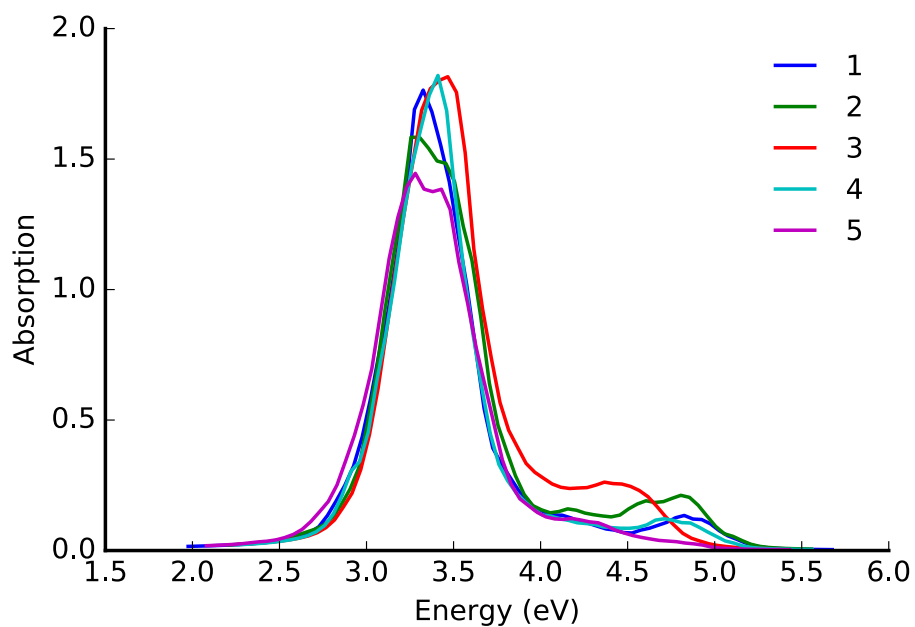


Figure S1: Absorption spectra of **1-5**, calculated at ADC(2)/def2-SV(P) level of theory

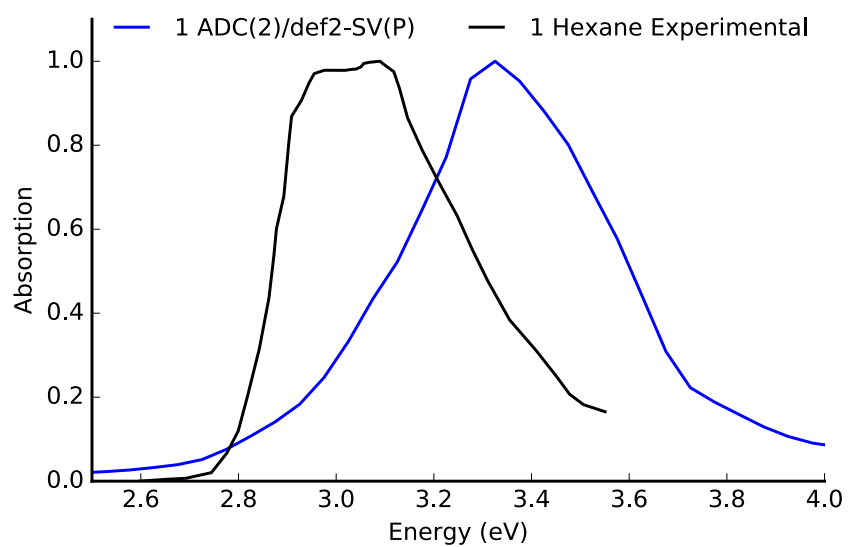


Figure S2: Calculated (vacuum/ ADC(2)/def2-SV(P)) and experimental (n-hexane)¹ absorption spectra of **1**.

SECTION S4. DIFFERENCE DENSITIES AND MOLECULAR ORBITALS

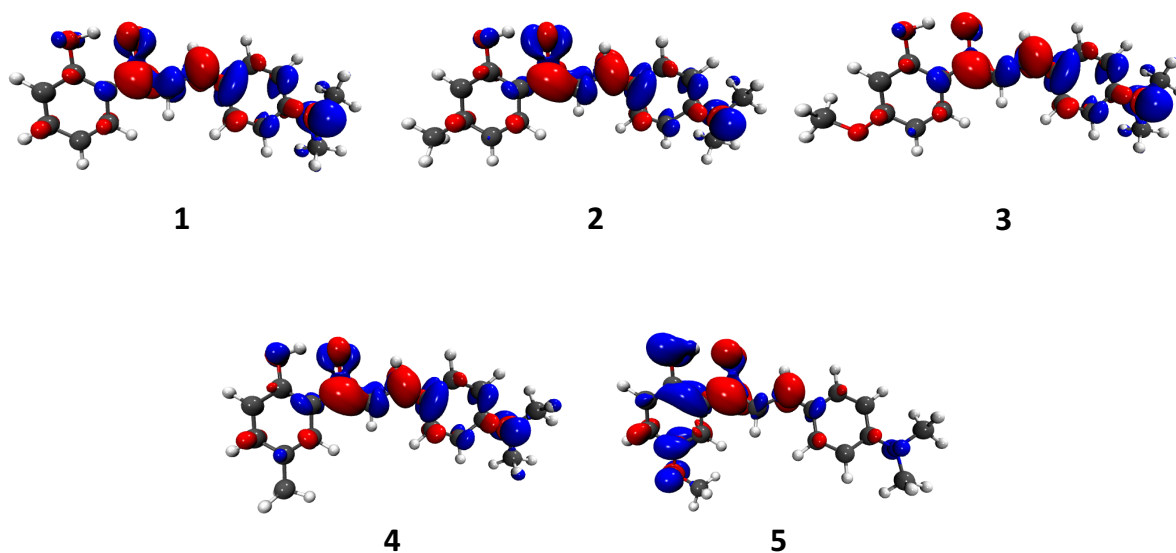


Figure S3: Difference of density between the S_0 (blue) and S_1 (red) states for compounds **1-5**, calculated at ADC(2)/def2-TZVP level of theory (Isovalue = 0.02).

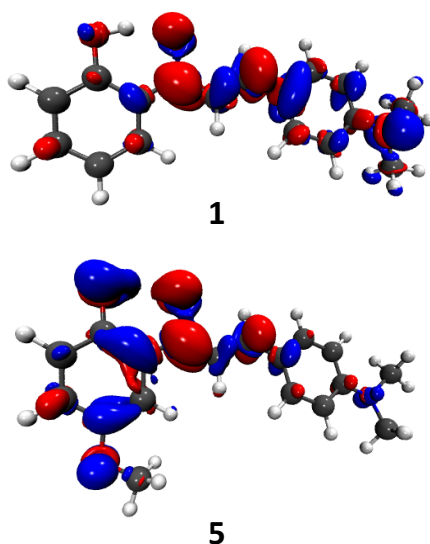


Figure S4: Difference of density between the S_0 (blue) and S_1 (red) states compounds **1** and **5**, calculated at CC2/def2-TZVP level of theory (Isovalue = 0.02).

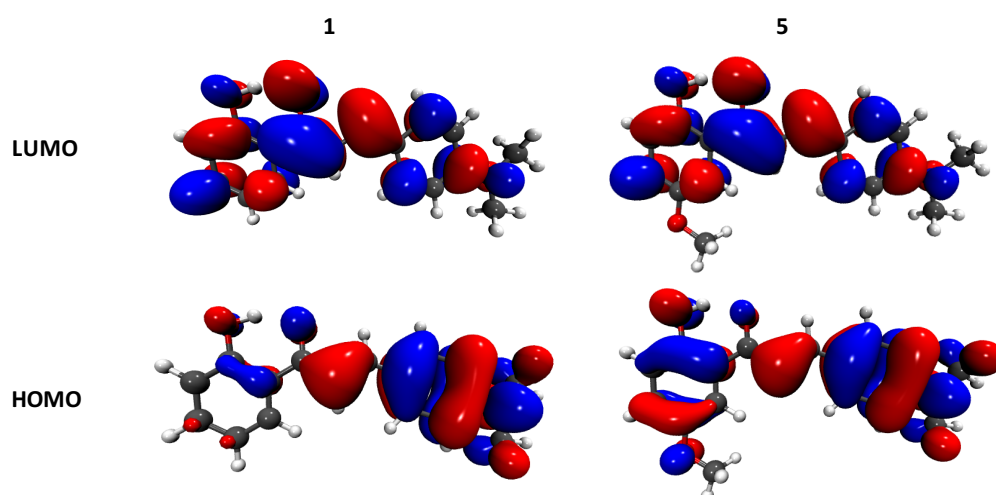


Figure S5: HOMO (Bottom) and LUMO (top) molecular orbitals for compounds **1** (left) and **5** (right), computed at CC2/def2-TZVP level of theory. Molecular orbitals for compounds **2-4** are identical to orbitals shown for **1** (Isovalue = 0.02).

SECTION S5. POTENTIAL ENERGY SURFACES

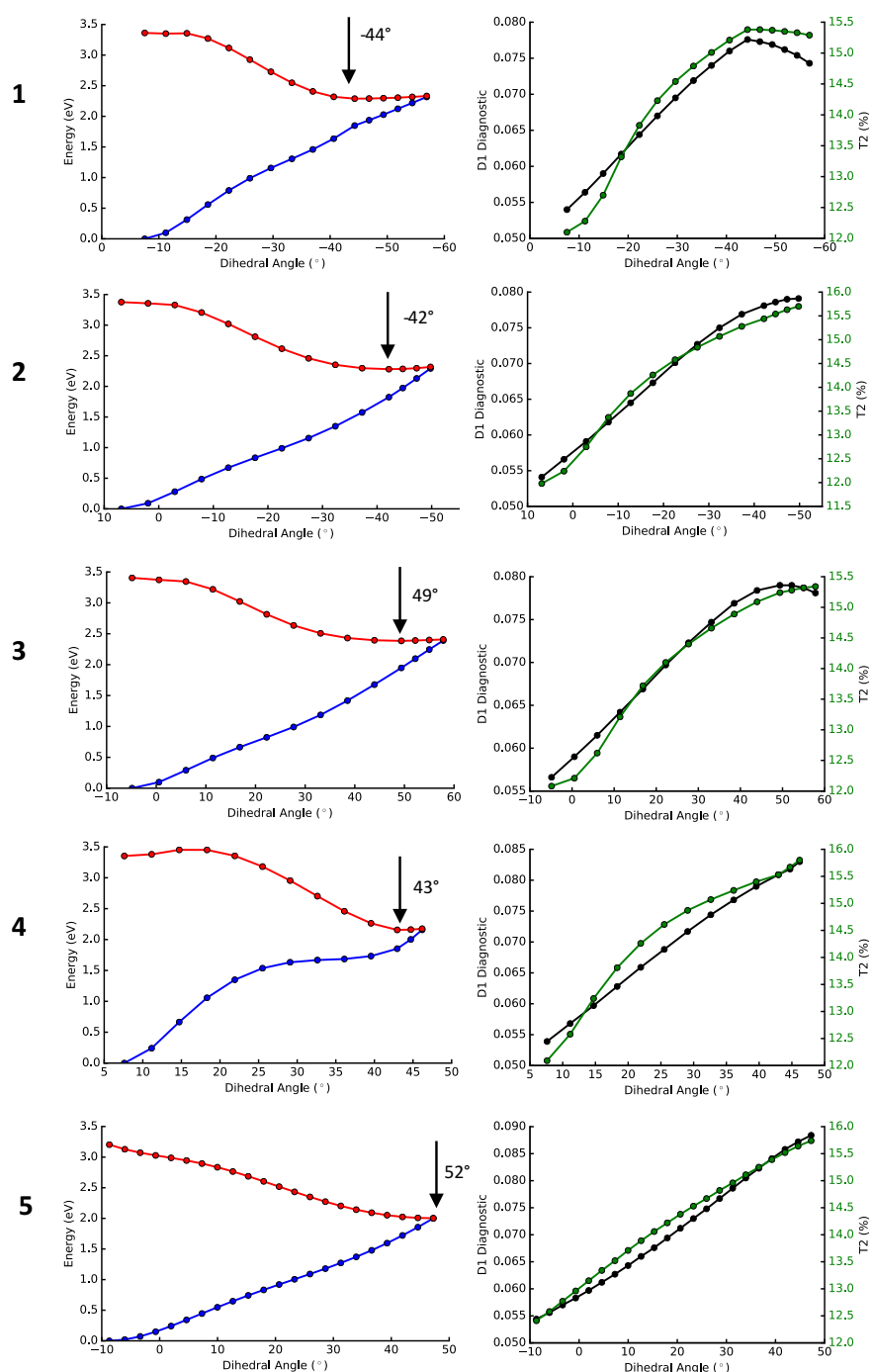


Figure S6: Linear interpolation of internal coordinates (LIIC) of 1-5 at ADC(2)/def2-TZVP level of theory. For 1-3, anchor points are the Franck Condon (FC) geometry, the K* minimum and the minimum energy conical intersection (MECI). For 4, anchor points are the FC geometry, the proton transfer geometry, the K* minimum and the LECl. In the dihedral angle plots, the points corresponding to proton transfer are omitted for clarity. For 5, LIIC is between the Franck Condon geometry and the K*/CI minimum. The dihedral angle at the K* minimum is given.

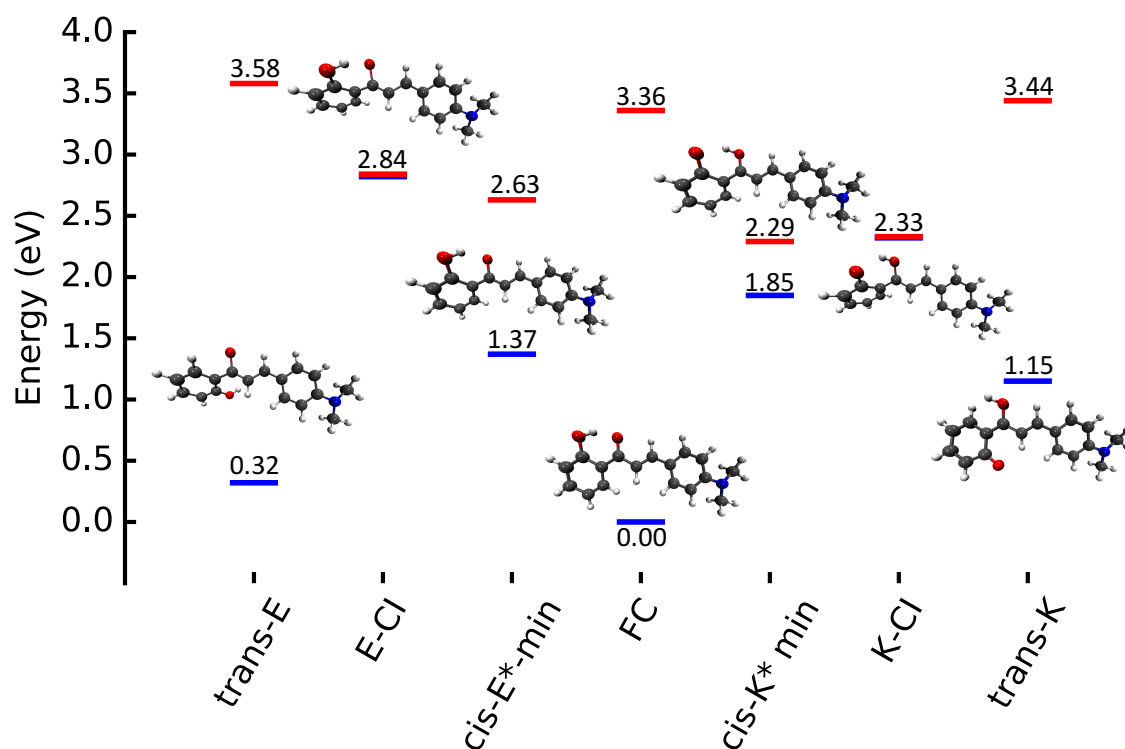


Figure S7. The ground state (blue) and first excited state (red) energies of important geometries on the potential energy surface of compound **1** at ADC(2)/def2-TZVP level. Energies are relative to the ground state Franck-Condon geometry.

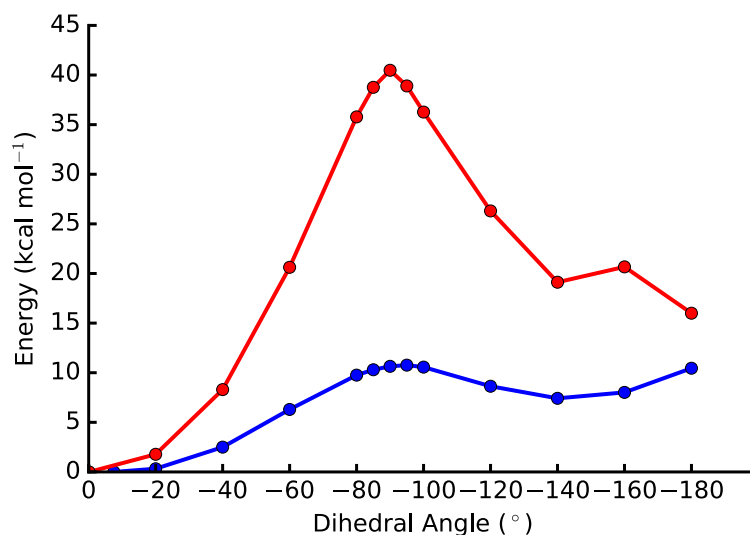


Figure S8: Relaxed geometry scan at MP2/def2-TZVP level of theory of dihedral rotation in S_0 for enol (blue) and keto (red) states. The dihedral angle O-C-C-C (defined in text) was fixed. The maxima are located at 10.76 kcal mol⁻¹ and 40.48 kcal mol⁻¹ for enol and keto states respectively.

SECTION S6. CONICAL INTERSECTIONS

Table S4: Important geometric parameters of located **keto-form** low energy conical intersections at respective level of theory

	ADC(2)/def2-TZVP			ADC(2)/def2-SV(P)		
	O-H (Å)	O...H (Å)	Θ (°)	O-H (Å)	O...H (Å)	Θ (°)
1	0.980	1.996	-56.9	0.989	1.998	-57.6
2	0.980	1.934	-49.8	0.990	1.927	-50.4
3	0.978	2.045	57.8	0.987	2.026	58.2
4	0.986	1.865	46.2	0.994	1.890	48.6
5	0.994	1.795	47.3	1.002	1.815	48.3

	CC2/def2-TZVP			CC2/def2-SV(P)		
	O-H (Å)	O...H (Å)	Θ (°)	O-H (Å)	O...H (Å)	Θ (°)
1	0.958	3.053	-88.3	0.979	2.979	-85.5
2	1.000	2.090	-70.0	1.000	2.091	-70.0
3	0.982	2.348	76.1	0.984	2.347	76.0
4	0.973	3.063	87.0	0.995	2.129	71.6
5	1.041	1.723	63.0	1.022	1.755	-64.3

	CAS(12,11)/6-31G(d)			CAS(6,6)/6-31G(d)		
	O-H (Å)	O...H (Å)	Θ (°)	O-H (Å)	O...H (Å)	Θ (°)
1	0.948	3.212	-89.3	0.948	3.151	-89.7

	CAS(14,13)/6-31G(d)		
	O-H (Å)	O...H (Å)	Θ (°)
1	0.948	3.201	-89.4

Table S5: Important geometric parameters of located **enol-form** low energy conical intersections at respective level of theory

	ADC(2)/def2-TZVP			ADC(2)/def2-SV(P)		
	O-H (Å)	O...H (Å)	Θ (°)	O-H (Å)	O...H (Å)	Θ (°)
1	0.972	2.144	-61.8	0.980	2.067	-59.2
2	0.973	2.126	61.9	0.981	2.051	59.1
3	0.975	2.088	-63.4	0.982	2.041	-59.4
4	0.972	2.098	-59.0	0.980	2.062	-58.0
5	0.981	2.043	-55.3	0.973	2.086	-57.3

	CC2/def2-TZVP			CC2/def2-SV(P)		
	O-H (Å)	O...H (Å)	Θ (°)	O-H (Å)	O...H (Å)	Θ (°)
1	0.977	3.332	-123.8	0.986	3.344	-123.1
2	0.991	2.100	72.4	0.990	2.133	75.0
3¹	0.996	1.988	-71.7	0.996	1.988	-71.7
4	0.987	2.147	-72.2	0.987	2.147	-71.8
5	0.978	2.367	-78.3	0.985	2.304	-76.4

	CAS(12,11)/6-31G(d)		
	O-H (Å)	O...H (Å)	Θ (°)
1	0.950	3.585	-143.6

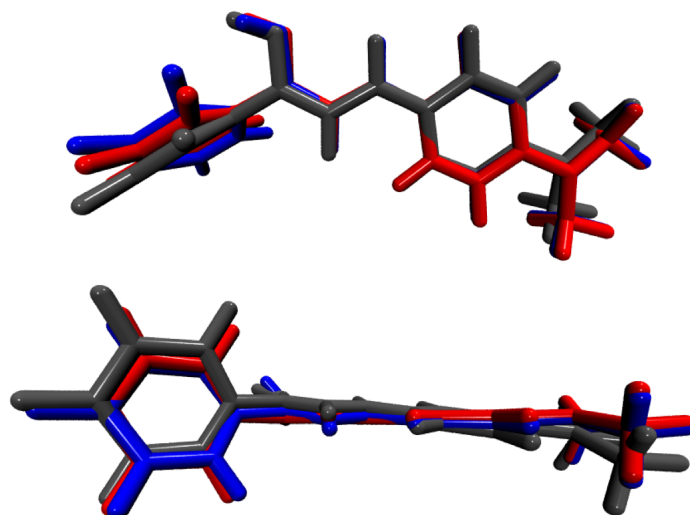
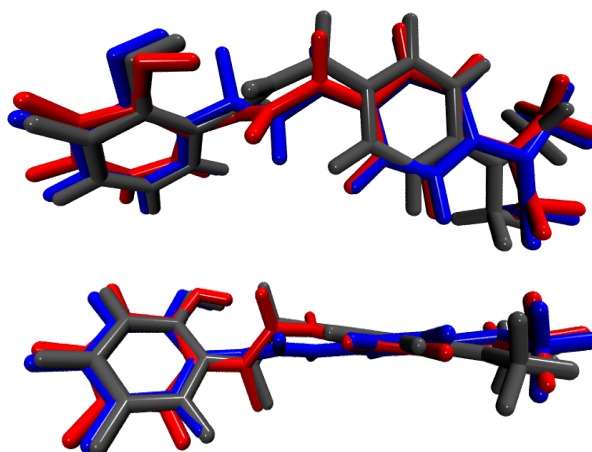
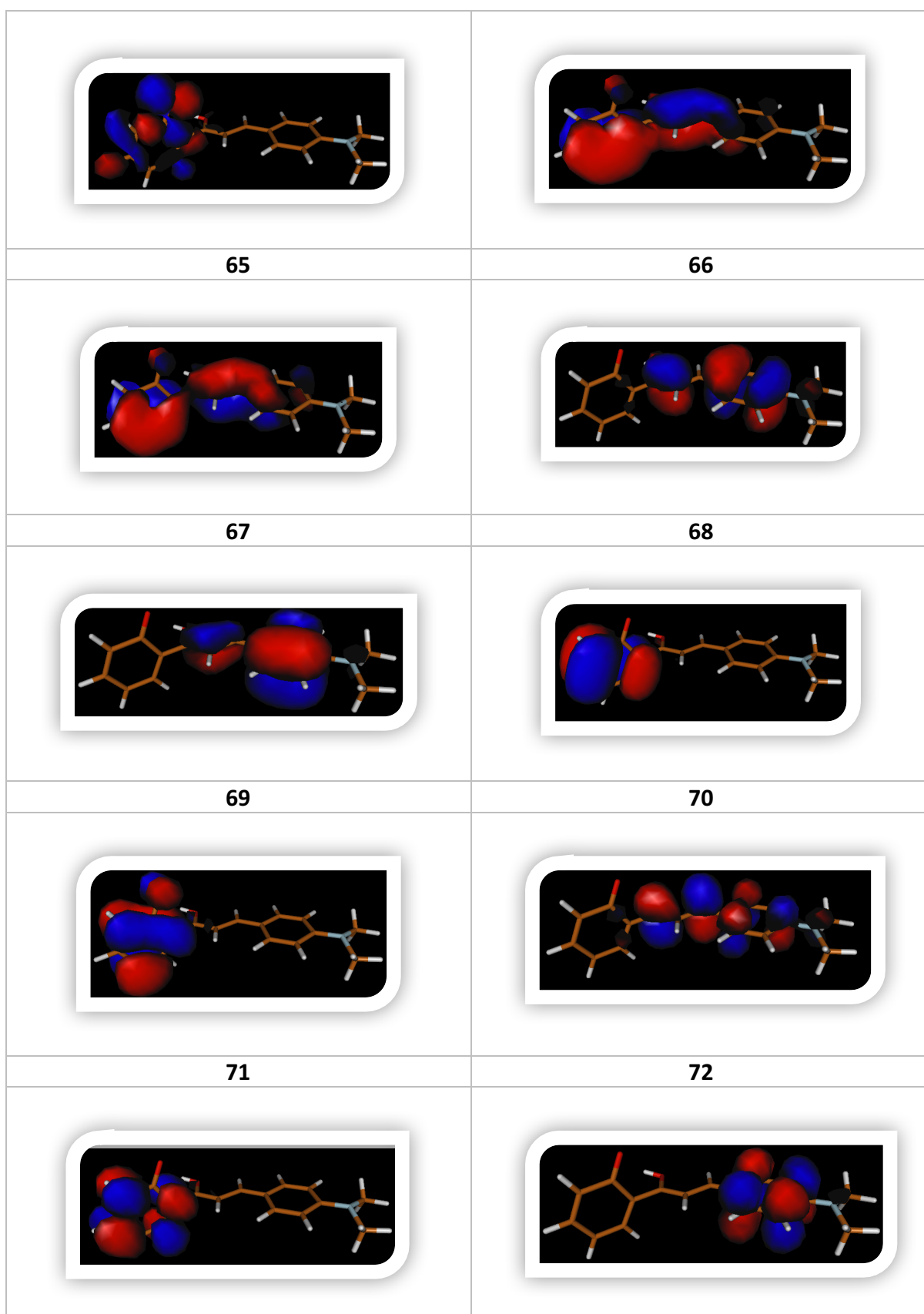
**Figure S9.** Two viewpoints of the superposition of the K^* conical intersections for compound **1** at different levels of theory. Blue: ADC(2)/def2-TZVP. Red: CC2/def2-TZVP (86 degrees). Grey: CAS(12,11)/6-31G(d).

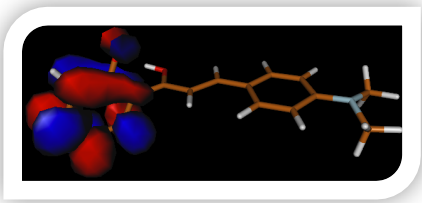
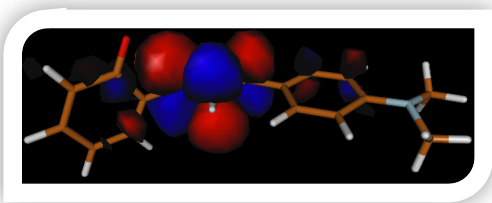
Table S5: RMSD values of the K* conical intersections between levels of theory

RMSD	<u>ADC(2)/def2-TZVP</u>	<u>CC2/def2-TZVP</u>	<u>CAS(12,11)/6-31G(d)</u>
ADC(2)/def2-TZVP	-	0.293	0.337
CC2/def2-TZVP	0.293	-	0.069
CAS(12,11)/6-31G(d)	0.337	0.069	-

**Figure S10.** Two viewpoints of the superposition of the E* conical intersections for compound **1** at different levels of theory. Blue: ADC(2)/def2-TZVP. Red: CC2/def2-TZVP. Grey: CAS(12,11)/6-31G(d).**Table S6:** RMSD values of the E* conical intersections between levels of theory

RMSD	<u>ADC(2)/def2-TZVP</u>	<u>CC2/def2-TZVP</u>	<u>CAS(12,11)/6-31G(d)</u>
ADC(2)/def2-TZVP	-	0.570	0.733
CC2/def2-TZVP	0.570	-	0.633
CAS(12,11)/6-31G(d)	0.733	0.633	-

Figure S11. Orbitals included in the active space, SA-2-CASSCF(14,13) calculations.

73	74
	
75	76
	
77	

SECTION S7. NON ADIABATIC DYNAMICS

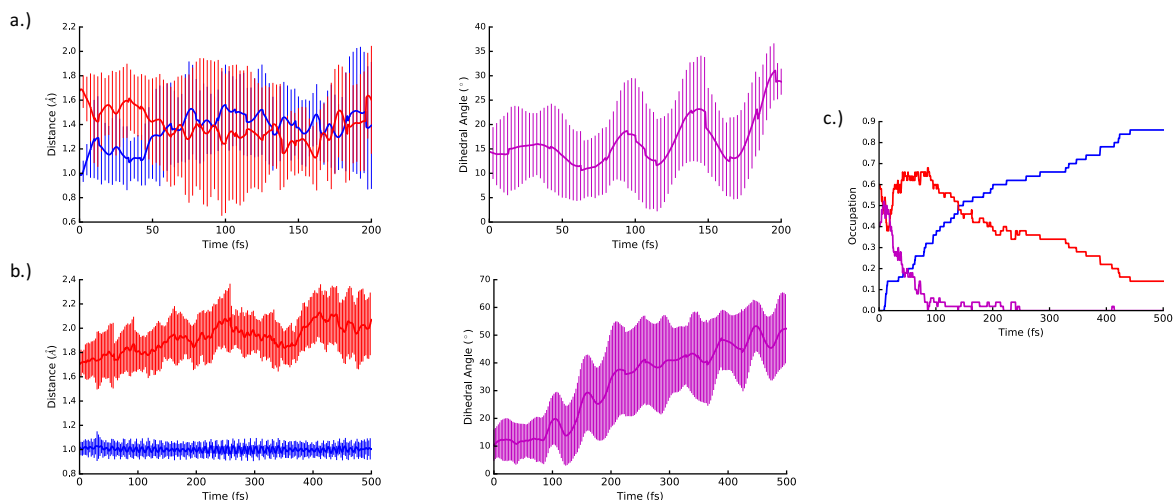


Figure S12: Compound 1: Average O-H distance (Å, left panel) and dihedral angle (degrees, central panel) for 24 trajectories undergoing proton transfer (top) and 26 trajectories not undergoing proton transfer (bottom). The occupation of the S_0 (blue), S_1 (red) and S_2 (purple) states for all 50 trajectories is displayed as a function of time (right). Error bars at time steps of 2.5 fs are shown. Average values were calculated at time steps with three or more trajectories.

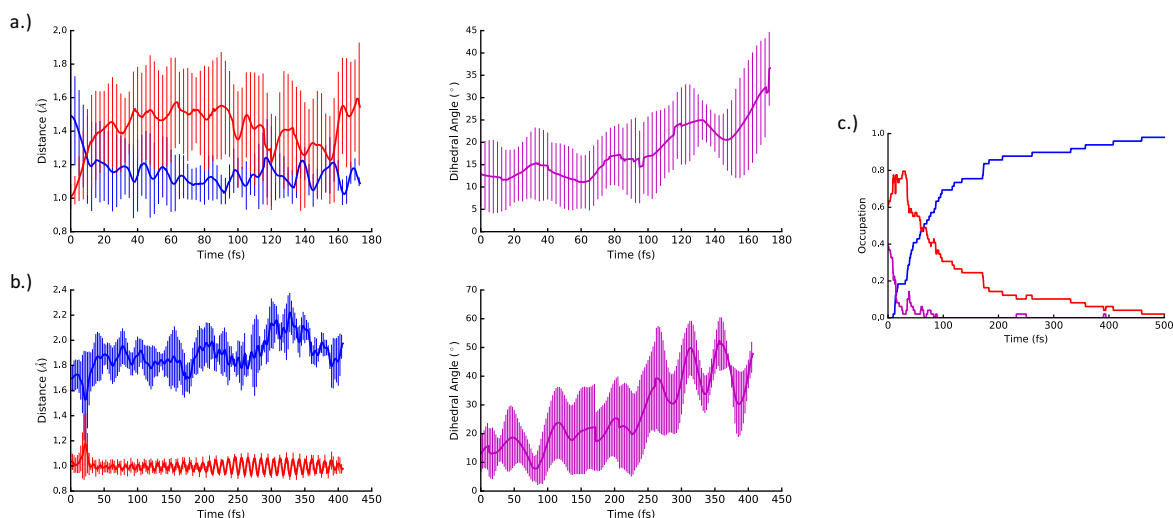


Figure S13: Compound 5: Average O-H distance (Å, left) and dihedral angle (degrees, centre) for 27 trajectories undergoing proton transfer (top) and 12 trajectories not undergoing proton transfer (bottom). The occupation of the S_0 (blue), S_1 (red) and S_2 (purple) states for all 49 trajectories is displayed as a function of time (right). Error bars at time steps of 2.5 fs are shown. Average values were calculated at time steps with three or more trajectories.

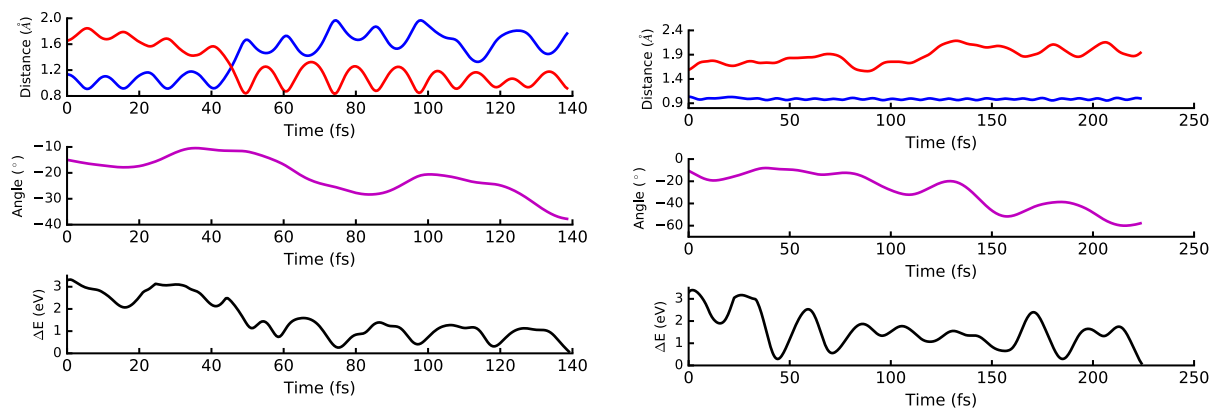


Figure S14: Example trajectories for compound 1. Trajectory 4 (Left) undergoes proton transfer in <50 fs, followed by intramolecular rotation. This rotational mode causes convergence of the S_0 and s_1 states. Trajectory 13 (right) does not undergo proton transfer.

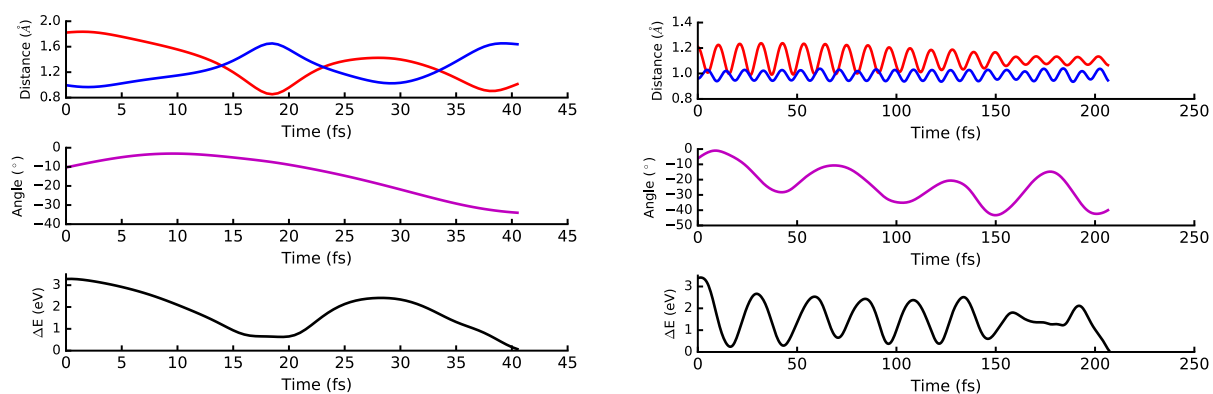


Figure S15: Example trajectories for compound 5. Trajectory 15 (Left) undergoes rapid proton transfer in <15 fs, followed by intramolecular rotation. This rotational mode causes convergence of the S_0 and s_1 states. Trajectory 2 (right) does not undergo proton transfer.

SECTION S8. OPTIMIZED GEOMETRIES

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Compound 1 - Enol S1 ADC(2)/def2-SV(P)

C	0.9679404	0.7154853	0.2129802
C	1.2462783	-0.4190994	-0.5875150
C	2.0246298	1.6453050	0.3744138
C	2.4894567	-0.6077986	-1.1854669
C	3.2699723	1.4628664	-0.2174420
C	3.5453000	0.3243245	-1.0177930
C	4.9298333	-0.8942829	-2.6114091
C	5.7346393	1.2177616	-1.6072387
C	-0.3009261	0.9636185	0.8341610
C	-1.4755982	0.1906274	0.6771786
C	-2.6164133	0.4477280	1.3782079
C	-3.9229321	-0.1952561	1.2760842
C	-4.4646150	-0.4959369	0.0054535
C	-4.6218011	-0.5971262	2.4444381
C	-5.6560528	-1.2097639	-0.1094660
C	-5.8239691	-1.3080915	2.3139880
C	-6.3343235	-1.6162530	1.0518282
H	0.4767469	-1.1851369	-0.7426642
H	1.8528250	2.5435141	0.9827749
H	2.6324316	-1.5047226	-1.7935003
H	4.0331308	2.2282622	-0.0556267
H	4.2948987	-0.6965427	-3.5017513
H	4.6709054	-1.8922613	-2.2179003
H	5.3632721	2.0947047	-2.1800834
H	5.9740445	1.5512667	-0.5829120
H	5.9813428	-0.9347363	-2.9359109
H	6.6747550	0.8746705	-2.0667010
H	-0.3754132	1.8428431	1.4948111
H	-1.5143425	-0.6552891	-0.0194651
H	-3.4218384	0.2684279	3.6661883
H	-3.9306748	-0.1484397	-0.8864375
H	-6.0659442	-1.4387307	-1.0994444
H	-6.3376948	-1.6141897	3.2315844
H	-7.2765577	-2.1713486	0.9723785
N	4.7939166	0.1174833	-1.5845974
O	-2.6431700	1.4590448	2.3872065
O	-4.1740527	-0.3629280	3.6996481

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Compound 1 - Enol S1 ADC(2)/def2-TZVP

C	0.9694978	0.7218467	0.2274443
C	1.2198409	-0.3881639	-0.6035930
C	2.0433024	1.6147831	0.4246001
C	2.4564540	-0.5885571	-1.1951832
C	3.2798584	1.4187871	-0.1637064
C	3.5301419	0.3001218	-0.9852053
C	4.8630142	-0.8584900	-2.6486052
C	5.7061188	1.1857874	-1.5878836
C	-0.2856161	0.9812756	0.8527282
C	-1.4532657	0.2060380	0.7015222
C	-2.6037495	0.4597502	1.3651916
C	-3.8898685	-0.2096983	1.2694625
C	-4.3874077	-0.5757211	0.0052723
C	-4.6248237	-0.5486559	2.4246418
C	-5.5677694	-1.2929534	-0.1099129

SUPPORTING INFORMATION

C	-5.8137747	-1.2641268	2.2956833
C	-6.2803486	-1.6368682	1.0412314
H	0.4365186	-1.1140521	-0.7947861
H	1.8890429	2.4887919	1.0513995
H	2.5832087	-1.4583329	-1.8264116
H	4.0577875	2.1472341	0.0231252
H	4.2456676	-0.5529902	-3.5052966
H	4.5522717	-1.8566907	-2.3386434
H	5.3157023	2.0372061	-2.1632975
H	5.9004505	-0.9253810	-2.9725057
H	5.9456373	1.5311060	-0.5816792
H	6.6342301	0.8501021	-2.0478374
H	-0.3492840	1.8575796	1.4982833
H	-1.4743809	-0.6547554	0.0423193
H	-3.4528711	0.3522792	3.6336864
H	-3.8307780	-0.2740622	-0.8749407
H	-5.9400814	-1.5711714	-1.0884884
H	-6.3544580	-1.5236668	3.1985042
H	-7.2087812	-2.1907228	0.9615297
N	4.7807676	0.0717795	-1.5406288
O	-2.6775707	1.5138308	2.3276870
O	-4.2146838	-0.2532390	3.6842929

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Compound 1 - Keto S1 ADC(2)/def2-SV(P)

C	0.9603334	0.7252473	0.2654714
C	1.1464591	-0.3068389	-0.6856560
C	2.0873285	1.5402664	0.5329358
C	2.3729380	-0.5180097	-1.3111688
C	3.3164201	1.3370298	-0.0884059
C	3.5017940	0.2927892	-1.0287782
C	4.7910326	-0.8212758	-2.7738013
C	5.7602273	1.0726305	-1.5133932
C	-0.2789790	0.9839000	0.9447396
C	-1.4746540	0.2487226	0.8059982
C	-2.6362626	0.5697208	1.4612596
C	-3.8997282	-0.2170608	1.2905705
C	-4.3937302	-0.5599384	0.0543763
C	-4.6299726	-0.5988756	2.4759200
C	-5.5550917	-1.3945875	-0.0539465
C	-5.7696629	-1.4242833	2.3446787
C	-6.2323850	-1.8253903	1.0739179
H	0.3114781	-0.9659407	-0.9536629
H	1.9874628	2.3613973	1.2555291
H	2.4405303	-1.3294507	-2.0407404
H	4.1376625	2.0127559	0.1644109
H	4.1830635	-0.4591841	-3.6307319
H	4.4449334	-1.8353105	-2.5095121
H	5.4653441	2.0428145	-1.9681342
H	5.8381691	-0.9099476	-3.1033760
H	6.0196941	1.2522627	-0.4559678
H	6.6720665	0.7150173	-2.0170466
H	-0.3057405	1.8327834	1.6446451
H	-1.5148542	-0.6229592	0.1392314
H	-3.2993111	1.3429463	3.0400161
H	-3.8769353	-0.2281694	-0.8545573
H	-5.9003919	-1.6918106	-1.0512403
H	-6.2790417	-1.7242623	3.2679094
H	-7.1170657	-2.4669050	0.9857316

SUPPORTING INFORMATION

N 4.7324317 0.0597001 -1.6268850
O -2.7312542 1.6470662 2.2814424
O -4.2743084 -0.1368498 3.6382207
37

Compound 1 - Keto S1 ADC(2)/def2-TZVP

C 0.9725936 0.7120752 0.2997871
C 1.1487803 -0.3219845 -0.6406170
C 2.0964458 1.5239135 0.5562492
C 2.3645302 -0.5335725 -1.2711755
C 3.3134942 1.3170614 -0.0710441
C 3.4900859 0.2694493 -0.9967301
C 4.7358476 -0.8001452 -2.7845840
C 5.7077898 1.0835018 -1.5504963
C -0.2538025 0.9754923 0.9821943
C -1.4460323 0.2464431 0.8332330
C -2.6020300 0.5509596 1.4851793
C -3.8594038 -0.2337037 1.2980303
C -4.2928324 -0.6254198 0.0628456
C -4.6536425 -0.5554038 2.4500522
C -5.4678255 -1.4269082 -0.0724036
C -5.8040480 -1.3479787 2.2936983
C -6.2099890 -1.7930642 1.0256803
H 0.3198293 -0.9743407 -0.8952340
H 1.9996661 2.3408638 1.2660134
H 2.4319397 -1.3419226 -1.9879340
H 4.1285363 -0.3818180 -3.5998113
H 4.1328704 1.9823001 0.1684723
H 4.3708092 -1.8036524 -2.5633677
H 5.3628936 2.0068937 -2.0370764
H 5.7643206 -0.8955015 -3.1297518
H 5.9761493 1.3173001 -0.5197765
H 6.6104614 0.7400909 -2.0537393
H -0.2709908 1.8129450 1.6777411
H -1.4829907 -0.6087081 0.1648414
H -3.3096107 1.3021491 3.0386004
H -3.7335060 -0.3411475 -0.8224777
H -5.7637698 -1.7518909 -1.0638009
H -6.3616808 -1.5980713 3.1902529
H -7.0976280 -2.4055102 0.9183308
N 4.7188825 0.0259573 -1.5949028
O -2.7008933 1.6143852 2.3237584
O -4.3352495 -0.0810378 3.6199627
37

Compound - 1 Keto S1 ADC(2)/def2-TZVP

C 0.9851160 0.6820994 0.3104922
C 1.1633387 -0.3701841 -0.6089904
C 2.1117107 1.4909232 0.5636399
C 2.3824412 -0.5971780 -1.2280209
C 3.3319793 1.2682963 -0.0516227
C 3.5092923 0.2063354 -0.9604298
C 4.7567155 -0.8852540 -2.7330419
C 5.7291828 1.0096308 -1.5175052
C -0.2464492 0.9701799 0.9734235
C -1.4420515 0.2446293 0.8362527
C -2.5871228 0.5507825 1.5067775
C -3.8363628 -1.6131204 1.3716873
C -3.8412755 -0.2468851 1.3618065
C -5.0478374 -2.3429355 1.1701947

SUPPORTING INFORMATION

C -5.0934968 0.4459191 1.2447808
C -6.2486475 -1.6955335 0.9971016
C -6.2723395 -0.2927897 1.0424121
H 0.3319086 -1.0206054 -0.8608485
H 2.0136347 2.3199156 1.2590947
H 2.4515592 -1.4178001 -1.9305588
H 4.1496545 -0.4736171 -3.5518424
H 4.1529247 1.9330406 0.1835606
H 4.3910996 -1.8866958 -2.5034334
H 5.3848442 1.9266440 -2.0165382
H 5.7850504 -0.9838310 -3.0776623
H 5.9951954 1.2563793 -0.4891305
H 6.6327801 0.6601914 -2.0149656
H -0.2639128 1.8241531 1.6486597
H -1.4876642 -0.6164829 0.1759046
H -2.9041455 -2.1493779 1.5165256
H -3.5676407 1.9440489 2.2653954
H -5.0041611 -3.4262325 1.1479409
H -7.1637985 -2.2538994 0.8384765
H -7.1956153 0.2648418 0.9247059
N 4.7401824 -0.0486230 -1.5503893
O -2.6551958 1.5821760 2.3877480
O -5.1408935 1.7408589 1.3683994
37

Compound 1 - Enol S1 CC2/def2-SV(P)

C 0.9477281 0.7232806 0.1687932
C 1.2222052 -0.3832380 -0.6839237
C 2.0249121 1.6296256 0.3837377
C 2.4698860 -0.5702147 -1.2704762
C 3.2753778 1.4520621 -0.1952760
C 3.5417918 0.3388534 -1.0432163
C 4.9509007 -0.8736790 -2.6277795
C 5.7795718 1.1937449 -1.5184206
C -0.3161746 0.9608567 0.7771431
C -1.4999165 0.1783781 0.6161780
C -2.6254432 0.4457557 1.3265708
C -3.9340012 -0.1980130 1.2601592
C -4.4997437 -0.5420635 0.0094188
C -4.6112948 -0.5644602 2.4582139
C -5.6892056 -1.2682784 -0.0610755
C -5.8080679 -1.2982195 2.3730024
C -6.3402277 -1.6455838 1.1289493
H 0.4381335 -1.1231065 -0.8883850
H 1.8576789 2.5031998 1.0291702
H 2.6075904 -1.4397278 -1.9193520
H 4.0506376 2.1958653 0.0086080
H 4.3361292 -0.6697655 -3.5300187
H 4.6793415 -1.8725010 -2.2429165
H 5.4591416 2.1229303 -2.0357175
H 6.0014336 1.4431048 -0.4657949
H 6.0096708 -0.9116973 -2.9285494
H 6.7159547 0.8428428 -1.9799099
H -0.4044729 1.8328981 1.4473778
H -1.5392924 -0.6675379 -0.0822630
H -3.3954773 0.3650275 3.6086559
H -3.9825064 -0.2214327 -0.9029409
H -6.1177146 -1.5302621 -1.0354494
H -6.3031529 -1.5792906 3.3093118

H -7.2791987 -2.2111587 1.0849379
N 4.7900023 0.1373767 -1.6011133
O -2.6675003 1.4822952 2.3280489
O -4.1446970 -0.2778674 3.6943014

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Compound 1 - Enol S1 CC2/def2-TZVP

C 0.9573165 0.7198361 0.1990331
C 1.2140160 -0.3755441 -0.6623433
C 2.0407275 1.6064662 0.4243796
C 2.4527514 -0.5689668 -1.2485772
C 3.2804145 1.4209438 -0.1563193
C 3.5305998 0.3153133 -1.0058185
C 4.8926640 -0.8451224 -2.6534794
C 5.7390426 1.1856298 -1.5345449
C -0.2927040 0.9636512 0.8122662
C -1.4690647 0.1779313 0.6473796
C -2.6042524 0.4310105 1.3234127
C -3.8988099 -0.2217416 1.2563722
C -4.4267554 -0.6041178 0.0076167
C -4.6169865 -0.5348153 2.4348078
C -5.6170089 -1.3133892 -0.0740110
C -5.8140733 -1.2487228 2.3414483
C -6.3078247 -1.6350004 1.1000665
H 0.4262947 -1.0910031 -0.8769975
H 1.8828291 2.4661246 1.0711759
H 2.5830216 -1.4226394 -1.9018280
H 4.0614819 2.1412840 0.0515166
H 4.2926791 -0.5501572 -3.5257319
H 4.5775552 -1.8410789 -2.3379704
H 5.3856452 2.0699183 -2.0831527
H 5.9382063 -0.9079513 -2.9523525
H 5.9602583 1.4815385 -0.5077846
H 6.6676862 0.8403642 -1.9871252
H -0.3739835 1.8301967 1.4709486
H -1.4891422 -0.6735687 -0.0261685
H -3.4159816 0.3947562 3.5859598
H -3.8832495 -0.3220802 -0.8882449
H -6.0126771 -1.6028450 -1.0407807
H -6.3401899 -1.4893838 3.2587415
H -7.2427164 -2.1826748 1.0474103
N 4.7788128 0.0983550 -1.5572969
O -2.6769644 1.5031124 2.3081874
O -4.1796182 -0.2156291 3.6798046

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Compound 1 - Keto S1 CC2/def2-SV(P)

C 0.9515661 0.7282456 0.2165557
C 1.1677689 -0.3218907 -0.7175733
C 2.0657865 1.5708638 0.4812711
C 2.4026075 -0.5249369 -1.3251189
C 3.3053559 1.3792645 -0.1196482
C 3.5172699 0.3149066 -1.0403859
C 4.8686884 -0.8602609 -2.7051548
C 5.7955090 1.0902242 -1.4654941
C -0.2928598 0.9694548 0.8770904
C -1.4777845 0.2132477 0.7410288
C -2.6604409 0.5533337 1.3599218
C -3.9238544 -0.2355836 1.2290496
C -4.5152851 -0.6914596 2.4770010

SUPPORTING INFORMATION

C	-4.5908300	-0.4278304	0.0396406
C	-5.6486962	-1.5450954	2.4060182
C	-5.7515186	-1.2657615	-0.0019193
C	-6.2622643	-1.8218731	1.1693252
H	0.3444610	-0.9974859	-0.9820887
H	1.9411026	2.4038533	1.1869774
H	2.4940308	-1.3461257	-2.0417158
H	4.1130864	2.0740039	0.1270570
H	4.2741736	-0.5699128	-3.5968378
H	4.5413748	-1.8639354	-2.3817190
H	5.5271185	2.0659013	-1.9224845
H	5.9267613	-0.9363303	-3.0010673
H	6.0221807	1.2579818	-0.3979939
H	6.7151407	0.7207909	-1.9457857
H	-0.3457864	1.8318736	1.5598564
H	-1.5045096	-0.6751020	0.0953231
H	-3.3262314	1.3007904	2.9322910
H	-4.1892572	-0.0035004	-0.8906799
H	-6.0415484	-1.9457429	3.3490850
H	-6.2266950	-1.4743821	-0.9687150
H	-7.1434386	-2.4749428	1.1311257
N	4.7515588	0.0956082	-1.6208265
O	-2.7807592	1.6433160	2.1511841
O	-4.0437819	-0.2315080	3.5954065

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Compound 1 - Keto S1 CC2/def2-TZVP

C	0.9653993	0.7178587	0.2597247
C	1.1646069	-0.3272016	-0.6737614
C	2.0812860	1.5501734	0.5168499
C	2.3859158	-0.5319725	-1.2911158
C	3.3065971	1.3544674	-0.0943219
C	3.5013545	0.2941221	-1.0109156
C	4.8010014	-0.8297544	-2.7367911
C	5.7443636	1.0980457	-1.5074620
C	-0.2636510	0.9645014	0.9267523
C	-1.4472000	0.2140760	0.7814732
C	-2.6209462	0.5344008	1.4023242
C	-3.8803221	-0.2544877	1.2493564
C	-4.4430400	-0.5384710	0.0360675
C	-4.5674544	-0.6254392	2.4639316
C	-5.6261119	-1.3360304	-0.0412871
C	-5.7262087	-1.4258063	2.3634500
C	-6.2443022	-1.7864613	1.1104126
H	0.3427809	-0.9894115	-0.9286766
H	1.9654877	2.3731468	1.2178664
H	2.4721296	-1.3444347	-2.0019598
H	4.1168716	2.0325572	0.1425085
H	4.2035461	-0.4734301	-3.5871615
H	4.4541844	-1.8280417	-2.4643103
H	5.4314706	2.0349846	-1.9883434
H	5.8407265	-0.9138732	-3.0501702
H	5.9865460	1.3088019	-0.4643990
H	6.6511435	0.7403504	-1.9933843
H	-0.3034377	1.8124331	1.6099973
H	-1.4724938	-0.6558103	0.1307729
H	-3.3332191	1.2481567	2.9554456
H	-3.9676612	-0.1887162	-0.8765184
H	-6.0200640	-1.6011820	-1.0170527

H -6.1988330 -1.7464495 3.2872098
H -7.1355947 -2.4021848 1.0496516
N 4.7299625 0.0650515 -1.5973377
O -2.7491800 1.6085805 2.2178277
O -4.1456540 -0.1525499 3.6033466

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Compound 1 - MP2/def2-SV(P)

C 0.9919212 0.6217082 0.2320644
C 1.1774762 -0.3267973 -0.7933040
C 2.0902756 1.4434194 0.5480900
C 2.3955100 -0.4620708 -1.4493791
C 3.3163092 1.3183899 -0.0985505
C 3.5112598 0.3476494 -1.1115046
C 4.8142247 -0.6393887 -2.9192115
C 5.7690247 1.1687527 -1.5099886
C -0.2557044 0.7927088 0.9601051
C -1.3725188 0.0275471 0.8760055
C -2.5472140 0.3543177 1.7081382
C -3.8449900 -0.3093026 1.4353438
C -4.0738502 -1.0683438 0.2667065
C -4.8975648 -0.1861087 2.3836986
C -5.2890754 -1.7069547 0.0437958
C -6.1132653 -0.8564334 2.1584619
C -6.3089828 -1.6055486 1.0036440
H 0.3468389 -0.9727261 -1.1016197
H 1.9780697 2.2058442 1.3295832
H 2.4722335 -1.2085375 -2.2431027
H 4.1250302 1.9926812 0.1914110
H 4.1840744 -0.2638710 -3.7524638
H 4.5121834 -1.6780224 -2.6998098
H 5.4850443 2.1848052 -1.8557245
H 5.8595289 -0.6681540 -3.2616826
H 6.0287149 1.2290545 -0.4389769
H 6.6763779 0.8598647 -2.0504326
H -0.2964346 1.6284033 1.6736305
H -1.4116241 -0.8412697 0.2141701
H -3.2925664 -1.1378127 -0.4956163
H -3.9093493 0.9984420 3.4671751
H -5.4469065 -2.2823679 -0.8746604
H -6.8970116 -0.7501280 2.9157609
H -7.2688265 -2.1105423 0.8425341
N 4.7304279 0.1873664 -1.7348825
O -2.4440196 1.1698260 2.6386856
O -4.7946212 0.5435995 3.5019060

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Compound 1 - MP2/def2-TZVP

C 1.0114985 0.5818465 0.2827220
C 1.1871786 -0.3614916 -0.7409748
C 2.1098514 1.3926426 0.6016115
C 2.3965493 -0.4948422 -1.4005690
C 3.3263589 1.2688381 -0.0511458
C 3.5097904 0.3068816 -1.0644091
C 4.7605406 -0.5992963 -2.9378544
C 5.7166931 1.1921798 -1.5436117
C -0.2288736 0.7611997 1.0092875
C -1.3657945 0.0476397 0.8657572
C -2.5366453 0.3576344 1.6969310
C -3.8226379 -0.3114614 1.4214077

SUPPORTING INFORMATION

C -4.0275236 -1.1142005 0.2844552
C -4.8938739 -0.1422206 2.3322363
C -5.2391188 -1.7445096 0.0582186
C -6.1079745 -0.7984223 2.1028981
C -6.2791895 -1.5900781 0.9795143
H 0.3633073 -1.0004639 -1.0406785
H 2.0021393 2.1417302 1.3804405
H 2.4733708 -1.2331620 -2.1871971
H 4.1323165 -0.1467116 -3.7171394
H 4.1350786 1.9274221 0.2346197
H 4.4316816 -1.6275484 -2.7830806
H 5.3663556 2.1610830 -1.9249406
H 5.7878172 -0.6346258 -3.2957075
H 5.9933523 1.3136841 -0.4956722
H 6.6141865 0.9064632 -2.0890091
H -0.2437522 1.5538611 1.7552551
H -1.4255429 -0.7632142 0.1543181
H -3.2346137 -1.2281668 -0.4431539
H -3.8891514 1.0327019 3.3763029
H -5.3773900 -2.3527383 -0.8273951
H -6.9054503 -0.6574912 2.8233835
H -7.2296628 -2.0854617 0.8147395
N 4.7274982 0.1436559 -1.6936467
O -2.4416308 1.1685305 2.6366588
O -4.7967389 0.6281124 3.4254279
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Compound - 2 Enol S1 ADC(2)/def2-SV(P)

C 0.1623220 2.2120253 -3.2188763
C 0.2794302 0.8188947 -3.4269977
C 0.3227058 -1.2522586 4.1199372
C 0.4966150 -0.0240178 -1.0329202
C 0.7372134 -2.4272105 6.2136902
C 0.7877631 -0.0426955 -2.3642932
C 0.8297247 -0.9901339 1.2939705
C 1.1309825 -0.8833697 -0.1042137
C 1.3719036 -1.9650169 3.4847150
C 1.6128899 -1.8325933 2.1213552
C -0.1797443 0.2673211 -4.6504948
C -0.2282204 -0.2945428 1.9286447
C -0.4330719 3.0280814 -4.1766194
C -0.4736926 -0.4191534 3.2936365
C -0.7727691 1.1069431 -5.6031601
C -0.9066591 2.4832830 -5.3877141
C -1.1403724 -0.8297229 6.0229463
C -1.5857847 3.3574391 -6.4103018
H 0.4406257 -3.4339626 5.8480998
H 0.4536809 -1.5048756 -4.2841238
H 0.4652001 -2.3493254 7.2779064
H 0.5534504 2.6373962 -2.2872650
H 1.8360931 -2.3472856 6.1505094
H 1.9352121 -1.5262029 -0.4978912
H 2.0138067 -2.6391670 4.0573299
H 2.4371202 -2.4016768 1.6705529
H -0.2659511 0.6969787 -0.7151637
H -0.5131766 4.1071974 -3.9970719
H -0.8918281 0.3520007 1.3416117
H -1.1235391 0.6433721 -6.5325775
H -1.1301694 4.3624984 -6.4381868

SUPPORTING INFORMATION

H -1.1430965 -0.9703108 7.1151285
H -1.2260014 0.2539671 5.8327956
H -1.3142015 0.1389922 3.7139278
H -1.5147451 2.9176570 -7.4198110
H -2.0404478 -1.3283354 5.6028613
H -2.6586709 3.4820822 -6.1713887
N 0.0986017 -1.3510848 5.4854354
O 1.6925838 -1.0007482 -2.9110733
O -0.1157827 -1.0524393 -4.9449101

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Compound 2 - Enol S1 ADC(2)/def2-TZVP

C 0.1241364 2.1905590 -3.1863244
C 0.2468736 0.8056543 -3.4010634
C 0.3507209 -1.2144832 4.1041683
C 0.4968564 -0.0454455 -1.0235571
C 0.7184714 -2.4152188 6.1791449
C 0.7714661 -0.0446542 -2.3459149
C 0.8445805 -0.9847953 1.2913907
C 1.1413187 -0.8962762 -0.0999421
C 1.3816593 -1.9432165 3.4755994
C 1.6195257 -1.8252017 2.1179981
C -0.1926352 0.2654121 -4.6264724
C -0.2000246 -0.2770148 1.9189813
C -0.4417408 -0.3920584 3.2784800
C -0.4554561 3.0061548 -4.1431748
C -0.7682594 1.1023772 -5.5795000
C -0.9121323 2.4688331 -5.3543208
C -1.1388134 -0.8283279 5.9796605
C -1.5645404 3.3474430 -6.3828436
H 0.3590259 -3.3834339 5.8024359
H 0.4290364 -1.4991144 -4.2577253
H 0.4635114 -2.3351407 7.2347709
H 0.5026136 2.6046109 -2.2582894
H 1.8060863 -2.3985026 6.1030410
H 1.9408801 -1.5313529 -0.4821646
H 2.0110216 -2.6099960 4.0501353
H 2.4259113 -2.4000515 1.6708605
H -0.2706926 0.6513896 -0.7048660
H -0.5425206 4.0722645 -3.9615673
H -0.8530207 0.3622745 1.3341415
H -1.0978660 4.3333630 -6.4106072
H -1.1056076 0.6549141 -6.5088474
H -1.1514473 -0.9518739 7.0614951
H -1.2651773 0.1711667 3.6977380
H -1.2753986 0.2329892 5.7700153
H -1.4986637 2.9075735 -7.3785792
H -1.9890890 -1.3789112 5.5524962
H -2.6236194 3.4907981 -6.1517243
N 0.1378344 -1.2905546 5.4737134
O 1.7027049 -0.9647335 -2.9141601
O -0.1275299 -1.0574199 -4.9246220

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Compound - 2 Keto S1 ADC(2) def2-SV(P)

C 0.0240709 -0.1553441 1.8984645
C 0.2531370 -0.3713345 -1.1523110
C 0.2910228 1.8694690 -5.4755420
C 0.3381106 -0.5391879 -2.5119880
C 0.4690689 -1.1745781 4.0867154

SUPPORTING INFORMATION

C	0.6005396	-1.2473200	1.2057907
C	0.6904100	-1.3394379	-0.2252927
C	0.6918343	0.8329203	-4.6056021
C	0.7008834	-2.3345008	6.2176033
C	1.0381271	-2.2747050	3.3977123
C	1.0992123	-2.3033070	2.0071506
C	-0.0395979	-0.1178170	3.2894487
C	-0.1488353	0.4927492	-3.4820814
C	-0.4099467	-0.1301277	6.1072382
C	-0.9426401	2.5511607	-5.3167122
C	-1.3326172	3.6513165	-6.2700372
C	-1.3696905	1.1070399	-3.3612758
C	-1.7522558	2.1566861	-4.2654515
H	0.6565277	-2.1108207	7.2951403
H	0.9783143	2.1166693	-6.2948828
H	1.1432956	-2.2496279	-0.6466140
H	1.3433326	-1.3650139	-3.8688195
H	1.4363667	-3.1319112	3.9468979
H	1.5479872	-3.1759564	1.5137571
H	1.7158321	-2.7105866	6.0033259
H	-0.0242261	-3.1474428	5.9973030
H	-0.0975776	0.8899721	5.8254002
H	-0.1936516	0.5689540	-0.8030025
H	-0.3014194	-0.2135924	7.2001047
H	-0.3926035	0.6922043	1.3403287
H	-0.5057999	0.7543552	3.7555244
H	-0.5935518	4.4725600	-6.2509497
H	-1.3865713	3.2748937	-7.3075377
H	-1.4851597	-0.2472030	5.8513698
H	-2.0495750	0.8246706	-2.5477397
H	-2.3185961	4.0701953	-6.0066369
H	-2.7175317	2.6543654	-4.1069607
N	0.4332470	-1.1217022	5.4740329
O	0.8362981	-1.6717481	-3.0684450
O	1.7742291	0.1530832	-4.8454261

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Compound 2 - Keto S1 ADC(2)/def2-TZVP

C	0.0466258	-0.1574668	1.8781780
C	0.2421369	1.8185003	-5.4912501
C	0.2845155	-0.3825249	-1.1419560
C	0.3788669	-0.5306619	-2.4932633
C	0.4896019	-1.1551550	4.0615341
C	0.6220927	-1.2497911	1.1996401
C	0.6579821	-2.3198886	6.1831506
C	0.6673576	0.8017171	-4.6201096
C	0.7222497	-1.3491278	-0.2216091
C	1.0491737	-2.2584374	3.3870050
C	1.1151610	-2.2973259	2.0042974
C	-0.0218711	-0.1133745	3.2617036
C	-0.1115615	0.5050751	-3.4505122
C	-0.4447601	-0.1342650	6.0554532
C	-0.9535558	2.5371828	-5.2791941
C	-1.2935774	1.1616445	-3.2731802
C	-1.3699307	3.6199657	-6.2323686
C	-1.7035310	2.1907030	-4.1810448
H	0.6120665	-2.1031458	7.2494487
H	0.8787168	2.0308176	-6.3460785
H	1.1764326	-2.2503016	-0.6302117

SUPPORTING INFORMATION

H 1.3507751 -1.3240524 -3.8747120
H 1.4415776 -3.1003993 3.9423618
H 1.5560024 -3.1645170 1.5203770
H 1.6429681 -2.7394505 5.9763575
H -0.0996710 -3.0800748 5.9452523
H -0.1623156 0.5426943 -0.7905112
H -0.1838563 0.8847162 5.7678131
H -0.3502797 -0.2021776 7.1382892
H -0.3653039 0.6759875 1.3185105
H -0.4817689 0.7523500 3.7207706
H -0.6241718 4.4174737 -6.2675230
H -1.4779335 3.2284254 -7.2464263
H -1.4942400 -0.3141133 5.7818742
H -1.9295143 0.9154162 -2.4287692
H -2.3226412 4.0584727 -5.9346761
H -2.6352046 2.7116981 -3.9812414
N 0.4620743 -1.0868538 5.4484995
O 0.8937020 -1.6514228 -3.0597464
O 1.7356093 0.1116873 -4.8961327

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Compound 2 - Keto S1 ADC(2)/def2-TZVP

C 0.1240147 2.1901738 -3.1856931
C 0.2468801 0.8053844 -3.4010436
C 0.3499458 -1.2145574 4.1041793
C 0.4963471 -0.0459011 -1.0235545
C 0.7190161 -2.4140471 6.1796552
C 0.7708060 -0.0453739 -2.3459731
C 0.8437801 -0.9853265 1.2913646
C 1.1406015 -0.8968630 -0.0999625
C 1.3815939 -1.9425634 3.4759009
C 1.6194023 -1.8248087 2.1182699
C -0.1918085 0.2658302 -4.6270797
C -0.2015332 -0.2783146 1.9186446
C -0.4432482 -0.3931539 3.2781555
C -0.4548272 3.0063249 -4.1425438
C -0.7666188 1.1033309 -5.5800957
C -0.9106351 2.4696889 -5.3542954
C -1.1402480 -0.8295597 5.9794177
C -1.5624948 3.3486582 -6.3828594
H 0.3607361 -3.3828673 5.8033896
H 0.4289409 -1.4991241 -4.2585695
H 0.4639902 -2.3337997 7.2352493
H 0.5018162 2.6037568 -2.2571786
H 1.8066051 -2.3960436 6.1035109
H 1.9402207 -1.5319184 -0.4821197
H 2.0114921 -2.6086251 4.0506804
H 2.4263302 -2.3990644 1.6713622
H -0.2708013 0.6513295 -0.7047890
H -0.5419405 4.0723371 -3.9604381
H -0.8551421 0.3600725 1.3335101
H -1.1010325 4.3371587 -6.4045197
H -1.1032563 0.6563915 -6.5099620
H -1.1528670 -0.9528642 7.0612747
H -1.2672844 0.1693773 3.6971648
H -1.2781056 0.2315330 5.7694894
H -1.4891894 2.9128989 -7.3798977
H -1.9897914 -1.3812877 5.5522762
H -2.6235332 3.4853293 -6.1566997

N 0.1370103 -1.2904021 5.4737307
O 1.7014458 -0.9662678 -2.9140100
O -0.1266179 -1.0568422 -4.9259411
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Compound - 2 Enol S1 CC2/def2-SV(P)

C 0.1402396 2.2496860 -3.2364402
C 0.2706163 0.8521584 -3.4168029
C 0.3086930 -1.2863049 4.1273804
C 0.4663823 0.0349016 -1.0129981
C 0.7521811 -2.4708269 6.2163416
C 0.7647438 0.0046187 -2.3366832
C 0.8129542 -0.9753014 1.2993805
C 1.1080597 -0.8423482 -0.0859154
C 1.3475359 -2.0091224 3.4737396
C 1.5848287 -1.8524080 2.1136376
C -0.1632238 0.2736155 -4.6431256
C -0.2353381 -0.2721299 1.9578230
C -0.4490673 3.0457321 -4.2167318
C -0.4804578 -0.4195850 3.3196095
C -0.7597773 1.0923942 -5.6170054
C -0.9034084 2.4725244 -5.4262854
C -1.1163429 -0.8383065 6.0599680
C -1.5726880 3.3252928 -6.4727309
H 0.4691369 -3.4826983 5.8558789
H 0.4856438 -2.3929278 7.2821494
H 0.5055480 -1.4690939 -4.2291017
H 0.5123591 2.6929650 -2.3046779
H 1.8492974 -2.3714444 6.1407903
H 1.9120698 -1.4741251 -0.5005078
H 1.9768624 -2.7080651 4.0316662
H 2.3968234 -2.4269748 1.6464502
H -0.2907565 0.7604560 -0.6882126
H -0.5398328 4.1279880 -4.0584691
H -0.8873178 0.3984619 1.3840203
H -1.0924508 0.6113799 -6.5449731
H -1.1034072 -0.9987759 7.1495437
H -1.1044672 4.3238988 -6.5290108
H -1.1552401 0.2513533 5.8858311
H -1.3109803 0.1426020 3.7557735
H -1.5094503 2.8554050 -7.4695058
H -2.0445082 -1.2895185 5.6489605
H -2.6435061 3.4697520 -6.2341663
N 0.0864340 -1.4095746 5.4866763
O 1.6856801 -0.9477481 -2.8982789
O -0.0738685 -1.0479059 -4.9139974
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Compound - 2 Enol S1 CC2/def2-TZVP

C 0.1011554 2.2292479 -3.2043158
C 0.2403793 0.8398229 -3.3908068
C 0.3412057 -1.2454778 4.1110612
C 0.4729407 0.0126427 -1.0022713
C 0.7210266 -2.4668169 6.1792478
C 0.7504487 0.0069628 -2.3171980
C 0.8363178 -0.9706101 1.2967308
C 1.1267996 -0.8578863 -0.0813832
C 1.3626533 -1.9857367 3.4666647
C 1.5985235 -1.8450545 2.1127493
C -0.1761146 0.2724086 -4.6179124

SUPPORTING INFORMATION

C	-0.1984466	-0.2526037	1.9464778
C	-0.4413735	-0.3876678	3.3025106
C	-0.4742588	3.0241096	-4.1831965
C	-0.7557305	1.0870964	-5.5928029
C	-0.9136597	2.4569743	-5.3914353
C	-1.1157842	-0.8300307	6.0136397
C	-1.5599456	3.3135460	-6.4421629
H	0.3625413	-3.4364983	5.8060345
H	0.4615821	2.6622868	-2.2766878
H	0.4720078	-2.3842577	7.2364858
H	0.4863077	-1.4607284	-4.2039026
H	1.8083994	-2.4434943	6.0918955
H	1.9245518	-1.4834189	-0.4859431
H	1.9781696	-2.6763796	4.0291217
H	2.3927858	-2.4265180	1.6508119
H	-0.2904244	0.7117698	-0.6737621
H	-0.5740040	4.0932631	-4.0227807
H	-0.8383159	0.4105872	1.3726646
H	-1.0560173	4.2786555	-6.5263927
H	-1.0766550	0.6208763	-6.5195244
H	-1.1110595	-0.9691386	7.0940248
H	-1.2046421	0.2396499	5.8174543
H	-1.2539851	0.1813531	3.7365312
H	-1.5394961	2.8266240	-7.4183583
H	-1.9980986	-1.3351554	5.5958853
H	-2.6056611	3.5097070	-6.1874392
N	0.1275699	-1.3466963	5.4735086
O	1.7035137	-0.9195339	-2.9039080
O	-0.0852071	-1.0538798	-4.8913160

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Compound - 2 Keto S1 CC2/def2-SV(P)

C	0.1786983	-0.3378774	-1.1230142
C	0.2253396	-0.5106166	-2.4891840
C	0.3765321	1.9426805	-5.3896811
C	0.4522447	-1.2036523	4.1029760
C	0.5335836	-1.2530515	1.2176963
C	0.6095514	-1.3234398	-0.2076799
C	0.7236927	0.8920256	-4.5032772
C	0.7964229	-2.3526317	6.2321470
C	1.0018922	-2.3096028	3.3955294
C	1.0365782	-2.3249329	2.0052785
C	-0.0274337	-0.1593067	1.9330738
C	-0.0678968	-0.1310355	3.3232977
C	-0.2310604	0.5219336	-3.4714096
C	-0.3044345	-0.1166125	6.1583436
C	-0.9078966	2.5385270	-5.3744915
C	-1.2327067	3.6623773	-6.3260756
C	-1.5077390	1.0272279	-3.5200140
C	-1.8372318	2.0725333	-4.4469533
H	0.0745969	0.8809868	5.8736399
H	0.1104721	-3.2032799	6.0363526
H	0.7653678	-2.1203703	7.3081711
H	1.0430145	-2.2350702	-0.6479201
H	1.1389106	2.2530194	-6.1176116
H	1.2386531	-1.2918546	-3.8471456
H	1.4011111	-3.1741198	3.9334296
H	1.4687463	-3.1966608	1.4946012
H	1.8248598	-2.6744912	5.9899879

SUPPORTING INFORMATION

H	-0.1676597	-0.2258815	7.2455802
H	-0.2476839	0.6096572	-0.7664516
H	-0.4496053	0.6933366	1.3862371
H	-0.5224554	0.7381507	3.8073211
H	-0.6965193	4.5875784	-6.0436892
H	-0.9335031	3.4052859	-7.3581963
H	-1.3915604	-0.1524003	5.9360740
H	-2.2632692	0.6843397	-2.7996083
H	-2.3149355	3.8810320	-6.3266913
H	-2.8436792	2.5112127	-4.4128194
N	0.4368385	-1.1641331	5.4832965
O	0.6939688	-1.6396165	-3.0635944
O	1.8161952	0.1987333	-4.6275250

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Compound - 2 Keto S1 CC2/def2-TZVP

C	0.0202858	-0.1530558	1.9124843
C	0.2403720	-0.3397373	-1.1125385
C	0.2999350	-0.4929105	-2.4695285
C	0.3074095	1.8638292	-5.4490592
C	0.4787615	-1.1824805	4.0783046
C	0.5859596	-1.2455277	1.2125390
C	0.6749154	-1.3230386	-0.2026315
C	0.6986579	0.8513924	-4.5493886
C	0.7172310	-2.3524831	6.1987821
C	1.0282639	-2.2883511	3.3873688
C	1.0794904	-2.3096121	2.0052161
C	-0.0362933	-0.1214829	3.2947818
C	-0.1701823	0.5426646	-3.4384592
C	-0.3772583	-0.1380811	6.1044831
C	-0.9318278	2.5288763	-5.3314609
C	-1.3045875	3.6074479	-6.3087028
C	-1.4014675	1.1263185	-3.3737788
C	-1.7778314	2.1438780	-4.3099379
H	0.6905098	-2.1269335	7.2640647
H	1.0026197	2.1172034	-6.2466322
H	1.1143842	-2.2240835	-0.6297022
H	1.2799449	-1.2364918	-3.8570491
H	1.4176301	-3.1391018	3.9324000
H	1.5099167	-3.1738853	1.5053081
H	1.7104678	-2.7397937	5.9654788
H	-0.0214550	-3.1371770	5.9846995
H	-0.0718633	0.8686260	5.8141454
H	-0.1909954	0.5910223	-0.7544319
H	-0.2518304	-0.2244714	7.1830073
H	-0.3923221	0.6870735	1.3621401
H	-0.4885605	0.7398791	3.7705446
H	-0.6136277	4.4517947	-6.2392663
H	-1.2644667	3.2354291	-7.3356166
H	-1.4415174	-0.2629118	5.8614682
H	-2.0956116	0.8418122	-2.5869554
H	-2.3139116	3.9768317	-6.1196604
H	-2.7431563	2.6292563	-4.1936366
N	0.4583088	-1.1322738	5.4583762
O	0.7895620	-1.6095509	-3.0567292
O	1.7841404	0.1501001	-4.7304268

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Compound 2 - MP2/def2-SV(P)

C	0.0920302	0.6194044	-3.4664349
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SUPPORTING INFORMATION

C	0.2210344	0.3837183	-4.8630552
C	0.2391800	-0.2831361	-1.0778657
C	0.3557112	-1.2189580	4.1268990
C	0.5809353	-0.4032216	-2.5109359
C	0.6738640	-1.0856110	1.2761165
C	0.8022920	-2.3678329	6.2292039
C	0.8761958	-1.0619931	-0.1663110
C	1.2348053	-2.0932812	3.4394603
C	1.3869970	-2.0170926	2.0565512
C	-0.2083814	-0.2222591	1.9584214
C	-0.2891240	1.3243342	-5.7762977
C	-0.3695190	-0.2854191	3.3391215
C	-0.5021525	1.8320865	-3.0483106
C	-0.8628344	-0.5299343	6.1247718
C	-0.8811259	2.5137514	-5.3515528
C	-0.9800940	2.7606004	-3.9662724
C	-1.4411777	3.4967059	-6.3466653
H	0.3681136	-3.3478824	5.9384620
H	0.6305220	-2.2173047	7.3060485
H	1.1606454	-1.2294695	-4.5967946
H	1.6252015	-1.7601588	-0.5678489
H	1.8096430	-2.8473531	3.9819124
H	1.8941343	-2.4137244	6.0733837
H	2.0780983	-2.7105559	1.5599100
H	-0.1754012	1.0971863	-6.8427156
H	-0.5347223	0.4260188	-0.7724609
H	-0.5690449	2.0648785	-1.9811761
H	-0.7839463	0.5517754	5.9189069
H	-0.7884440	0.5235673	1.4017460
H	-0.7992508	-0.6608390	7.2158584
H	-1.0080980	3.3379723	-7.3489778
H	-1.0729530	0.4073788	3.8069888
H	-1.2297531	4.5357536	-6.0385953
H	-1.4252964	3.6976147	-3.6099685
H	-1.8631453	-0.8759529	5.7887479
H	-2.5387789	3.3894019	-6.4307288
N	0.2234260	-1.2575964	5.5012787
O	0.8075588	-0.7103382	-5.3701159
O	1.2628549	-1.3622343	-2.9107053

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Compound 2 - MP2/def2-TZVP

C	0.0780982	0.6134415	-3.4428392
C	0.2256405	0.3879204	-4.8318808
C	0.2787376	-0.2560516	-1.0624802
C	0.3895750	-1.1823102	4.1049942
C	0.5735190	-0.3992384	-2.4949401
C	0.6692971	-1.0885427	1.2683593
C	0.7918175	-2.3527710	6.1908312
C	0.8574603	-1.0852327	-0.1684047
C	1.2515349	-2.0652413	3.4247197
C	1.3853379	-2.0092194	2.0460703
C	-0.2033792	-0.2218306	1.9435000
C	-0.2674479	1.3258418	-5.7443553
C	-0.3465689	-0.2681855	3.3194006
C	-0.5388861	1.8077403	-3.0277141
C	-0.8599254	-0.5303916	6.0818158
C	-0.8829049	2.4949054	-5.3208091
C	-1.0052461	2.7323844	-3.9438160

SUPPORTING INFORMATION

C -1.4260822 3.4818959 -6.3136323
H 0.3005011 -3.2876918 5.8881659
H 0.6348274 -2.2056261 7.2577775
H 1.1387045 -1.2090457 -4.5246105
H 1.5404257 -1.8317659 -0.5699364
H 1.8250162 -2.8026144 3.9695392
H 1.8649573 -2.4588302 6.0279596
H 2.0598054 -2.7024711 1.5522880
H -0.1410881 1.1142062 -6.8012741
H -0.4097847 0.5124562 -0.7420220
H -0.6312625 2.0280126 -1.9719968
H -0.7943223 0.4983774 1.3876460
H -0.7961042 -0.6370242 7.1631312
H -0.8455777 0.5364924 5.8562610
H -1.0085766 3.3151822 -7.3070213
H -1.0397646 0.4181866 3.7865123
H -1.2000249 4.5064505 -6.0124066
H -1.4676310 3.6501354 -3.5958739
H -1.8196921 -0.9445008 5.7437796
H -2.5133766 3.3948187 -6.3883542
N 0.2780734 -1.1980714 5.4814257
O 0.8273305 -0.7049900 -5.3244800
O 1.2269863 -1.3768014 -2.9053292
41

Compound - 3 Enol S1 ADC(2)/def2-SV(P)

C 0.0073172 0.1040067 6.4443369
C 0.1245190 -0.3997077 -0.8216520
C 0.1857635 -0.0372540 2.2204114
C 0.2045997 0.0441370 3.6106054
C 0.2418743 -0.5568555 -2.1690748
C 0.3218193 0.6768540 -4.3400861
C 0.7784926 -1.2540628 0.1000094
C 0.7859915 -1.1168887 1.5274878
C 0.8314736 -0.9480623 4.4062623
C 1.2755924 -2.0128812 6.5524654
C 1.4068940 -2.1078789 2.3276904
C 1.4315479 -2.0324538 3.7164881
C -0.3071397 1.4671574 -5.3133559
C -0.4227543 0.1619971 -3.2502230
C -1.6603415 3.0431258 -7.2028239
C -1.6757482 1.7449270 -5.2172757
C -1.8114093 0.4333476 -3.1880965
C -2.4316161 1.2204540 -4.1458289
H 0.1856220 0.0645151 7.5304000
H 0.2288486 1.1335354 6.1147476
H 0.3201786 1.8419936 -6.1250108
H 0.5950437 -2.8793526 6.4052770
H 1.2832732 -1.7540795 7.6229162
H 1.3317963 -2.1057801 -0.3283641
H 1.8803677 -2.9676764 1.8346625
H 1.9215148 -2.8401563 4.2661141
H 1.9396897 -0.2289841 -3.8719530
H 2.2985827 -2.3289915 6.2857045
H -0.2825382 0.9039844 4.0776141
H -0.3039096 0.7701523 1.6623826
H -0.5067131 0.4310769 -0.4836720
H -0.8605593 3.7278812 -6.8650340
H -1.0699779 -0.0960622 6.2576051

SUPPORTING INFORMATION

H -1.2212389 2.2514911 -7.8378418
H -2.3914373 0.0075159 -2.3613678
H -2.4016322 3.6085182 -7.7863451
H -3.5030311 1.4409455 -4.1073828
N 0.8813032 -0.8469974 5.7902343
O 1.1023469 -1.5371778 -2.7409612
O 1.6516539 0.4800154 -4.4896715
O -2.3660595 2.4936712 -6.1073941

41

Compound - 3 Enol S1 ADC(2)/def2-TZVP

C 0.1378511 -0.4148230 -0.8160184
C 0.1675732 -0.0599733 2.1979132
C 0.1970668 0.0362599 3.5800680
C 0.2083047 -0.5731905 -2.1527046
C 0.3025681 0.6691157 -4.3091951
C 0.7832274 -1.2770806 0.1006514
C 0.7899742 -1.1257964 1.5171227
C 0.8609376 -0.9190732 4.3749543
C 1.2841656 -1.9767089 6.5157863
C 1.4418858 -2.0867581 2.3188703
C 1.4735494 -1.9942783 3.6988216
C -0.0222731 0.0914858 6.3954196
C -0.3127537 1.4629197 -5.2759500
C -0.4392619 0.1689194 -3.2217916
C -1.6153192 3.0376267 -7.1591989
C -1.6717706 1.7490419 -5.1764491
C -1.8194814 0.4471325 -3.1600994
C -2.4299396 1.2349092 -4.1126630
H 0.1155636 1.1177044 6.0536875
H 0.1544260 0.0788286 7.4699272
H 0.3036543 1.8332080 -6.0834977
H 0.5813205 -2.8075608 6.3591689
H 1.2937819 -1.7227470 7.5747153
H 1.3166809 -2.1323841 -0.3147897
H 1.8947081 -0.2583298 -3.8499377
H 1.9260567 -2.9304219 1.8345977
H 1.9850011 -2.7705872 4.2526038
H 2.2854329 -2.3187550 6.2524132
H -0.3042130 0.8771082 4.0414772
H -0.3524227 0.7125029 1.6411539
H -0.4433502 0.4355353 -0.4757095
H -0.8162242 3.6957876 -6.8090241
H -1.0654122 -0.2000622 6.2065754
H -1.1899760 2.2384220 -7.7713933
H -2.3273013 3.6092299 -7.7483665
H -2.3932986 0.0310921 -2.3397739
H -3.4880329 1.4620876 -4.0694948
N 0.9303752 -0.7941526 5.7569413
O 0.9784991 -1.5935187 -2.7729569
O 1.6340452 0.4604144 -4.4557176
O -2.3556188 2.5068694 -6.0681370

41

Compound - 3 Keto S1 ADC(2)/def2-SV(P)

C 0.0009812 0.8478228 -3.1770977
C 0.1405824 -0.2443314 2.1298217
C 0.5953956 -0.0300826 -0.8951451
C 0.8614242 0.0631405 -2.2346618
C 0.9147218 -1.1270579 4.2854079

SUPPORTING INFORMATION

C	1.2132917	-0.8481242	1.4294974
C	1.4098072	-0.7465038	0.0111067
C	1.5826653	-2.2202748	6.3595238
C	1.9850992	-1.7412231	3.5879748
C	2.1245550	-1.6014418	2.2100507
C	-0.0062727	-0.3792026	3.5082166
C	-0.3313356	2.1684157	-2.9691708
C	-0.4560975	0.1922169	-4.3783328
C	-0.4647146	-0.8375400	6.2756790
C	-1.2324801	2.8321212	-3.8475334
C	-1.3628315	0.8666004	-5.2436025
C	-1.7463446	2.1901420	-4.9794751
C	-3.1455982	2.3002363	-6.8886481
H	0.0543928	2.7007625	-2.0908066
H	1.3677433	-3.2599800	6.0310366
H	1.3796304	-2.1474047	7.4395812
H	1.6299008	-0.8787121	-3.6648878
H	2.2805029	-1.2641281	-0.4191390
H	2.6598646	-2.0290129	6.2156970
H	2.7239740	-2.3460971	4.1201054
H	2.9678001	-2.0959086	1.7091969
H	-0.2931179	0.5072987	-0.5372142
H	-0.3843669	-0.9636576	7.3668508
H	-0.6080501	0.3462795	1.5874895
H	-0.6777290	0.2283468	6.0851551
H	-0.8641447	0.1076268	3.9797410
H	-1.3305586	-1.4343273	5.9162010
H	-1.5390885	3.8665746	-3.6568625
H	-1.6993751	0.3043003	-6.1187327
H	-2.3576602	2.0087377	-7.6080193
H	-3.7396145	1.4081040	-6.6155527
H	-3.8034174	3.0493583	-7.3523523
N	0.7865000	-1.2316342	5.6638016
O	0.0035794	-0.9707515	-4.6901743
O	1.9545790	-0.5128044	-2.8013339
O	-2.5941931	2.9221158	-5.7433923

41

Compound - 3 Keto S1 ADC(2)/def2-TZVP

C	0.0144311	-0.3580471	3.4856262
C	0.1540793	-0.2431249	2.1118475
C	0.5944247	-0.0590003	-0.8877323
C	0.8323476	0.0208338	-2.2218602
C	0.9400326	-1.0803043	4.2659003
C	1.2217125	-0.8524128	1.4222536
C	1.4132185	-0.7724238	0.0114148
C	1.5733390	-2.1903649	6.3283945
C	2.0002657	-1.7052151	3.5791485
C	2.1351770	-1.5878745	2.2063056
C	-0.0346691	0.8076035	-3.1507594
C	-0.3998297	2.1018820	-2.8995572
C	-0.4590305	-0.8216396	6.2325482
C	-0.4630245	0.1930090	-4.3743572
C	-1.2765690	2.7888405	-3.7772242
C	-1.3437018	0.8880832	-5.2383844
C	-1.7560788	2.1849076	-4.9320156
C	-3.0882020	2.3196936	-6.8780390
H	1.3027219	-3.2008667	5.9907488
H	1.3806131	-2.1164355	7.3977091

SUPPORTING INFORMATION

H 1.5591512 -0.8983443 -3.6702543
H 2.2695507 -1.2958849 -0.4105433
H 2.6445952 -2.0528262 6.1782815
H 2.7338202 -2.2909983 4.1177526
H 2.9666724 -2.0831470 1.7124200
H -0.0396341 2.6043682 -2.0076985
H -0.2747347 0.4815919 -0.5242432
H -0.3881774 -0.9271571 7.3141615
H -0.5934707 0.3241094 1.5669139
H -0.7221357 0.2153927 6.0216357
H -0.8325615 0.1276219 3.9530468
H -1.2713660 -1.4666344 5.8685323
H -1.5947390 3.8007751 -3.5514266
H -1.6583128 0.3625208 -6.1310147
H -2.2704812 2.0702349 -7.5593524
H -3.6580983 1.4165240 -6.6444113
H -3.7402503 3.0534557 -7.3432450
N 0.8235376 -1.1547047 5.6474140
O 1.9073500 -0.5725191 -2.8070639
O -0.0051369 -0.9660585 -4.7095227
O -2.5968366 2.9345362 -5.6933499

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Compound - 3 Keto S1 ADC(2)/def2-TZVP

C 0.4378916 1.4062516 -4.1740403
C 0.4929805 -0.2226646 -0.9058917
C 0.7218580 -0.1853622 -2.2434759
C 0.7363428 -1.2821066 4.2458693
C 1.0789156 -1.0267281 1.4112784
C 1.3051347 -0.9262096 0.0069704
C 1.3373552 -2.4002690 6.3138009
C 1.8183908 -1.8897448 3.5778453
C 1.9820673 -1.7599496 2.2092826
C -0.0120295 -0.4373539 2.0814288
C -0.1663576 0.5497993 -3.1943611
C -0.1802703 -0.5643812 3.4509359
C -0.3818044 2.1709604 -5.0392518
C -0.7074492 -1.0527516 6.1837147
C -1.5268326 0.4060365 -3.1933192
C -1.7708002 2.0579360 -4.9790344
C -2.0670850 3.6528289 -6.6960572
C -2.3354685 1.1724863 -4.0705910
H 0.1291250 2.8232626 -5.7359791
H 1.0857431 -3.4114251 5.9635817
H 1.1208306 -2.3360440 7.3791799
H 2.0648739 -0.2417330 -3.5335157
H 2.1749052 -1.4388200 -0.4006125
H 2.4099516 -2.2495470 6.1878370
H 2.5463564 -2.4718379 4.1279185
H 2.8302270 -2.2412488 1.7301406
H -0.3795750 0.3207696 -0.5549968
H -0.6586691 -1.1655784 7.2658067
H -0.7530369 0.1269884 1.5246945
H -0.9766502 -0.0168894 5.9746819
H -1.0429593 -0.0922315 3.9032602
H -1.4293924 3.1277500 -7.4121058
H -1.4853219 4.4248872 -6.1856281
H -1.5051927 -1.7032388 5.7977776
H -1.9998509 -0.2802031 -2.4983493

SUPPORTING INFORMATION

H -2.9029428 4.1099043 -7.2179882
H -3.4158296 1.0836165 -4.0367817
N 0.5906066 -1.3684385 5.6238368
O 1.7218670 1.4383327 -4.2998532
O 1.7544704 -0.8532541 -2.8247280
O -2.6423755 2.7462003 -5.7632810

41

Compound - 3 Enol S1 CC2/def2-TZVP

C 0.0002130 0.0796960 6.4253630
C 0.1009319 -0.3711640 -0.7985915
C 0.1530501 -0.0498519 2.2217961
C 0.1592209 -0.5451223 -2.1276896
C 0.1856926 0.0357232 3.6034244
C 0.2910714 0.6759408 -4.2917498
C 0.7640114 -1.2456900 0.1165710
C 0.7855969 -1.1078410 1.5217567
C 0.8635003 -0.9265420 4.3875842
C 1.3180750 -1.9968013 6.5217225
C 1.4554913 -2.0709152 2.3197535
C 1.4914715 -1.9927754 3.6987787
C -0.3009901 1.4710774 -5.2759075
C -0.4813762 0.1746977 -3.2158650
C -1.5633492 3.0409311 -7.1916511
C -1.6691053 1.7354814 -5.2169358
C -1.8704637 0.4265970 -3.2051374
C -2.4613308 1.2054444 -4.1788272
H 0.1513836 1.1048111 6.0838623
H 0.1928427 0.0564847 7.4973940
H 0.3339480 1.8449696 -6.0683082
H 0.6334272 -2.8424595 6.3645925
H 1.2894643 -2.0960483 -0.3213637
H 1.3266496 -1.7446397 7.5815471
H 1.8311324 -0.2915413 -3.7965159
H 1.9477309 -2.9042686 1.8240399
H 2.0129139 -2.7680300 4.2459729
H 2.3258168 -2.3130253 6.2483116
H -0.3240070 0.8655978 4.0769240
H -0.3780710 0.7205382 1.6713614
H -0.4746497 0.4815358 -0.4498901
H -0.7863629 3.7040290 -6.8024800
H -1.0495608 -0.1949163 6.2483674
H -1.1070435 2.2517269 -7.7948213
H -2.2654162 3.6089043 -7.7968758
H -2.4628474 0.0069542 -2.3987890
H -3.5235984 1.4206879 -4.1722569
N 0.9286834 -0.8201298 5.7672801
O 0.8903062 -1.5770725 -2.7994005
O 1.6227200 0.4613281 -4.3956081
O -2.3371730 2.4856776 -6.1277389

41

Compound - 3 Keto S1 CC2/def2-TZVP

C 0.1070239 -0.2492939 2.1603539
C 0.5272004 0.0115048 -0.8414264
C 0.7980008 0.1590398 -2.1711938
C 0.9159447 -1.1480754 4.2812104
C 1.1828401 -0.8271226 1.4443942
C 1.3619642 -0.7033867 0.0419958
C 1.6212435 -2.2596658 6.3285909

SUPPORTING INFORMATION

C	1.9879233	-1.7409550	3.5724878
C	2.1122272	-1.5773205	2.2048847
C	-0.0272497	-0.4067799	3.5282144
C	-0.0557928	0.9225283	-3.1229797
C	-0.2651178	2.2767603	-3.0503541
C	-0.4507758	-0.9059190	6.2828777
C	-0.5471477	0.1894730	-4.2646973
C	-1.1161313	2.9215421	-3.9807200
C	-1.4190219	0.8413702	-5.1760519
C	-1.7029276	2.2001105	-5.0224160
C	-3.1038784	2.2016227	-6.9308665
H	0.1782416	2.8538717	-2.2434647
H	1.4130513	-3.2823940	5.9860974
H	1.4250177	-2.2015786	7.3983249
H	1.5314268	-0.7304277	-3.6137780
H	2.2322025	-1.1903511	-0.3970839
H	2.6813705	-2.0520462	6.1726291
H	2.7289972	-2.3350548	4.0924654
H	2.9475301	-2.0453702	1.6898724
H	-0.3518475	-1.0419050	7.3589711
H	-0.3641386	0.5151759	-0.4776704
H	-0.6448402	0.3299517	1.6331619
H	-0.6811953	0.1451870	6.1003935
H	-0.8769291	0.0533205	4.0173086
H	-1.2931010	-1.5138922	5.9258634
H	-1.3453680	3.9776901	-3.8827722
H	-1.8140878	0.2427127	-5.9882976
H	-2.3346616	1.8016238	-7.5977762
H	-3.7152802	2.9243241	-7.4660686
H	-3.7313749	1.3836408	-6.5653877
N	0.8022914	-1.2727448	5.6505696
O	1.8991815	-0.3825092	-2.7525193
O	-0.0952170	-1.0051576	-4.4766793
O	-2.5175945	2.9205001	-5.8484635

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Compound - 3 MP2/def2-SV(P)

C	0.1468901	-0.1645706	2.2488113
C	0.1492639	-0.2111454	3.6399817
C	0.4091198	-0.0951779	-0.8090301
C	0.5483521	-0.2523188	-2.2733161
C	1.0236556	-0.9580864	1.4805740
C	1.0345242	-1.0652948	4.3498700
C	1.0559347	-0.9496437	0.0236904
C	1.7831501	-2.1576719	6.3940375
C	1.8910114	-1.8166728	2.1842748
C	1.9051121	-1.8737212	3.5764662
C	-0.0225181	-0.4605246	6.4631543
C	-0.0907064	0.4804400	-4.5779491
C	-0.3434823	0.5012573	-3.1787781
C	-0.8926781	1.2291817	-5.4595602
C	-1.4353963	1.2782101	-2.7192229
C	-1.9531078	1.9930217	-4.9708687
C	-2.2331421	2.0052110	-3.5867455
C	-2.5463252	2.7551098	-7.1357328
H	0.1681210	-0.5687445	7.5420626
H	1.3338212	-0.7360756	-4.3806312
H	1.3924514	-3.1679483	6.1478927
H	1.6831637	-1.7129852	-0.4592628

H	1.7138059	-2.0128474	7.4830624
H	2.5788754	-2.4596621	1.6198605
H	2.5977691	-2.5675314	4.0583341
H	2.8532643	-2.1267577	6.1260626
H	-0.0645250	0.6204641	6.2442573
H	-0.2071781	0.7154678	-0.4117389
H	-0.5651792	0.4180245	4.1761534
H	-0.5719961	0.4976025	1.7513242
H	-0.6395451	1.1694528	-6.5202755
H	-1.0171167	-0.9004705	6.2368359
H	-1.5424473	3.1516180	-7.3755226
H	-1.6858311	1.2889986	-1.6544809
H	-2.6548212	1.7444314	-7.5709086
H	-3.0814455	2.5977670	-3.2304085
H	-3.3123824	3.4198067	-7.5614678
N	1.0544479	-1.0956868	5.7317129
O	0.8958327	-0.2390341	-5.1284819
O	1.4168054	-1.0155807	-2.7335773
O	-2.7755479	2.7420877	-5.7404595

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Compound - 3 MP2/def2-TZVP

C	0.1598198	-0.1529014	2.2327010
C	0.1667078	-0.1953960	3.6163365
C	0.3613012	-0.1420530	-0.8047540
C	0.5264810	-0.2596517	-2.2607312
C	1.0268736	-0.9504641	1.4709281
C	1.0548248	-1.0367303	4.3216905
C	1.0668771	-0.9418065	0.0219617
C	1.7654061	-2.1503531	6.3556853
C	1.8917041	-1.8033676	2.1706209
C	1.9091323	-1.8545422	3.5559684
C	-0.0282000	-0.4664259	6.4182052
C	-0.1025992	0.4796764	-4.5475657
C	-0.3445619	0.5119941	-3.1542575
C	-0.8968609	1.2233490	-5.4267423
C	-1.4213569	1.2962150	-2.6940957
C	-1.9441293	1.9898381	-4.9353074
C	-2.2122540	2.0209875	-3.5577897
C	-2.5227502	2.7247290	-7.1066004
H	0.1582055	-0.5537700	7.4870344
H	1.3034212	-0.7189014	-4.3086073
H	1.3193610	-3.1235228	6.1082924
H	1.7107732	-2.0052239	7.4330458
H	1.7442960	-1.6513914	-0.4496263
H	2.5653640	-2.4445635	1.6099246
H	2.5950864	-2.5371510	4.0386462
H	2.8203924	-2.1747464	6.0804268
H	-0.1261202	0.5950932	6.1883026
H	-0.3196721	0.5979628	-0.4097894
H	-0.5297856	0.4350411	4.1523162
H	-0.5469482	0.5068799	1.7406843
H	-0.6593348	1.1620157	-6.4799504
H	-0.9808575	-0.9619593	6.1858554
H	-1.5251781	3.1087358	-7.3338757
H	-1.6564523	1.3249052	-1.6383179
H	-2.6278138	1.7162175	-7.5141851
H	-3.0420415	2.6184030	-3.2009424
H	-3.2736877	3.3761124	-7.5459354

N 1.0913629 -1.0459156 5.7027730
 O 0.8831853 -0.2508527 -5.0851271
 O 1.4096701 -1.0055571 -2.7297569
 O -2.7696413 2.7390908 -5.7074414
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Compound - 4 Keto S1 ADC(2)/def2-SV(P)

C 0.3187713 -1.3266094 -0.4777504
 C 0.5598374 -2.4530534 -1.2220840
 C 0.7018731 2.5917348 3.0772075
 C 0.9588773 0.2576556 1.4011846
 C 1.1313539 -0.9245256 0.6035912
 C 1.6318239 4.0345514 4.8083723
 C 1.7258523 1.6349515 3.2896780
 C 1.8442766 0.5105126 2.4775008
 C -0.0528975 1.2240179 1.1838678
 C -0.1792541 2.3513210 1.9922829
 C -0.3069317 -2.8579562 -2.3761148
 C -0.3136609 4.7733585 3.4736894
 C -0.6857486 -1.9760474 -3.3529075
 C -0.7207595 -4.2419769 -2.4662977
 C -1.5943504 -2.3661017 -4.4068855
 C -1.6119342 -4.6115789 -3.4984903
 C -2.0272548 -1.3295718 -5.4029223
 C -2.0468125 -3.6762628 -4.4600309
 H 0.0146761 5.2407014 2.5202785
 H 1.2760945 -4.1871676 -1.1345584
 H 1.3380596 4.9137430 5.4031703
 H 1.8232857 3.2099722 5.5162670
 H 1.9726489 -1.5878555 0.8555499
 H 2.4521152 1.7645337 4.0963641
 H 2.5824580 4.2681188 4.2822213
 H 2.6525918 -0.2057358 2.6775382
 H -0.3265090 -0.9384813 -3.3196706
 H -0.3324372 5.5508403 4.2535637
 H -0.5510690 -0.7238374 -0.7710618
 H -0.7636961 1.1005831 0.3574234
 H -0.9801168 3.0584641 1.7601294
 H -1.1487203 -0.8918546 -5.9109969
 H -1.3497466 4.4162571 3.3437499
 H -1.9394274 -5.6576813 -3.5249837
 H -2.5604411 -0.5046802 -4.8959071
 H -2.6957415 -1.7610528 -6.1656452
 H -2.7404649 -3.9878907 -5.2511922
 N 0.5532373 3.6971747 3.9039100
 O 1.6215282 -3.2636362 -0.9872704
 O -0.2313867 -5.1249342 -1.6527708

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Compound - 4 Keto S1 ADC(2)/def2-TZVP

C 0.3189204 -1.3267735 -0.4768387
 C 0.5577926 -2.4536808 -1.2185513
 C 0.7041162 2.5909956 3.0706913
 C 0.9594552 0.2570244 1.3988400
 C 1.1305166 -0.9247196 0.6033136
 C 1.6314858 4.0316926 4.8022021
 C 1.7292378 1.6369776 3.2811333
 C 1.8460831 0.5121668 2.4717198
 C -0.0532960 1.2206691 1.1835252
 C -0.1781299 2.3485240 1.9889044

C -0.3075058 -2.8567498 -2.3721721
 C -0.3190204 4.7659780 3.4717441
 C -0.6845622 -1.9745671 -3.3475004
 C -0.7229580 -4.2383963 -2.4632781
 C -1.5912789 -2.3621537 -4.4017715
 C -1.6121586 -4.6059484 -3.4958389
 C -2.0211873 -1.3254741 -5.3965370
 C -2.0445851 -3.6704979 -4.4562550
 H 1.2696757 -4.1886417 -1.1297576
 H 1.3389530 4.9132524 5.3934661
 H 1.8166777 3.2083161 5.5130056
 H 1.9712850 -1.5881884 0.8557288
 H 2.4568711 1.7685149 4.0859253
 H 2.5857507 4.2602996 4.2811980
 H 2.6556437 -0.2026565 2.6704630
 H -0.0050604 5.2327579 2.5136403
 H -0.3240279 -0.9377782 -3.3131177
 H -0.3330445 5.5457116 4.2489891
 H -0.5492746 -0.7228924 -0.7717404
 H -0.7662989 1.0945901 0.3597271
 H -0.9805808 3.0540137 1.7583962
 H -1.1418714 -0.8887079 -5.9034308
 H -1.3546865 4.4035946 3.3544906
 H -1.9407862 -5.6513860 -3.5231217
 H -2.5532666 -0.5000446 -4.8899132
 H -2.6894910 -1.7546817 -6.1602402
 H -2.7373136 -3.9807704 -5.2483850
 N 0.5581989 3.6971712 3.8932675
 O 1.6166464 -3.2655946 -0.9824408
 O -0.2369254 -5.1219459 -1.6494812
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Compound - 4 Keto S1 ADC(2)/def2-TZVP

C 0.0802606 1.3059022 1.0442009
 C 0.4455312 -3.2176878 -3.7307494
 C 0.5146539 -1.1713489 -0.6598098
 C 0.7348561 -2.2944003 -1.3972230
 C 0.8049407 2.6544224 2.9455317
 C 1.1200386 0.3748066 1.2363448
 C 1.3247345 -0.7787163 0.4202389
 C 1.7436204 4.1251178 4.6313972
 C 1.8567557 1.7353586 3.1312196
 C 2.0018460 0.6328716 2.3059527
 C -0.0689605 2.4113567 1.8666618
 C -0.1544561 -2.7029879 -2.5272732
 C -0.2155515 4.8221949 3.3333354
 C -0.3886435 -3.5487350 -4.8123438
 C -1.5112170 -2.6426034 -2.4356975
 C -1.7836955 -3.4263563 -4.7229838
 C -2.3559951 -2.9872728 -3.5492996
 C -3.8359973 -2.8427509 -3.3907659
 H 0.0906896 -3.9040941 -5.7188610
 H 0.1546765 5.2785894 2.4042892
 H 1.4477375 4.9797786 5.2381019
 H 2.0143165 3.3178680 5.3126140
 H 2.0391435 -3.4670022 -2.0288203
 H 2.1762386 -1.4151129 0.6555764
 H 2.5743162 1.8757378 3.9291597
 H 2.6336192 4.3990823 4.0472027

SUPPORTING INFORMATION

H	2.8250982	-0.0541515	2.4814965
H	-0.2554478	5.5883898	4.1062721
H	-0.3476684	-0.5739086	-0.9406504
H	-0.6227383	1.1768247	0.2276505
H	-0.8840807	3.0929227	1.6597628
H	-1.2354327	4.4753992	3.1638325
H	-1.9763464	-2.3125138	-1.5104577
H	-2.4086647	-3.6856136	-5.5714034
H	-4.0947961	-1.8042255	-3.1699714
H	-4.1883783	-3.4475176	-2.5515051
H	-4.3663053	-3.1500335	-4.2909935
N	0.6250552	3.7371955	3.7965343
O	1.7273244	-3.4125327	-3.7944388
O	1.7589219	-3.1442532	-1.1341281

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Compound - 4 Keto S1 CC2/def2-SV(P)

C	0.2626418	-1.2550122	-0.4905394
C	0.5103771	-2.3636593	-1.2714229
C	0.7545798	2.6145705	3.1033417
C	0.9633870	0.3043216	1.3854943
C	1.1055777	-0.8614748	0.5720826
C	1.6968491	3.9980511	4.8839277
C	1.7942254	1.6568728	3.2718268
C	1.8871347	0.5469429	2.4393312
C	-0.0628852	1.2744391	1.2153485
C	-0.1676194	2.3887215	2.0411728
C	-0.3168677	4.7512625	3.6187837
C	-0.3698282	-2.7936322	-2.4063380
C	-0.6789319	-1.9875072	-3.4721655
C	-0.7844899	-4.1881752	-2.3988332
C	-1.5849062	-2.4307294	-4.5049056
C	-1.6903808	-4.6062164	-3.4058428
C	-1.9864479	-1.4688174	-5.5867494
C	-2.0807526	-3.7321216	-4.4411503
H	1.1837679	-4.1025818	-1.2187831
H	1.4085032	4.8733424	5.4867153
H	1.8517018	3.1519221	5.5768409
H	1.9567805	-1.5272254	0.7844954
H	2.5458131	1.7807323	4.0565931
H	2.6626488	4.2190725	4.3833283
H	2.7035590	-0.1706929	2.6002279
H	-0.0922630	5.2500829	2.6528449
H	-0.2849855	-0.9609054	-3.5119476
H	-0.2959816	5.5108622	4.4157765
H	-0.6215363	-0.6593502	-0.7551715
H	-0.7987152	1.1567912	0.4097590
H	-0.9764785	3.0990617	1.8474077
H	-1.0968254	-1.0678000	-6.1082972
H	-1.3439443	4.3478158	3.5697352
H	-2.0563657	-5.6399701	-3.3605390
H	-2.5363987	-0.6054782	-5.1652494
H	-2.6357872	-1.9577785	-6.3331418
H	-2.7810314	-4.0846144	-5.2107415
N	0.6355506	3.7060391	3.9398596
O	1.5741420	-3.1672332	-1.0796186
O	-0.2538167	-4.9999282	-1.5334561

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Compound - 4 Keto S1 CC2/def2-TZVP

C	0.2692741	-1.2891245	-0.4533913
C	0.5005562	-2.3984663	-1.2189954
C	0.7202393	2.5750374	3.0926592
C	0.9467962	0.2615285	1.4127959
C	1.0974603	-0.9058483	0.6193032
C	1.6862199	4.0111407	4.8037024
C	1.7506573	1.6243209	3.2859758
C	1.8510117	0.5094293	2.4737310
C	-0.0680897	1.2283928	1.2151213
C	-0.1776762	2.3474232	2.0214165
C	-0.2837352	4.7547102	3.5061488
C	-0.3689377	-2.8084385	-2.3663813
C	-0.7171100	-4.2082279	-2.4567395
C	-0.7389087	-1.9501912	-3.3578716
C	-1.5660394	-4.6096137	-3.5079740
C	-1.5995665	-2.3717593	-4.4318841
C	-2.0086129	-3.6926359	-4.4754820
C	-2.0403739	-1.3617502	-5.4441683
H	0.0427917	5.2169014	2.5644064
H	1.1337501	-4.1401012	-1.2052616
H	1.4001624	4.8759083	5.4009120
H	1.8974831	3.1884347	5.4889555
H	1.9297570	-1.5689556	0.8541357
H	2.4798853	1.7566517	4.0753579
H	2.6062615	4.2503868	4.2529493
H	2.6531951	-0.2029633	2.6501079
H	-0.2899878	5.5153070	4.2857388
H	-0.4053998	-0.9140994	-3.3276973
H	-0.5911403	-0.6859412	-0.7297280
H	-0.7824401	1.1054245	0.4067036
H	-0.9715759	3.0542311	1.8141229
H	-1.1763889	-0.8981216	-5.9300855
H	-1.3079396	4.3993290	3.3803081
H	-1.8674532	-5.6527365	-3.5414795
H	-2.6100622	-0.5576300	-4.9678408
H	-2.6653153	-4.0273721	-5.2737740
H	-2.6666058	-1.8173042	-6.2121313
N	0.5863394	3.6708676	3.9212569
O	1.5433817	-3.2287697	-1.0095493
O	-0.1918629	-5.0553744	-1.6153743

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Compound - 4 MP2/def2-SV(P)

C	0.1375808	-1.3636961	-0.3549256
C	0.3812206	-2.6641210	-1.0144111
C	0.7256575	2.6589407	3.0208889
C	0.8475623	0.2732108	1.4279830
C	0.9393865	-0.9646201	0.6653383
C	1.6113318	1.5997141	3.3424068
C	1.6469945	4.0197267	4.8196988
C	1.6644653	0.4461540	2.5628237
C	-0.0170408	1.3362121	1.0939365
C	-0.0768812	4.9456814	3.2957126
C	-0.0800764	2.4946583	1.8626496
C	-0.2503516	-4.3037023	-2.7983657
C	-0.2984977	-2.9741452	-2.2962167
C	-0.9473509	-4.6132570	-3.9814447
C	-1.0014922	-1.9946678	-3.0363553
C	-1.6405308	-3.6295521	-4.6776400

SUPPORTING INFORMATION

C	-1.6761980	-2.2954236	-4.2201894
C	-2.3936812	-1.2326705	-5.0131780
H	0.3679313	5.3536346	2.3632495
H	0.8967671	-4.8905136	-1.4219940
H	1.4068554	4.9478078	5.3607636
H	1.6517679	3.2000043	5.5587693
H	1.7358297	-1.6648463	0.9571428
H	2.2761693	1.6707291	4.2061995
H	2.3630104	-0.3525321	2.8443923
H	2.6703983	4.1139321	4.3985668
H	-0.0671528	5.7374561	4.0604736
H	-0.6497223	1.2696931	0.2005282
H	-0.6999842	-0.7448680	-0.6876115
H	-0.7614288	3.2867618	1.5435264
H	-0.9074556	-5.6483147	-4.3378867
H	-1.0071288	-0.9573127	-2.6851768
H	-1.1331482	4.6965250	3.0950128
H	-1.8629821	-1.0127487	-5.9578029
H	-2.1692347	-3.8988497	-5.6017563
H	-2.4674949	-0.2926276	-4.4398498
H	-3.4180115	-1.5549403	-5.2726135
N	0.6389639	3.7936752	3.8044444
O	0.4216961	-5.2962991	-2.1972213
O	1.1422561	-3.4948089	-0.4898682

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Compound - 4 MP2/def2-TZVP

C	0.1683600	-1.3384772	-0.3742514
C	0.3875878	-2.6414637	-1.0175173
C	0.6897691	2.6235036	3.0307997
C	0.8050415	0.2477730	1.4573291
C	0.9003613	-0.9860771	0.7036728
C	1.5695144	1.5719242	3.3559287
C	1.6159283	0.4187581	2.5880438
C	1.6619972	4.0107569	4.7667541
C	-0.0437386	4.9279361	3.2458890
C	-0.0553167	1.3036811	1.1205957
C	-0.1107548	2.4603731	1.8787058
C	-0.2155214	-4.2639154	-2.8057284
C	-0.2916341	-2.9489582	-2.2893375
C	-0.8896258	-4.5729230	-3.9919471
C	-1.0156479	-1.9815822	-3.0121441
C	-1.6006371	-3.5997940	-4.6721541
C	-1.6689018	-2.2810816	-4.1983668
C	-2.4180406	-1.2303822	-4.9683619
H	0.4520519	5.2853257	2.3329918
H	0.9061306	-4.8066954	-1.4183395
H	1.4394734	4.9326369	5.3008472
H	1.6380511	-1.7090199	1.0474469
H	1.7142825	3.2083180	5.5035036
H	2.2240035	1.6479405	4.2134252
H	2.3026750	-0.3746838	2.8675921
H	2.6468007	4.1089922	4.2897498
H	-0.0288655	5.7262711	3.9855509
H	-0.5923625	-0.6795982	-0.7673997
H	-0.6892281	1.2313784	0.2431867
H	-0.7866973	3.2455327	1.5681590
H	-0.8288979	-5.5899386	-4.3625830
H	-1.0541798	-0.9615304	-2.6488936

SUPPORTING INFORMATION

H -1.0878694 4.7172113 3.0118808
H -1.9382968 -1.0305858 -5.9295084
H -2.1113313 -3.8626040 -5.5941961
H -2.4600628 -0.2922417 -4.4135578
H -3.4426922 -1.5479341 -5.1731243
N 0.6021955 3.7596462 3.8106117
O 0.4747876 -5.2427315 -2.2013887
O 1.1312908 -3.4857408 -0.4838647

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Compound - 5 Keto S1 ADC(2)/def2-SV(P)

C 0.3253795 -0.0607913 -1.7237301
C 0.3465947 0.0062628 3.9380163
C 0.7718390 1.4676961 5.8738058
C 0.8065162 -0.2832221 -3.0114651
C 1.1096828 0.3439423 5.1134881
C 1.7954497 -0.4932451 -5.6679682
C 2.5364382 -1.5470697 4.8267229
C -0.0660745 -0.5643067 -4.0940088
C -0.3180232 2.2561322 5.4963169
C -0.5178432 -0.8287713 -6.4750787
C -0.6792406 0.8230083 3.5401124
C -0.8761690 0.3961112 1.0618518
C -1.0589422 -0.1002777 -1.4250388
C -1.1004758 1.9419296 4.3542536
C -1.4533216 -0.5956118 -3.8025325
C -1.4628470 0.5522821 2.2858874
C -1.6088856 0.1278171 -0.1207091
C -1.9259338 -0.3719919 -2.5128776
H 0.0257932 -1.0734948 -7.4011249
H 0.2195002 0.4676764 1.0315834
H 0.6063335 -0.8633029 3.3261020
H 1.0532598 0.1562660 -0.9321457
H 1.3762749 1.6997809 6.7577852
H 1.7129764 -2.2829383 4.8248103
H 1.8868824 -0.2267200 -3.1695373
H 2.0129306 -0.7781949 -6.7093346
H 2.0218186 0.5877928 -5.5454720
H 2.4840212 -1.0650973 -5.0223516
H 2.8348252 -1.3148160 3.7890427
H 3.3967917 -1.9578688 5.3732768
H -0.6169294 3.1311791 6.0854504
H -1.0319117 0.1461685 -6.6168173
H -1.2872428 -1.6067575 -6.3320580
H -2.1849848 -0.7895057 -4.5912401
H -2.7034177 0.0815019 -0.0142819
H -3.0088107 -0.4028014 -2.3315344
H -3.0140012 1.1938332 3.1106676
N 0.4169537 -0.8191550 -5.3697101
O 2.1666247 -0.3668253 5.5308223
O -2.1921401 2.5655297 4.0671675
O -2.7996913 0.4478552 2.4818534

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Compound - 5 Keto S1 ACD(2)/def2-TZVP

C 0.0258848 -0.6856335 -1.5837121
C 0.2579588 0.1064323 6.0856404
C 0.4005956 -1.2008381 -2.8140465
C 0.6026949 0.7341710 3.7397417
C 1.1193417 0.3806988 5.0320371

SUPPORTING INFORMATION

C	1.3778365	-2.0466689	-5.3270755
C	3.3512020	0.5865933	4.2330490
C	-0.2385153	-0.8063691	-4.0073045
C	-0.3221084	-0.6624553	-6.4283334
C	-0.7432559	0.7725585	3.5392839
C	-0.9102661	0.5119661	1.0475050
C	-1.0073455	0.2660569	-1.4620299
C	-1.1144204	0.2055378	5.8847180
C	-1.2591341	0.1594700	-3.8935294
C	-1.3197264	1.1072467	2.1944517
C	-1.4379269	0.8257175	-0.2252355
C	-1.6300848	0.6708876	-2.6621464
C	-1.6553534	0.5639191	4.6319460
H	0.0195295	-1.2196055	-7.2994435
H	0.0738905	0.3612514	-6.4874875
H	0.5552328	-1.0304110	-0.7013227
H	0.6766836	-0.1648163	7.0480180
H	1.2045709	-1.9252848	-2.8390327
H	1.2689592	0.9501155	2.9137820
H	1.4024905	-2.9064757	-4.6566981
H	1.4987880	-2.4207647	-6.3426415
H	2.2308958	-1.3957348	-5.0881636
H	3.2209247	1.6161563	3.8951820
H	3.2251448	-0.1019087	3.3956624
H	4.3380997	0.4618964	4.6681972
H	-0.1255863	-0.2327778	1.1451807
H	-1.4103807	-0.6137535	-6.4767302
H	-1.7753509	0.5189779	-4.7742274
H	-1.8107007	0.0147764	6.6947057
H	-2.2393397	1.5622339	-0.2563544
H	-2.4233117	1.4118921	-2.6142720
H	-2.7816755	1.8657421	3.0503465
N	0.1067869	-1.3587493	-5.2326421
O	2.4330053	0.2779407	5.2866111
O	-2.2654198	2.0770284	2.2269999
O	-2.9206141	0.7629801	4.4593706

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Compound - 5 Keto S1 ADC(2)/def2-TZVP

C	0.3081060	-0.0876322	-1.6811898
C	0.3573772	0.0570695	3.8646581
C	0.7561954	1.4097582	5.8714761
C	0.7996574	-0.3337305	-2.9529544
C	1.1093922	0.3450725	5.0536151
C	1.8096795	-0.5365599	-5.5843712
C	2.5564167	-1.4944182	4.6239595
C	-0.0575474	-0.6181609	-4.0356244
C	-0.3539801	2.1799751	5.5427780
C	-0.4787425	-0.8305516	-6.4157990
C	-0.6928051	0.8526016	3.5221059
C	-0.9051925	0.4097462	1.0597273
C	-1.0748151	-0.0962415	-1.4064341
C	-1.1230648	1.9161886	4.3898399
C	-1.4420061	-0.6113989	-3.7700210
C	-1.4829777	0.6009232	2.2710254
C	-1.6366881	0.1548093	-0.1219639
C	-1.9283354	-0.3637786	-2.4981117
H	0.0566964	-1.0899576	-7.3279443
H	0.1801649	0.4448143	1.0335391

H	0.6268585	-0.7724322	3.2227194
H	1.0189373	0.1307868	-0.8908023
H	1.3467070	1.6076068	6.7587356
H	1.7470909	-2.2254821	4.5833252
H	1.8718400	-0.3029036	-3.0988820
H	1.9849632	0.5435921	-5.4801715
H	2.0466534	-0.8312215	-6.6056471
H	2.4996295	-1.0626483	-4.9237437
H	2.8280536	-1.1789457	3.6150936
H	3.4200387	-1.9255528	5.1210913
H	-0.6642738	3.0066390	6.1733494
H	-0.9139578	0.1716530	-6.5357597
H	-1.2921088	-1.5472233	-6.2982481
H	-2.1539719	-0.8019203	-4.5625653
H	-2.7219220	0.1399035	-0.0342156
H	-2.9842130	1.2790775	3.1261202
H	-3.0021634	-0.3674770	-2.3323078
N	0.4396688	-0.9102706	-5.2981357
O	2.1836882	-0.3683311	5.4249322
O	-2.2162989	2.5545896	4.1297325
O	-2.8227504	0.5520315	2.4670688

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Compound - 5 Keto S1 CC2/def2-SV(P)

C	0.3530248	-0.0657024	-1.7644783
C	0.3950389	0.0248491	3.9593381
C	0.6744430	1.4380357	5.9485722
C	0.8148714	-0.2847646	-3.0575465
C	1.0976827	0.3520745	5.1710803
C	1.7768128	-0.5692288	-5.7191503
C	2.6127647	-1.4688700	4.8882970
C	-0.0844979	-0.5353665	-4.1343402
C	-0.4417244	2.1915257	5.5600748
C	-0.5742330	-0.8481545	-6.5078271
C	-0.6402343	0.8280941	3.5400332
C	-0.8147372	0.4164444	1.0329687
C	-1.0341338	-0.0788938	-1.4472523
C	-1.1665291	1.8839229	4.3790423
C	-1.4072277	0.5611472	2.2708757
C	-1.4751535	-0.5440037	-3.8278445
C	-1.5568347	0.1511261	-0.1393028
C	-1.9233984	-0.3233993	-2.5306518
H	0.2810510	0.4858203	1.0016074
H	0.7097039	-0.8158656	3.3299949
H	1.0922477	0.1242405	-0.9759542
H	1.2337656	1.6712542	6.8625674
H	1.8165929	-2.2347582	4.8364936
H	1.8940685	-0.2504960	-3.2322311
H	1.9564255	-0.8407902	-6.7710359
H	2.0944120	0.4837091	-5.5695535
H	2.4170502	-1.2165280	-5.0935500
H	2.9344976	-1.1995914	3.8647728
H	3.4714032	-1.8689910	5.4476642
H	-0.0311815	-1.0845538	-7.4361143
H	-0.7994360	3.0281475	6.1735562
H	-1.1260427	0.1033886	-6.6563195
H	-1.3112287	-1.6530971	-6.3376447
H	-2.2184935	-0.7146097	-4.6116374
H	-2.6507878	0.1147406	-0.0165769

SUPPORTING INFORMATION

H -2.8911260 1.2504526 3.1670649
H -3.0042220 -0.3342263 -2.3329515
N 0.3741751 -0.7750601 -5.4129143
O 2.1816940 -0.3251032 5.6127681
O -2.3033916 2.4377250 4.0603121
O -2.7271118 0.4853560 2.4677934

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Compound - 5 Keto S1 CC2/def2-TZVP

C 0.3313187 -0.1003107 -1.7142898
C 0.4041038 0.0836922 3.8796997
C 0.6569950 1.3644151 5.9493392
C 0.8065957 -0.3485711 -2.9893037
C 1.0974227 0.3493415 5.1057500
C 1.7954988 -0.6198578 -5.6273356
C 2.6441287 -1.4040173 4.6600562
C -0.0755649 -0.5989750 -4.0691864
C -0.4820414 2.0972279 5.6152201
C -0.5273496 -0.8456018 -6.4477951
C -0.6643483 0.8586352 3.5257658
C -0.8520509 0.4267570 1.0359036
C -1.0549302 -0.0733298 -1.4253120
C -1.1911140 1.8552378 4.4189729
C -1.4381781 0.6152228 2.2586109
C -1.4638148 -0.5587676 -3.7938312
C -1.5918539 0.1838629 -0.1385175
C -1.9278981 -0.3090510 -2.5157102
H 0.0065351 -1.1242123 -7.3552983
H 0.2339444 0.4468276 1.0115677
H 0.7275912 -0.7110233 3.2158361
H 1.0519104 0.0897133 -0.9245612
H 1.2017658 1.5531793 6.8685832
H 1.8665184 -2.1655964 4.5604623
H 1.8777956 -0.3458075 -3.1484210
H 1.9995040 -0.9262339 -6.6523836
H 2.0525705 0.4426461 -5.5183688
H 2.4444978 -1.2021268 -4.9708766
H 2.9333447 -1.0358387 3.6722920
H 3.5103926 -1.8236926 5.1651856
H -0.8508128 2.8780704 6.2738519
H -0.9704081 0.1496232 -6.5894473
H -1.3341085 -1.5658397 -6.3014807
H -2.1858496 -0.7212979 -4.5841220
H -2.6771145 0.1889409 -0.0384283
H -2.8699547 1.3487169 3.1804864
H -3.0001333 -0.2845610 -2.3374182
N 0.3997599 -0.8840013 -5.3324492
O 2.2021275 -0.3298152 5.4951079
O -2.3240569 2.4408879 4.1275785
O -2.7627389 0.6055306 2.4542665

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Compound - 5 MP2/def2-SV(P)

C 1.0415033 0.2514330 4.9495558
C 0.3827762 0.2795950 3.7199186
C -0.8708622 0.9305082 3.5826235
C -1.4692083 1.5368225 4.7177601
C -0.7779755 1.5152048 5.9465240
C 0.4525784 0.8864261 6.0636275
C -1.5659240 1.0099423 2.2760645

C	-0.8417851	0.6332151	1.0429473
C	-1.5304720	0.4279205	-0.1087453
C	-0.9910332	0.0602579	-1.4112906
C	-1.8691855	-0.0902300	-2.5028932
C	-1.4164786	-0.4387963	-3.7737272
C	-0.0396601	-0.6685456	-4.0214474
C	-0.4821345	-0.9727181	-6.3984451
C	0.3803455	-0.1562349	-1.6601063
C	0.8471141	-0.5057117	-2.9236299
C	2.8763170	-0.9768073	4.0910621
C	1.8430395	-1.0205459	-5.5316677
H	-1.2523229	1.9998068	6.8067264
H	0.9894034	0.8586436	7.0183356
H	0.2471424	0.5386384	1.0733582
H	-2.6207365	0.5603991	-0.0487052
H	-2.9431082	0.0790420	-2.3506923
H	-2.1509198	-0.5280026	-4.5774519
H	-0.8350286	0.0611139	-6.5989511
H	-1.3659268	-1.6151670	-6.2421342
H	-3.0375485	2.0005043	3.7791825
H	0.8098076	-0.2324033	2.8565652
H	0.0377503	-1.3430119	-7.2952658
H	1.1107577	-0.0475376	-0.8492435
H	1.9221948	-0.6515771	-3.0524942
H	2.2689168	-1.8061301	3.6805733
H	3.0965334	-0.2536306	3.2822246
H	3.8220865	-1.3815433	4.4816918
H	2.3854040	-1.7022806	-4.8538015
H	2.0220085	-1.3711300	-6.5596704
H	2.2803708	-0.0051212	-5.4268692
N	0.4190346	-1.0502647	-5.2671431
O	-2.7439105	1.4007823	2.2114163
O	-2.6677858	2.1412292	4.6920302
O	2.2369220	-0.3540953	5.1821876

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Compound - 5 MP2/def2-TZVP

C	0.3760281	-0.1607456	-1.6462539
C	0.3985890	0.2937884	3.6989568
C	0.4442237	0.8757069	6.0375661
C	0.8379676	-0.5282630	-2.8982108
C	1.0409054	0.2607443	4.9276159
C	1.8299740	-1.0081675	-5.4960937
C	2.8621216	-0.9596893	4.0514445
C	-0.0462318	-0.7062948	-3.9851014
C	-0.4760389	-0.9618982	-6.3585033
C	-0.7844027	1.4943423	5.9185530
C	-0.8450730	0.5860360	1.0407820
C	-0.8537427	0.9320997	3.5602243
C	-0.9878958	0.0631391	-1.4052885
C	-1.4133382	-0.4611969	-3.7476273
C	-1.4593988	1.5212615	4.6914990
C	-1.5260543	0.4492826	-0.1163979
C	-1.5473840	1.0034174	2.2632286
C	-1.8629725	-0.0918582	-2.4894199
H	0.0274768	-1.3367327	-7.2476595
H	0.2190023	0.4006867	1.0827913
H	0.8389815	-0.1948113	2.8432403
H	0.9648934	0.8460458	6.9881838

H	1.0987209	-0.0317681	-0.8474028
H	1.9010473	-0.6782696	-3.0294479
H	2.0186268	-1.3693062	-6.5053648
H	2.1988836	0.0235928	-5.4173184
H	2.2401800	-1.7644074	3.6480376
H	2.4042107	-1.6334824	-4.8115251
H	3.0741249	-0.2338116	3.2603698
H	3.7960584	-1.3747262	4.4222117
H	-0.7640155	0.0841089	-6.5314202
H	-1.2582347	1.9626855	6.7735906
H	-1.3833762	-1.5512461	-6.2213667
H	-2.1360366	-0.5577277	-4.5462599
H	-2.5957083	0.6476602	-0.0767411
H	-2.9233541	0.0879841	-2.3392507
H	-2.9843177	1.9792557	3.7196307
N	0.4105452	-1.1153289	-5.2222454
O	2.2427171	-0.3395193	5.1639201
O	-2.6616055	2.1186733	4.6491289
O	-2.7160971	1.4287399	2.1979243

Dimer Geometries:

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Dimer 1

C	-5.8069833	-2.0928815	1.7798447
C	-6.9935783	-1.3683016	1.5865391
H	-7.7530719	-1.4238299	2.3592090
C	-7.1837041	-0.6320686	0.4325882
H	-8.1129891	-0.0868142	0.2937395
C	-6.1971545	-0.5940832	-0.5593992
H	-6.3560720	-0.0330543	-1.4741485
C	-5.0173823	-1.2884963	-0.3637605
H	-4.2673655	-1.2668664	-1.1469063
C	-4.7808862	-2.0370531	0.8031100
C	-3.5085805	-2.7643677	1.0462341
C	-2.3594480	-2.5326444	0.1690746
H	-2.4265581	-1.7540111	-0.5805447
C	-1.2244491	-3.2458420	0.3222300
H	-1.2311474	-3.9999932	1.1085126
C	0.0021619	-3.1079179	-0.4263030
C	0.1751818	-2.1853499	-1.4644810
H	-0.6545056	-1.5556213	-1.7735727
C	-1.4529110	3.0942521	2.0501169
H	-1.5264469	3.8263387	2.8458500
C	-2.5664950	2.2885202	1.7233676
C	-2.3987610	1.3668854	0.6781076
H	-3.2208301	0.7251694	0.3803092
C	-1.1967235	1.2579654	0.0261607
H	-1.1048063	0.5312545	-0.7779514
C	-4.8522317	1.5027415	2.1321826
H	-4.5509307	0.4526217	2.2269524
H	-5.6503713	1.6849013	2.8507890
H	-5.2634680	1.6404399	1.1241156
N	-3.7458894	2.3997177	2.3960105
O	-3.4205315	-3.5448496	2.0086548
O	-5.6981488	-2.8034334	2.9035261
C	1.1079817	-3.8845383	-0.0997730
C	1.3641603	-2.0482479	-2.1237241

C	-0.2639299	2.9571517	1.3908756
C	-0.0909102	2.0345824	0.3526968
C	-3.9035116	3.3626830	3.4675651
H	-4.8348525	-3.2849291	2.8468029
C	2.3100016	-3.7756172	-0.7517132
H	1.0192433	-4.6083978	0.7077714
H	1.4412096	-1.3126998	-2.9156630
C	2.4777512	-2.8539785	-1.7969734
H	0.5626321	3.6011310	1.6799599
C	1.1357006	1.8966596	-0.3958368
H	-3.7197173	4.3874395	3.1191971
H	-4.9246012	3.3190869	3.8450981
H	-3.2219748	3.1613388	4.3061733
H	3.1320136	-4.4128763	-0.4468051
N	3.6571201	-2.7427960	-2.4696034
H	1.0870153	1.2049783	-1.2372073
C	2.3424980	2.4607896	-0.1906492
C	3.8147636	-1.7798062	-3.5411702
C	4.7635302	-3.6397591	-2.2058162
C	3.4469618	2.1139837	-1.0940026
H	2.5169665	3.1413177	0.6338755
H	3.1910596	-2.0264913	-4.4122720
H	3.5551722	-0.7704751	-3.2025941
H	4.8568123	-1.7585491	-3.8595933
H	4.4696489	-4.6913714	-2.3269254
H	5.5705600	-3.4336027	-2.9078786
H	5.1576585	-3.5108291	-1.1886078
O	3.2133397	1.4896659	-2.1470198
C	4.8399345	2.4899424	-0.7606159
C	5.8787538	2.1984750	-1.6820623
C	5.1888193	3.1096011	0.4533336
O	5.6588110	1.5932162	-2.8532253
C	7.2017949	2.5490870	-1.3778223
H	4.4199305	3.3183210	1.1884386
C	6.4954821	3.4458275	0.7510737
H	4.6855300	1.4193035	-2.8899882
H	7.9694538	2.3182563	-2.1087040
C	7.5030663	3.1640027	-0.1780825
H	6.7353577	3.9204109	1.6965538
H	8.5338399	3.4243849	0.0447560

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Dimer 2

C	8.5951724	-0.0987354	-1.2042805
C	8.3426704	-0.6337544	1.2025275
C	6.4136584	-0.7523254	-0.2969735
C	5.8050684	-0.5957714	-1.5520595
C	2.4877654	4.2367296	0.5369905
C	5.5954174	-1.2173074	0.7567365
C	4.4794184	-0.8998674	-1.7307705
C	2.7738834	1.9116576	-0.2722715
C	4.2800544	-1.5226874	0.5478535
C	3.6715004	-1.3742904	-0.7037795
C	0.5338054	2.8268826	0.0855845
C	-0.3416826	3.8704516	0.4241335
C	2.2742394	-1.6421504	-0.9482215
C	-0.0511066	1.5864516	-0.2539105
C	-1.6988616	3.6711556	0.4337535

SUPPORTING INFORMATION

C	1.3205944	-1.8943644	-0.0298495
C	-1.4061666	1.4130116	-0.2257225
C	-2.2818906	2.4492656	0.1178905
C	-0.0878006	-2.0096264	-0.4387035
C	-3.7191426	2.3142956	0.1118935
C	-1.1407756	-2.2511524	0.5715235
C	-0.8546466	-2.5718504	1.9111325
C	-4.4437536	1.2283286	-0.2223095
C	-2.5015006	-2.1377244	0.1928045
C	-1.8570686	-2.7468364	2.8451885
C	-5.9099126	1.2767086	-0.1275385
C	-3.5152446	-2.2983134	1.1444795
C	-3.1923176	-2.5976854	2.4544305
C	-6.7208206	0.1008476	-0.5236975
C	-6.1581016	-1.0404654	-1.1241695
C	-8.1196736	0.1129596	-0.2884145
C	-6.9286746	-2.1393174	-1.4584815
C	-8.8933246	-1.0076714	-0.6249545
C	-8.3035286	-2.1172104	-1.1996805
H	9.6148224	0.0248756	-0.8411935
H	8.2824734	0.8500446	-1.6608095
H	9.3778424	-0.2958054	1.1628575
H	8.6057834	-0.8663614	-1.9897175
H	7.8261604	-0.0332354	1.9620235
H	8.3386534	-1.6814164	1.5350705
H	6.3778954	-0.2346544	-2.3983565
H	3.5729734	4.1440806	0.4998815
H	2.1990074	5.0851526	-0.0986405
H	3.8038994	2.2676376	-0.2947505
H	2.2024434	4.4764506	1.5709665
H	6.0143954	-1.3651044	1.7451695
H	4.0444024	-0.7647384	-2.7189985
H	2.5397224	1.5130526	-1.2675135
H	2.7182044	1.0759436	0.4388005
H	0.0463854	4.8490026	0.6837165
H	3.7030964	-1.9000024	1.3875515
H	1.9405384	-1.5759524	-1.9835175
H	0.5754974	0.7484286	-0.5343965
H	-2.3444036	4.5062626	0.6988385
H	1.5618454	-1.9350834	1.0251165
H	-1.8046586	0.4455336	-0.5141595
H	-4.2855346	3.1925496	0.4213215
H	0.1751274	-2.6998254	2.2251575
H	-2.0436916	-1.8121624	-1.6039305
H	-3.9632916	0.3135366	-0.5469755
H	-1.6101816	-2.9934394	3.8722545
H	-5.0962906	-1.0745204	-1.3394425
H	-8.0660976	1.8538896	0.3945415
H	-4.5461696	-2.1859764	0.8246505
H	-3.9871976	-2.7206124	3.1840375
H	-6.4662426	-3.0054904	-1.9200555
H	-9.9589646	-0.9663634	-0.4254595
H	-8.9181226	-2.9754814	-1.4573385
N	7.7328624	-0.4738094	-0.1024615
N	1.8851994	2.9984046	0.0878475
O	-0.3957376	-1.8408784	-1.6314425
O	-2.8739566	-1.8461034	-1.0632135
O	-6.4721076	2.2967886	0.3077415

O -8.7538336 1.1557446 0.2536945

SECTION S9. CONICAL INTERSECTION GEOMETRIES

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1_ADC2_SVP

C	3.6273856	1.7762277	3.2654699
C	4.0790078	2.5017206	2.1733641
C	4.3030568	1.8959846	4.4944587
C	5.2219349	3.3582026	2.2717635
C	5.4212804	2.7554436	4.6249982
C	5.9176368	3.4409272	3.4540561
C	7.1713638	4.2370137	3.6029407
C	8.2836125	4.0096624	2.8418865
C	9.4791480	4.7491379	2.9769793
C	10.7276189	4.4739742	2.3193766
C	10.9670598	3.3395700	1.5082392
C	11.8227374	5.3491956	2.5117413
C	12.2185223	3.0871097	0.9485303
C	13.0755503	5.1050198	1.9554143
C	13.3176769	3.9568768	1.1620140
C	14.7115940	2.6352781	-0.3457966
C	15.5813247	4.7210476	0.6614250
H	2.7516089	1.1234613	3.1780195
H	3.5596247	2.4244563	1.2110456
H	3.9858178	1.3481343	5.3891740
H	5.5626981	3.9177568	1.3921828
H	6.7014798	4.7832468	5.3406645
H	8.2059291	3.2067417	2.0949096
H	9.4535482	5.5881512	3.6887530
H	10.1635626	2.6153714	1.3228638
H	11.6782692	6.2485000	3.1253495
H	12.3340011	2.1845822	0.3422784
H	13.8726569	5.8257355	2.1540328
H	14.1370075	2.8398732	-1.2748446
H	14.3825852	1.6618601	0.0580307
H	15.2900935	5.6146900	0.0682535
H	15.7751350	2.5333979	-0.6125382
H	15.7993834	5.0468597	1.6933452
H	16.5177080	4.3188338	0.2436635
N	14.5770013	3.6792522	0.6463861
O	5.9589626	2.9818328	5.7816015
O	7.1178068	5.2140509	4.5541177

37

1_ADC2_SVP_E

C	1.0015575	0.7460624	0.2779701
C	1.2544308	-0.3756539	-0.5525670
C	2.0881645	1.6457902	0.4480466
C	2.4884685	-0.5787582	-1.1655747
C	3.3228340	1.4462290	-0.1612384
C	3.5657690	0.3219376	-0.9909950
C	4.8842614	-0.8663630	-2.6583495
C	5.7580299	1.1870983	-1.6102513
C	-0.2551426	1.0072736	0.8967929
C	-1.4235857	0.1460869	0.7963790
C	-2.6248534	0.4079785	1.2674939
C	-3.9305879	-0.2397715	1.2139616
C	-4.5200305	-0.5302581	-0.0385004
C	-4.5949437	-0.6235866	2.4065886
C	-5.7167541	-1.2382594	-0.1108903
C	-5.8059063	-1.3294663	2.3222966
C	-6.3585330	-1.6325037	1.0771948

H	0.4635143	-1.1106352	-0.7416705
H	1.9469543	2.5349527	1.0782731
H	2.5966023	-1.4595190	-1.8034237
H	4.1046856	2.1912091	0.0098193
H	4.2519722	-0.5966450	-3.5322978
H	4.5812588	-1.8690502	-2.3118495
H	5.3909663	2.0737057	-2.1719036
H	5.9298291	-0.9430820	-2.9959921
H	6.0153430	1.5098305	-0.5869534
H	6.6885723	0.8362181	-2.0840432
H	-0.3686728	1.9452277	1.4638706
H	-1.3578714	-0.8124608	0.2668085
H	-3.3954434	0.3029920	3.5792028
H	-3.9995976	-0.2023088	-0.9449095
H	-6.1638955	-1.4683386	-1.0840385
H	-6.2933624	-1.6310001	3.2555371
H	-7.3074531	-2.1806553	1.0286823
N	4.8066770	0.0973606	-1.5812981
O	-2.9216124	1.6627269	2.0968610
O	-4.1016447	-0.3743548	3.6409378

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1_ADC2_TZVP

C	5.4336371	2.7586916	4.6087608
C	4.3069711	1.9204453	4.4878038
C	3.6417454	1.7878281	3.2635739
C	4.1017211	2.5018781	2.1768904
C	5.2556635	3.3361734	2.2670690
C	5.9457851	3.4250792	3.4424544
C	7.1918832	4.2239462	3.5872665
C	8.3040161	4.0009886	2.8478991
C	9.4968012	4.7388112	2.9880626
C	10.7330710	4.4622330	2.3254958
C	10.9651909	3.3405590	1.5077099
C	12.2094958	3.0951821	0.9461678
C	13.3044000	3.9508713	1.1736658
C	13.0636592	5.0996699	1.9502238
C	11.8212235	5.3370054	2.5132015
C	14.6875752	2.6416736	-0.3348049
C	15.5538745	4.7196222	0.6733380
H	3.9743631	1.4000320	5.3795180
H	2.7742635	1.1432563	3.1768594
H	3.5874094	2.4275423	1.2246466
H	5.5975860	3.8834923	1.3945399
H	8.2438807	3.2049024	2.1092818
H	9.4822338	5.5727897	3.6872719
H	10.1685578	2.6271028	1.3219614
H	12.3258933	2.2124296	0.3314548
H	13.8536834	5.8162186	2.1307209
H	11.6750170	6.2236884	3.1239067
H	14.3461809	1.6763564	0.0438126
H	15.7371496	2.5349003	-0.6044078
H	14.1145784	2.8776887	-1.2424060
H	15.2385040	5.5869231	0.0763049
H	16.4831942	4.3310697	0.2591623
H	15.7645377	5.0619599	1.6883876
H	6.7062063	4.7771664	5.3087581
N	14.5691076	3.6598054	0.6848580
O	5.9671509	2.9807071	5.7682045

O 7.1251887 5.2104801 4.5365261
 37
 1_ADC2_TZVP Positive Dihedral
 C 0.9783536 0.6887597 0.2916296
 C 1.1579188 -0.3539285 -0.6375485
 C 2.1022041 1.5024232 0.5420302
 C 2.3776155 -0.5706424 -1.2643083
 C 3.3217079 1.2914699 -0.0807438
 C 3.5019814 0.2329526 -0.9920644
 C 4.7734629 -0.8865376 -2.7339146
 C 5.7438959 1.0140602 -1.5101564
 C -0.2449780 0.9670975 0.9732296
 C -1.4565009 0.2512027 0.8265239
 C -2.5775318 0.5159792 1.5294035
 C -3.8430342 -0.2710218 1.3760325
 C -3.8686007 -1.6299508 1.4539850
 C -5.0790885 0.4321988 1.1863348
 C -5.0913374 -2.3431146 1.2283908
 C -6.2699383 -0.2828091 0.9796118
 C -6.2731360 -1.6878233 0.9866545
 H 0.3313789 -1.0133083 -0.8837253
 H 2.0025528 2.3247328 1.2453636
 H 2.4489583 -1.3871641 -1.9730162
 H 4.1415769 1.9594141 0.1532602
 H 4.1625182 -0.5074438 -3.5653383
 H 4.4258367 -1.8897221 -2.4810003
 H 5.4213756 1.9504482 -1.9867617
 H 5.8051417 -0.9730724 -3.0705357
 H 6.0120047 1.2301441 -0.4746484
 H 6.6412414 0.6579044 -2.0130394
 H -0.2473036 1.7974143 1.6761851
 H -1.5099633 -0.5795606 0.1265767
 H -2.9524155 -2.1779091 1.6487924
 H -3.4998371 1.9196104 2.3628284
 H -5.0632991 -3.4274190 1.2394826
 H -7.1746347 0.2945423 0.8193979
 H -7.1916462 -2.2351707 0.8131768
 N 4.7388278 -0.0249938 -1.5722266
 O -2.6352932 1.4797302 2.5050004
 O -5.1100148 1.7314872 1.2751476
 37
 1_ADC2_TZVP_E
 C -4.5613698 -0.6262956 2.3900304
 C -5.7781973 -1.3072141 2.3195309
 C -6.3322283 -1.6097655 1.0843155
 C -5.6999120 -1.2220845 -0.1034148
 C -4.5081662 -0.5223498 -0.0408486
 C -3.9110058 -0.2388839 1.2019082
 C -2.6127738 0.4102043 1.2382868
 C -1.4156511 0.1515769 0.7846290
 C -0.2484906 1.0078223 0.8881917
 C 0.9931399 0.7392205 0.2641507
 C 1.2422383 -0.3797874 -0.5613472
 C 2.4777261 -0.5847588 -1.1585798
 C 3.5532052 0.3008634 -0.9640658
 C 3.3042443 1.4319678 -0.1586614
 C 2.0733611 1.6375815 0.4356032
 C 4.8705930 -0.8607962 -2.6345160

C	5.7224499	1.1833431	-1.5907486
H	-6.2628671	-1.5976982	3.2443792
H	-7.2719017	-2.1489324	1.0449833
H	-6.1461001	-1.4577966	-1.0614840
H	-3.9981883	-0.1940569	-0.9390319
H	-1.3429605	-0.8097038	0.2855895
H	-0.3497031	1.9283234	1.4619096
H	0.4542310	-1.0986185	-0.7620191
H	2.5956756	-1.4588462	-1.7861863
H	4.0796422	2.1674959	0.0125052
H	1.9218324	2.5239071	1.0469129
H	4.5619685	-1.8599141	-2.3252500
H	5.9018315	-0.9301237	-2.9782342
H	4.2389274	-0.5501612	-3.4793870
H	5.3187964	2.0265312	-2.1699005
H	6.6500823	0.8535780	-2.0569219
H	5.9690914	1.5412833	-0.5906127
H	-3.3041548	0.2201651	3.5461705
N	4.8081056	0.0625307	-1.5205415
O	-4.0459999	-0.4027387	3.6216909
O	-2.9474614	1.6741517	2.0109336

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1_CAS1413_6-31G(d)

C	-4.1248931	-1.1353230	2.3521709
C	-5.3233146	-1.9710750	2.2366025
C	-6.1850478	-1.8460521	1.1798144
C	-5.9391486	-0.9021012	0.1447272
C	-4.7947950	-0.0976661	0.1967011
C	-3.8825495	-0.2040703	1.2435698
C	-2.6756454	0.6414692	1.3006470
C	-1.4982723	0.2833273	0.7374454
C	-0.3384321	1.0879453	0.7694377
C	0.9277240	0.7812282	0.1738502
C	1.2032818	-0.4012051	-0.5501133
C	2.4461113	-0.6438588	-1.1036360
C	3.5092280	0.2802668	-0.9657983
C	3.2339071	1.4575251	-0.2573011
C	1.9948385	1.6935488	0.2922011
C	4.9113106	-1.0533197	-2.4569542
C	5.7432595	1.0825511	-1.5263050
H	-5.4918278	-2.6758133	3.0291514
H	-7.0613232	-2.4672410	1.1273112
H	-6.6219537	-0.8148174	-0.6792619
H	-4.6046180	0.6047193	-0.5952210
H	-1.4808577	-0.6696240	0.2463502
H	-0.4114540	2.0233838	1.2913212
H	0.4385026	-1.1427339	-0.6855417
H	2.5893716	-1.5591698	-1.6417902
H	3.9925107	2.2033503	-0.1277365
H	1.8371773	2.6123795	0.8292603
H	4.6669906	-2.0103423	-2.0114371
H	5.9432637	-1.1008950	-2.7727179
H	4.2905797	-0.9193378	-3.3419713
H	5.4210200	1.9411200	-2.1145844
H	6.6600997	0.7036942	-1.9540196
H	5.9714772	1.4237968	-0.5235971
H	-3.5866240	1.8722197	2.4145936
N	4.7588213	0.0222894	-1.4998291

O -3.3883068 -1.1941560 3.3125541
 O -2.7852445 1.8340349 1.9091371
 37
 1_CAS1211_6-31G(d)
 C -4.1245612 -1.1322408 2.3498232
 C -5.3244034 -1.9656367 2.2354592
 C -6.1859368 -1.8406724 1.1787394
 C -5.9392613 -0.8986045 0.1416252
 C -4.7949346 -0.0959137 0.1926891
 C -3.8835526 -0.2021061 1.2415153
 C -2.6759910 0.6411768 1.2995053
 C -1.4966414 0.2795640 0.7376759
 C -0.3375421 1.0814178 0.7726109
 C 0.9316383 0.7719257 0.1811928
 C 1.2084065 -0.4113622 -0.5374190
 C 2.4547698 -0.6550842 -1.0863029
 C 3.5149263 0.2680020 -0.9479545
 C 3.2371796 1.4473531 -0.2430743
 C 1.9977185 1.6853078 0.3012757
 C 4.9117309 -1.0422060 -2.4596374
 C 5.7328890 1.0868861 -1.5404264
 H -5.4938374 -2.6696404 3.0284877
 H -7.0629602 -2.4609330 1.1272394
 H -6.6222742 -0.8118554 -0.6822681
 H -4.6036110 0.6055072 -0.5999098
 H -1.4804725 -0.6739028 0.2478088
 H -0.4105510 2.0180415 1.2923895
 H 0.4442085 -1.1533468 -0.6733074
 H 2.5990668 -1.5718224 -1.6213896
 H 3.9952548 2.1932963 -0.1126680
 H 1.8379796 2.6054018 0.8355026
 H 4.6407324 -2.0053505 -2.0458066
 H 5.9466740 -1.1065412 -2.7631533
 H 4.3058411 -0.8673176 -3.3485327
 H 5.3918150 1.9160797 -2.1603799
 H 6.6579968 0.7122964 -1.9543913
 H 5.9563315 1.4691382 -0.5523167
 H -3.5928915 1.8802330 2.3965206
 N 4.7757484 0.0043339 -1.4689843
 O -3.3850558 -1.1930287 3.3084731
 O -2.7812623 1.8316522 1.9084192
 37
 1_CAS1211_6-31G(d)_E
 C -4.2057735 -0.6761930 2.0645252
 C -5.3905865 -1.4140033 2.0086665
 C -5.9709943 -1.7095548 0.7848681
 C -5.3823025 -1.2506910 -0.3939870
 C -4.2237430 -0.5140641 -0.3314781
 C -3.5948345 -0.2307937 0.8873438
 C -2.3164743 0.5703897 0.8349919
 C -1.2807396 0.2534562 1.7479327
 C -0.0500538 1.0259870 1.7034210
 C 1.0167060 0.8039674 0.8655905
 C 1.0135659 -0.2369539 -0.1105874
 C 2.0835396 -0.4347779 -0.9502083
 C 3.2377015 0.3937039 -0.8825289
 C 3.2487372 1.4372113 0.0873118
 C 2.1780159 1.6334056 0.9229802

C 4.2384485 -0.8214079 -2.7476971
 C 5.4490164 1.0761733 -1.6609915
 H -5.8364943 -1.7340033 2.9322758
 H -6.8807259 -2.2820525 0.7503793
 H -5.8365094 -1.4647788 -1.3449100
 H -3.7690129 -0.1327249 -1.2259776
 H -1.3136010 -0.6216058 2.3719256
 H 0.0658129 1.8675844 2.3762291
 H 0.1476576 -0.8641629 -0.1823656
 H 2.0293863 -1.2246099 -1.6708768
 H 4.0916540 2.0925789 0.1663991
 H 2.2063127 2.4339585 1.6393148
 H 4.1173674 -1.8124365 -2.3232738
 H 5.1624003 -0.8127915 -3.3047277
 H 3.4255621 -0.6417702 -3.4447441
 H 5.1890456 2.1005880 -1.9117645
 H 6.1866530 0.7362877 -2.3711293
 H 5.9094190 1.0667193 -0.6790307
 H -2.9909524 0.1883304 3.2458317
 N 4.2980623 0.1954763 -1.7146903
 O -3.7257189 -0.4112979 3.3061826
 O -2.2018178 1.4405363 -0.0188712
 37
 1_CAS66_6-31G(d)
 C -4.1638702 -1.1305131 2.3539302
 C -5.3659546 -1.9702116 2.2293995
 C -6.1972971 -1.8451480 1.1891579
 C -5.9431914 -0.8885528 0.1393870
 C -4.8077785 -0.0862729 0.1919594
 C -3.8952700 -0.1921407 1.2477293
 C -2.6881122 0.6455065 1.3100992
 C -1.4695669 0.2862177 0.7269426
 C -0.3520339 1.0568997 0.7590821
 C 0.9434591 0.7518520 0.1635422
 C 1.2316215 -0.4177039 -0.5445863
 C 2.4737769 -0.6559799 -1.0894768
 C 3.5221930 0.2677131 -0.9534788
 C 3.2370678 1.4462495 -0.2542839
 C 1.9865295 1.6685842 0.2860835
 C 4.9333373 -1.0471078 -2.4456852
 C 5.7308896 1.1047444 -1.5540558
 H -5.5391570 -2.6735388 3.0223427
 H -7.0763373 -2.4612215 1.1210171
 H -6.6279411 -0.8080723 -0.6832151
 H -4.6147382 0.6166003 -0.5979403
 H -1.4635895 -0.6650011 0.2276573
 H -0.4148891 1.9964805 1.2769081
 H 0.4731855 -1.1665959 -0.6803242
 H 2.6227868 -1.5736230 -1.6219506
 H 3.9865953 2.2002968 -0.1228275
 H 1.8159503 2.5884505 0.8180762
 H 4.6763753 -2.0065394 -2.0140668
 H 5.9681844 -1.1018838 -2.7516786
 H 4.3215835 -0.8963779 -3.3350476
 H 5.3779217 1.9282630 -2.1748559
 H 6.6572809 0.7377237 -1.9720628
 H 5.9559588 1.4933599 -0.5686469
 H -3.5079745 1.8603388 2.5208833

SUPPORTING INFORMATION

N 4.7846846 0.0137606 -1.4732935
 O -3.4438289 -1.1866670 3.3221931
 O -2.7826843 1.8501581 1.9101164
 37

1_CC2_SVP 72deg rotation

C 0.9383082 0.7434011 0.1978504
 C 1.1496945 -0.2919582 -0.7372460
 C 2.0249572 1.6141869 0.4335210
 C 2.3603713 -0.4477359 -1.3917032
 C 3.2423916 1.4658874 -0.2090493
 C 3.4387585 0.4354681 -1.1553881
 C 4.8725606 -0.9049649 -2.5952507
 C 5.7804503 1.0551631 -1.3697984
 C -0.2964450 0.9560077 0.8808779
 C -1.4316140 0.1408673 0.8139773
 C -2.6593552 0.5271938 1.2936353
 C -3.8832819 -0.2641184 1.2063964
 C -4.3394205 -0.9045561 2.4288939
 C -4.6779051 -0.3056583 0.0722600
 C -5.4860849 -1.7516221 2.3570304
 C -5.8250960 -1.1223543 0.0487444
 C -6.2185151 -1.8427241 1.1816057
 H 0.3444125 -0.9831088 -0.9688807
 H 1.9037435 2.4204397 1.1532978
 H 2.4618362 -1.2625007 -2.0988454
 H 4.0412497 2.1579557 0.0299720
 H 4.1311702 -1.0165150 -3.3895107
 H 4.8426641 -1.8039058 -1.9657293
 H 5.5845638 2.1285114 -1.4163131
 H 5.8536736 -0.8363662 -3.0625802
 H 6.0522797 0.7979017 -0.3376387
 H 6.6272137 0.8418465 -2.0202605
 H -0.3810214 1.8628540 1.4785373
 H -1.3986026 -0.8241905 0.3133941
 H -3.4492901 1.6494894 2.5787666
 H -4.3786409 0.2430286 -0.8169652
 H -5.7761251 -2.2840812 3.2581835
 H -6.3819449 -1.2229118 -0.8779662
 H -7.1068928 -2.4641312 1.1410050
 N 4.6325646 0.3072401 -1.8398279
 O -2.8158883 1.7777334 1.8480012
 O -3.7767404 -0.5917725 3.5370033
 37

1_CC2_SVP 82deg rotation

C 0.2236228 1.1146077 -0.2890236
 C 1.5771066 0.6480428 -0.1621240
 C 1.9201284 -0.7058825 0.0991677
 C 2.6579596 1.5619278 -0.2765070
 C 3.2362854 -1.1271850 0.2493214
 C 3.9826310 1.1547991 -0.1244340
 C 4.3132583 -0.2039641 0.1383788
 C 5.8977504 -2.0461629 0.2796121
 C 6.7025041 0.2775299 -0.0700863
 C -0.9298335 0.3359616 -0.1470409
 C -2.2147498 0.8179028 -0.3351341
 C -3.4155208 -0.0311437 -0.2804538
 C -3.8377751 -0.8327700 -1.3363547
 C -4.2220629 0.1269447 0.9149446

SUPPORTING INFORMATION

C -4.9810642 -1.6496577 -1.1653869
 C -5.3761012 -0.7155097 1.0523959
 C -5.7517247 -1.5671300 0.0107239
 H 0.0686969 2.1795133 -0.5219680
 H 1.1355087 -1.4641089 0.1832470
 H 2.4302477 2.6202819 -0.4862496
 H 3.4217190 -2.1869837 0.4539941
 H 4.7633508 1.9144046 -0.2103771
 H 5.3741415 -2.5591451 1.1047102
 H 5.5917048 -2.5213448 -0.6740524
 H 6.6612523 1.2014677 0.5316461
 H 6.6806420 0.5549579 -1.1435266
 H 6.9759525 -2.1976163 0.4259049
 H 7.6631924 -0.2164848 0.1447048
 H -0.8529869 -0.7335720 0.0736622
 H -3.2227683 -0.9097548 -2.2447128
 H -3.2491755 2.3924354 -0.3191764
 H -5.2453656 -2.3739216 -1.9457916
 H -5.9694180 -0.6316351 1.9712463
 H -6.6421124 -2.2018201 0.1146090
 N 5.6232497 -0.6196590 0.2941159
 O -2.4096579 2.1054332 -0.7449405
 O -3.9186783 1.0746116 1.7246055
 37

1_CC2_SVP 86deg rotation

C 0.9199921 0.8089356 0.1866574
 C 1.1701469 -0.3428780 -0.6029048
 C 2.0119067 1.6990957 0.3540806
 C 2.4186044 -0.5966497 -1.1660544
 C 3.2657718 1.4588594 -0.2046549
 C 3.5098928 0.2970363 -0.9852248
 C 4.8867076 -1.0213697 -2.5142345
 C 5.7603384 1.0813616 -1.5129308
 C -0.3451421 1.1026198 0.8026250
 C -1.4990328 0.3074945 0.7467945
 C -2.7070580 0.6453162 1.3321751
 C -3.9067301 -0.1969850 1.2416725
 C -4.1819886 -1.1135590 2.3527316
 C -4.8080424 -0.0914107 0.1865895
 C -5.3182888 -1.9918971 2.2163940
 C -5.9373113 -0.9417881 0.1203151
 C -6.1872896 -1.8860350 1.1349645
 H 0.3664689 -1.0675734 -0.7835446
 H 1.8652413 2.6102650 0.9504289
 H 2.5351257 -1.5041087 -1.7654311
 H 4.0579970 2.1937957 -0.0344061
 H 4.2715463 -0.8420700 -3.4219712
 H 4.5948725 -1.9965291 -2.0854554
 H 5.4459951 1.9877548 -2.0733657
 H 5.9425853 -1.0973475 -2.8185940
 H 5.9969732 1.3804544 -0.4763339
 H 6.6867927 0.6946823 -1.9660154
 H -0.4174276 2.0381126 1.3777453
 H -1.4886908 -0.6465782 0.2030147
 H -3.6090945 1.7660225 2.5966161
 H -4.6125291 0.6277992 -0.6196307
 H -5.4786334 -2.7174669 3.0236191
 H -6.6148059 -0.8696110 -0.7392478

SUPPORTING INFORMATION

H -7.0612898 -2.5458157 1.0629605
 N 4.7566279 0.0360238 -1.5311579
 O -2.8274757 1.8324952 2.0111423
 O -3.4627462 -1.0984623 3.4006211

37

1_CC2_SVP_E

C 0.9595973 0.5744867 0.3729084
 C 1.1620639 -0.3893702 -0.6604223
 C 2.0283419 1.4949595 0.5914326
 C 2.3534316 -0.4488463 -1.3870619
 C 3.1851127 1.4831664 -0.1659288
 C 3.4226005 0.4495053 -1.1143479
 C 4.9642668 -0.8126777 -2.5691585
 C 5.6815849 1.3331712 -1.5103990
 C -0.1842091 0.6629208 1.2135891
 C -1.4544514 -0.1249916 1.1341056
 C -2.6146373 0.4106234 0.6879877
 C -3.9425392 -0.2172455 0.8645825
 C -4.3273369 -0.5592247 2.1945214
 C -4.8236159 -0.4886465 -0.1920970
 C -5.5929716 -1.1371147 2.4279716
 C -6.0507352 -1.1050440 0.0373893
 C -6.4319102 -1.4255655 1.3536146
 H 0.3629353 -1.1118551 -0.8769084
 H 1.9079431 2.2774189 1.3525819
 H 2.4295247 -1.2066900 -2.1743713
 H 3.9102505 2.2840446 -0.0099423
 H 4.3981606 -0.8004712 -3.5278158
 H 4.7453055 -1.7661695 -2.0404909
 H 5.4813961 2.2664879 -2.0809695
 H 5.7688084 1.5941974 -0.4383980
 H 6.0451657 -0.7947847 -2.8143666
 H 6.6609449 0.9338255 -1.8319859
 H -0.0039612 1.2026593 2.1691336
 H -1.4914065 -1.1709809 1.5280949
 H -2.6177826 -0.1487513 2.8944415
 H -4.5049063 -0.2290197 -1.2137515
 H -5.8684254 -1.3753729 3.4612802
 H -6.7018651 -1.3515697 -0.8039452
 H -7.3892860 -1.9257855 1.5264420
 N 4.6600471 0.3254576 -1.7221108
 O -2.6135775 1.6367498 0.0665282
 O -3.5138633 -0.3394885 3.2578685

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1_CC2_TZVP 78deg rotation

C -4.3394205 -0.9045561 2.4288939
 C -5.4860849 -1.7516221 2.3570304
 C -6.2185151 -1.8427241 1.1816057
 C -5.8250960 -1.1223543 0.0487444
 C -4.6779051 -0.3056583 0.0722600
 C -3.8832819 -0.2641184 1.2063964
 C -2.6593552 0.5271938 1.2936353
 C -1.4316140 0.1408673 0.8139773
 C -0.2964450 0.9560077 0.8808779
 C 0.9383082 0.7434011 0.1978504
 C 1.1496945 -0.2919582 -0.7372460
 C 2.3603713 -0.4477359 -1.3917032
 C 3.4387585 0.4354681 -1.1553881

SUPPORTING INFORMATION

C 3.2423916 1.4658874 -0.2090493
 C 2.0249572 1.6141869 0.4335210
 C 4.8725606 -0.9049649 -2.5952507
 C 5.7804503 1.0551631 -1.3697984
 H -5.7761251 -2.2840812 3.2581835
 H -7.1068928 -2.4641312 1.1410050
 H -6.3819449 -1.2229118 -0.8779662
 H -4.3786409 0.2430286 -0.8169652
 H -1.3986026 -0.8241905 0.3133941
 H -0.3810214 1.8628540 1.4785373
 H 0.3444125 -0.9831088 -0.9688807
 H 2.4618362 -1.2625007 -2.0988454
 H 4.0412497 2.1579557 0.0299720
 H 1.9037435 2.4204397 1.1532978
 H 4.8426641 -1.8039058 -1.9657293
 H 5.8536736 -0.8363662 -3.0625802
 H 4.1311702 -1.0165150 -3.3895107
 H 5.5845638 2.1285114 -1.4163131
 H 6.6272137 0.8418465 -2.0202605
 H 6.0522797 0.7979017 -0.3376387
 H -3.4492901 1.6494894 2.5787666
 N 4.6325646 0.3072401 -1.8398279
 O -3.7767404 -0.5917725 3.5370033
 O -2.8158883 1.7777334 1.8480012
 37

1_CC2_TZVP 80deg rotation

C 0.9088407 0.8495476 -0.0794977
 C 1.2491403 -0.5050201 0.1734477
 C 1.9942003 1.7549805 -0.2001188
 C 2.5640819 -0.9344004 0.3174977
 C 3.3145065 1.3394406 -0.0571125
 C 3.6429794 -0.0143529 0.2070952
 C 5.2369834 -1.8423546 0.3532268
 C 6.0427857 0.4894556 -0.0000220
 C -0.4417515 1.3184970 -0.2029638
 C -1.5955135 0.5346709 -0.0642202
 C -2.8738835 1.0039126 -0.2780908
 C -4.0768984 0.1677394 -0.2142222
 C -4.5027125 -0.6368055 -1.2649465
 C -4.8902141 0.3273538 0.9783789
 C -5.6513087 -1.4428225 -1.0916445
 C -6.0396405 -0.5184057 1.1257790
 C -6.4149388 -1.3696209 0.0879188
 H 0.4648235 -1.2542842 0.2537438
 H 1.7808811 2.8054517 -0.4064422
 H 2.7302256 -1.9899914 0.5252962
 H 4.1070138 2.0753999 -0.1346566
 H 4.7109609 -2.3373472 1.1743037
 H 4.9256183 -2.3092159 -0.5931243
 H 6.0008664 1.4052531 0.5978295
 H 6.0267606 0.7650853 -1.0666719
 H 6.3070398 -1.9921927 0.4985427
 H 6.9928466 -0.0036003 0.2171492
 H -0.6045664 2.3706524 -0.4421009
 H -1.5126943 -0.5220942 0.1817802
 H -3.9117830 -0.6901463 -2.1803932
 H -3.9209692 2.5778905 -0.2608014
 H -5.9232785 -2.1566046 -1.8673483

H -6.6146615 -0.4482328 2.0491425
H -7.3015892 -1.9933284 0.1891728
N 4.9596836 -0.4155424 0.3652114
O -3.0818063 2.3071641 -0.6761224
O -4.6020287 1.2838680 1.7849841

37

1_CC2_TZVP 88deg rotation

C 0.9185658 0.7991425 0.1775651
C 1.1686418 -0.3425525 -0.6003039
C 1.9976678 1.6802575 0.3471221
C 2.4068068 -0.5917175 -1.1614499
C 3.2418838 1.4453565 -0.2070599
C 3.4879248 0.2904795 -0.9719129
C 4.8705128 -1.0151875 -2.5009359
C 5.7337188 1.0796225 -1.4995409
C -0.3534092 1.1048695 0.7894941
C -1.4939882 0.3310485 0.7364621
C -2.6925072 0.6546255 1.3355121
C -3.8982072 -0.2014555 1.2494321
C -4.1631492 -1.1304365 2.3350071
C -4.7795442 -0.1138915 0.1877461
C -5.3297662 -1.9805185 2.2184541
C -5.8976692 -0.9400495 0.1218431
C -6.1638732 -1.8774765 1.1432531
H 0.3766608 -1.0603195 -0.7809809
H 1.8504088 2.5828435 0.9320731
H 2.5301398 -1.4890385 -1.7527209
H 4.0262388 2.1706265 -0.0382579
H 4.2565858 -0.8305105 -3.3948689
H 4.5893508 -1.9878305 -2.0876029
H 5.4095428 1.9747895 -2.0506169
H 5.9131968 -1.0852095 -2.8092189
H 5.9793278 1.3779635 -0.4764079
H 6.6500158 0.7080975 -1.9571769
H -0.4073152 2.0335995 1.3478361
H -1.4855622 -0.6120535 0.2011971
H -3.5360832 1.7965145 2.6146481
H -4.5836132 0.5937595 -0.6093249
H -5.5064882 -2.6880695 3.0197221
H -6.5683082 -0.8703675 -0.7261129
H -7.0378882 -2.5140815 1.0652071
N 4.7393168 0.0281825 -1.5067569
O -2.8265222 1.8473115 1.9731321
O -3.4226112 -1.1683245 3.3355431

37

1_CC2_TZVP_E

C -4.3332373 -0.5709996 2.1848837
C -5.5843435 -1.1374642 2.4116669
C -6.4229764 -1.4211621 1.3452993
C -6.0450070 -1.0991304 0.0351739
C -4.8159053 -0.4908260 -0.1911424
C -3.9337341 -0.2354956 0.8694995
C -2.6006820 0.3736322 0.6992477
C -1.4396514 -0.1237529 1.1508522
C -0.1757147 0.6554938 1.2160461
C 0.9527102 0.5933649 0.3597977
C 1.1561916 -0.3639836 -0.6674271
C 2.3522776 -0.4379547 -1.3717858

SUPPORTING INFORMATION

C 3.4251653 0.4529824 -1.1192148
 C 3.1836929 1.4736994 -0.1668505
 C 2.0182953 1.5107109 0.5668332
 C 4.9540425 -0.8092958 -2.5689068
 C 5.6809363 1.3279498 -1.5126655
 H -5.8622783 -1.3778169 3.4369116
 H -7.3741430 -1.9079735 1.5303405
 H -6.6996021 -1.3392123 -0.7929476
 H -4.5078493 -0.2246312 -1.1998723
 H -1.4640750 -1.1452317 1.5211439
 H -0.0232925 1.1833960 2.1647620
 H 0.3765684 -1.0928809 -0.8783553
 H 2.4512137 -1.1987067 -2.1381142
 H 3.9152038 2.2515581 0.0039178
 H 1.8979712 2.2763005 1.3304192
 H 4.7361604 -1.7517427 -2.0570676
 H 6.0168246 -0.8014065 -2.8123940
 H 4.3966624 -0.7967342 -3.5120075
 H 5.4803689 2.2534155 -2.0677864
 H 6.6445799 0.9376639 -1.8390927
 H 5.7752882 1.5832459 -0.4544923
 H -2.6550059 -0.0996248 2.9213901
 N 4.6587666 0.3228687 -1.7179316
 O -3.5292156 -0.3701969 3.2639670
 O -2.6061961 1.5999311 0.0559118
 40

2_ADC2_SVP

C 0.0637081 -0.1619633 1.8833718
 C 0.2605232 1.8574427 -5.4993245
 C 0.3526525 -0.3641114 -1.1629472
 C 0.3825926 -0.5357491 -2.5142070
 C 0.4810505 -1.1665808 4.0841242
 C 0.6485888 -1.2557968 1.2010748
 C 0.6533127 -2.3256487 6.2222634
 C 0.6842172 0.8415667 -4.6207010
 C 0.7529277 -1.3543032 -0.2293447
 C 1.0565175 -2.2695709 3.4072491
 C 1.1326574 -2.3084993 2.0164050
 C -0.0147631 -0.1153685 3.2745377
 C -0.1201106 0.5083106 -3.4736534
 C -0.4527233 -0.1322907 6.0861981
 C -0.9640681 2.5564348 -5.3054248
 C -1.3307052 1.1255703 -3.3240691
 C -1.3796264 3.6496078 -6.2556180
 C -1.7296731 2.1837908 -4.2205502
 H 0.6044355 -2.0990939 7.2996480
 H 0.9221323 2.0836492 -6.3454871
 H 1.1668673 -2.2846279 -0.6473712
 H 1.3091833 -1.4286073 -3.8930256
 H 1.4474376 -3.1239656 3.9660150
 H 1.5845146 -3.1867617 1.5354201
 H 1.6597501 -2.7294763 6.0202545
 H -0.0377416 0.5973754 -0.8018952
 H -0.0916039 -3.1196476 5.9961908
 H -0.1659515 0.8933064 5.7981071
 H -0.3544686 0.6790758 1.3167994
 H -0.3552152 -0.2005669 7.1818424
 H -0.4877130 0.7596515 3.7280217

SUPPORTING INFORMATION

H -0.6263311 4.4570168 -6.2864691
H -1.4928107 3.2569484 -7.2820623
H -1.5217793 -0.2824726 5.8191064
H -1.9879370 0.8528934 -2.4896009
H -2.3438481 4.0900352 -5.9500588
H -2.6747787 2.7045308 -4.0173358
N 0.4269125 -1.1063528 5.4752477
O 0.7788324 -1.7023684 -3.1029107
O 1.7630549 0.1566470 -4.8898310
40

2_ADC_SVP_E

C 0.2067177 2.2772439 -3.2660033
C 0.2458184 0.8702984 -3.4123220
C 0.3324993 -1.2688015 4.1300693
C 0.4341326 -0.1154063 -1.0480159
C 0.7225114 -2.4267902 6.2412842
C 0.7360096 0.0406689 -2.3201300
C 0.8521163 -1.0380104 1.2925078
C 1.1637927 -0.9378341 -0.0932780
C 1.3896549 -1.9797725 3.5055398
C 1.6364320 -1.8649975 2.1420921
C -0.2132542 -0.3423107 1.9219258
C -0.2484194 0.2863206 -4.6052882
C -0.3747738 3.0752924 -4.2452812
C -0.4614685 -0.4530057 3.2890958
C -0.8202550 1.1074824 -5.5873850
C -0.8948253 2.4951708 -5.4225375
C -1.1428854 -0.8359362 6.0217348
C -1.5754652 3.3537130 -6.4559014
H 0.3710564 -1.4781888 -4.1936667
H 0.4077793 -3.4326044 5.8880343
H 0.4482102 -2.3312387 7.3035942
H 0.6143322 2.7143718 -2.3482213
H 1.8227972 -2.3697616 6.1833521
H 2.0344486 -2.6422359 4.0892989
H 2.0431490 -1.4844486 -0.4719420
H 2.4685963 -2.4330720 1.7031416
H -0.4094777 4.1626200 -4.1125072
H -0.4316842 0.4715065 -0.7172396
H -0.8710353 0.3100242 1.3345683
H -1.1266365 4.3612163 -6.4941934
H -1.1467246 -0.9520688 7.1168688
H -1.2048756 0.6222602 -6.4916748
H -1.2473597 0.2414113 5.8084446
H -1.3032111 0.1116291 3.6986131
H -1.5073847 2.9045016 -7.4615053
H -2.0335638 -1.3590673 5.6109492
H -2.6470371 3.4712493 -6.2089794
N 0.1069907 -1.3459659 5.5024716
O 1.8650057 -0.7367362 -2.9997553
O -0.2417331 -1.0487376 -4.8277185
40

2_ADC2_TZVP

C 0.0645487 -0.1571046 1.8825796
C 0.2592455 1.8514333 -5.4792741
C 0.3383813 -0.3653822 -1.1507710
C 0.3697240 -0.5259908 -2.4875771
C 0.4786030 -1.1648426 4.0625115

SUPPORTING INFORMATION

C 0.6435783 -1.2453383 1.2049911
 C 0.6552212 -2.3174488 6.1947850
 C 0.6789321 0.8451091 -4.5990043
 C 0.7483350 -1.3479530 -0.2155595
 C 1.0443774 -2.2629827 3.3925085
 C 1.1262817 -2.2958442 2.0114301
 C -0.0213226 -0.1212706 3.2652222
 C -0.1154810 0.5147938 -3.4526664
 C -0.4433212 -0.1381700 6.0611818
 C -0.9556847 2.5436998 -5.2912300
 C -1.3138939 1.1327355 -3.3124318
 C -1.3712882 3.6287350 -6.2383800
 C -1.7185604 2.1677212 -4.2205380
 H 0.6039469 -2.0884494 7.2585150
 H 0.9077154 2.0792417 -6.3202155
 H 1.1627896 -2.2682188 -0.6210104
 H 1.2762729 -1.4073752 -3.8696044
 H 1.4305879 -3.1072189 3.9485048
 H 1.5742131 -3.1613119 1.5320185
 H 1.6468284 -2.7243743 5.9973025
 H -0.0462065 0.5858715 -0.7954543
 H -0.0874798 -3.0958703 5.9702438
 H -0.1672387 0.8772943 5.7778069
 H -0.3439714 0.6776213 1.3235636
 H -0.3447899 -0.2118461 7.1433292
 H -0.4875046 0.7405139 3.7236198
 H -0.6275910 4.4272337 -6.2699200
 H -1.4815462 3.2452787 -7.2547885
 H -1.4981396 -0.2954443 5.7955599
 H -1.9678543 0.8689439 -2.4903573
 H -2.3230273 4.0662612 -5.9380960
 H -2.6623872 2.6697490 -4.0317143
 N 0.4418461 -1.0997525 5.4491272
 O 0.7664585 -1.6940223 -3.0834527
 O 1.7594116 0.1740150 -4.8727753

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2_ADC2_TZVP_E

C 0.2031113 2.2718696 -3.2570154
 C 0.2334595 0.8704335 -3.3917434
 C 0.3384172 -1.2541914 4.1168869
 C 0.4422358 -0.1055318 -1.0325206
 C 0.7292676 -2.4190600 6.2116093
 C 0.7339244 0.0612261 -2.2959743
 C 0.8430544 -1.0317511 1.2947837
 C 1.1623521 -0.9324502 -0.0814550
 C 1.3792664 -1.9731026 3.4928082
 C 1.6231252 -1.8593733 2.1372173
 C -0.2207300 -0.3446084 1.9197185
 C -0.2619129 0.2842355 -4.5740104
 C -0.3709559 3.0624316 -4.2336400
 C -0.4649393 -0.4579595 3.2809974
 C -0.8135616 1.0990997 -5.5638945
 C -0.8947221 2.4787446 -5.3997516
 C -1.1336034 -0.8336101 5.9985862
 C -1.5577381 3.3331288 -6.4421692
 H 0.3170631 -1.4856756 -4.1495056
 H 0.3894302 -3.3970527 5.8423032
 H 0.4673738 -2.3347352 7.2653051

SUPPORTING INFORMATION

H 0.6271416 2.7041187 -2.3578430
 H 1.8175441 -2.3866763 6.1433394
 H 2.0145032 -2.6289974 4.0740700
 H 2.0169904 -1.4966343 -0.4547570
 H 2.4422178 -2.4220154 1.6976475
 H -0.4077169 4.1397834 -4.1109280
 H -0.4283996 0.4561670 -0.7081504
 H -0.8780075 0.2930393 1.3384696
 H -1.1084680 4.3260417 -6.4831795
 H -1.1461180 -0.9454117 7.0815808
 H -1.1895466 0.6256385 -6.4648102
 H -1.2611565 0.2272541 5.7791372
 H -1.3001817 0.0933544 3.6933155
 H -1.4890496 2.8817845 -7.4322279
 H -1.9915518 -1.3779359 5.5791877
 H -2.6180312 3.4607333 -6.2075579
 N 0.1369651 -1.3092735 5.4936400
 O 1.8831949 -0.6210048 -3.0010809
 O -0.2642672 -1.0520735 -4.7983688

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2_CC2_SVP

C 0.0789200 -0.1644600 1.9134700
 C 0.2752000 -0.4197000 -2.4608800
 C 0.3978900 2.0233800 -5.3464800
 C 0.4782000 -1.1970600 4.0993200
 C 0.5219300 -0.2354500 -1.1173200
 C 0.6818400 -1.2433800 1.2105200
 C 0.7099600 -2.3568000 6.2429200
 C 0.7626100 0.9984900 -4.4498600
 C 0.7940000 -1.3033400 -0.2185600
 C 1.0353500 -2.3063200 3.4155600
 C 1.1172600 -2.3308900 2.0243700
 C -0.0105500 -0.1311900 3.3015900
 C -0.1773800 0.6208700 -3.3926200
 C -0.3838600 -0.1380200 6.1338300
 C -0.9163500 2.5597800 -5.3556500
 C -1.2971200 3.6337700 -6.3333900
 C -1.5201600 1.0062500 -3.5250600
 C -1.8545900 2.0263200 -4.4578700
 H 0.4058800 0.7857400 -0.7312300
 H 0.6737600 -2.1049800 7.3171300
 H 0.8166600 -1.4620700 -3.9192600
 H 1.0345800 -2.2844400 -0.6602200
 H 1.1577900 2.3114400 -6.0984000
 H 1.3871800 -3.1857800 3.9654000
 H 1.5428300 -3.2147600 1.5300900
 H 1.7290000 -2.7211200 6.0202900
 H -0.0117300 -3.1829300 6.0494300
 H -0.0458200 0.8733500 5.8480100
 H -0.2484600 -0.2345300 7.2241900
 H -0.3616500 0.6617200 1.3414000
 H -0.5135200 0.7242000 3.7620100
 H -0.6169500 4.5050500 -6.2733200
 H -1.2644000 3.2408100 -7.3669200
 H -1.4703800 -0.2242500 5.9084100
 H -2.2860300 0.5831600 -2.8744200
 H -2.3249100 3.9764500 -6.1309300
 H -2.8674600 2.4667300 -4.4249900

SUPPORTING INFORMATION

N 0.4116300 -1.1588900 5.4866400
 O 0.3487000 -1.6426700 -3.0530700
 O 1.8101300 0.2455200 -4.6041400
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2_CC2_SVP_E

C 0.2279428 1.0334940 -3.2992271
 C 0.2587412 2.4553445 -3.3088107
 C 0.2707682 -0.2034081 -1.0387061
 C 0.3507598 -1.2979914 4.1251000
 C 0.7258661 -2.4795785 6.2293274
 C 0.7270321 0.2430364 -2.1805027
 C 0.8382312 -1.0991069 1.2738420
 C 1.0497229 -1.0690618 -0.1070315
 C 1.4119084 -2.0177889 3.4962265
 C 1.6363500 -1.9270845 2.1325802
 C -0.2035665 -0.3599626 1.9250001
 C -0.2655367 0.3386787 -4.4443804
 C -0.3159921 3.1555689 -4.3555335
 C -0.4325640 -0.4527659 3.2922948
 C -0.8804427 1.0652490 -5.4820774
 C -0.8965290 2.4626184 -5.4570334
 C -1.1131082 -0.8379357 6.0202946
 C -1.5544599 3.2423618 -6.5631136
 H 0.4021867 -3.4807344 5.8703283
 H 0.4521777 -2.3842748 7.2922630
 H 0.4706729 -1.3006984 -3.8856316
 H 0.7085826 2.9694007 -2.4519051
 H 1.8265301 -2.4291039 6.1668429
 H 1.8687179 -1.6621254 -0.5488583
 H 2.0653934 -2.6689520 4.0843310
 H 2.4609571 -2.5009928 1.6858689
 H -0.3027128 4.2524295 -4.3557960
 H -0.7437112 0.1183024 -0.7663700
 H -0.8423344 0.3103505 1.3373146
 H -1.0096382 4.1821409 -6.7607923
 H -1.1175995 -0.9610830 7.1150108
 H -1.1764728 0.2434808 5.8091328
 H -1.2559713 0.1322157 3.7123687
 H -1.2771361 0.5088250 -6.3405584
 H -1.5909282 2.6552883 -7.4961591
 H -2.0224451 -1.3261906 5.6064835
 H -2.5921362 3.5077213 -6.2845880
 N 0.1167304 -1.3916043 5.4903277
 O 1.9385886 -0.0281131 -3.0048235
 O -0.2145649 -0.9979603 -4.5330493
 40

2_CC2_TZVP

C 0.0789205 -0.1644600 1.9134702
 C 0.2752005 -0.4197000 -2.4608798
 C 0.3978905 2.0233800 -5.3464797
 C 0.4782005 -1.1970600 4.0993202
 C 0.5219305 -0.2354500 -1.1173198
 C 0.6818405 -1.2433800 1.2105202
 C 0.7099605 -2.3568000 6.2429202
 C 0.7626105 0.9984900 -4.4498598
 C 0.7940005 -1.3033400 -0.2185598
 C 1.0353505 -2.3063200 3.4155602
 C 1.1172605 -2.3308900 2.0243702

SUPPORTING INFORMATION

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C -0.0105495 -0.1311900 3.3015902
C -0.1773795 0.6208700 -3.3926198
C -0.3838595 -0.1380200 6.1338303
C -0.9163495 2.5597800 -5.3556497
C -1.2971195 3.6337700 -6.3333897
C -1.5201595 1.0062500 -3.5250598
C -1.8545895 2.0263200 -4.4578698
H 0.4058805 0.7857400 -0.7312298
H 0.6737605 -2.1049800 7.3171302
H 0.8166605 -1.4620700 -3.9192598
H 1.0345805 -2.2844400 -0.6602198
H 1.1577905 2.3114400 -6.0983998
H 1.3871805 -3.1857800 3.9654002
H 1.5428305 -3.2147600 1.5300902
H 1.7290005 -2.7211200 6.0202902
H -0.0117295 -3.1829300 6.0494303
H -0.0458195 0.8733500 5.8480102
H -0.2484595 -0.2345300 7.2241903
H -0.3616495 0.6617200 1.3414002
H -0.5135195 0.7242000 3.7620102
H -0.6169495 4.5050500 -6.2733197
H -1.2643995 3.2408100 -7.3669198
H -1.4703795 -0.2242500 5.9084102
H -2.2860295 0.5831600 -2.8744198
H -2.3249095 3.9764500 -6.1309298
H -2.8674595 2.4667300 -4.4249897
N 0.4116305 -1.1588900 5.4866403
O 0.3487005 -1.6426700 -3.0530698
O 1.8101305 0.2455200 -4.6041398
40
2_CC2_TZVP_E
C 0.2060400 0.9933100 -3.3252800
C 0.2454600 2.4177100 -3.3131800
C 0.3104100 -0.1971600 -1.0402800
C 0.3403900 -1.3100200 4.1372600
C 0.7114800 -2.4846300 6.2495200
C 0.7219100 0.1910300 -2.2215800
C 0.8710100 -1.0708600 1.2885400
C 1.1015600 -1.0309000 -0.0925300
C 1.4098600 -2.0188000 3.5096500
C 1.6571100 -1.9056800 2.1541200
C -0.1854600 -0.3511500 1.9367400
C -0.2806800 0.3211100 -4.4872400
C -0.3173200 3.1385300 -4.3505300
C -0.4377500 -0.4638300 3.2967300
C -0.8947400 1.0709200 -5.5088500
C -0.9050700 2.4659100 -5.4619100
C -1.1246400 -0.8369500 6.0296400
C -1.5602000 3.2699500 -6.5517900
H 0.3912600 -3.4926700 5.9067000
H 0.4408600 -2.3753000 7.3118700
H 0.4631700 -1.3305400 -3.9786400
H 0.6974200 2.9143300 -2.4460500
H 1.8119600 -2.4307000 6.1844200
H 1.9470400 -1.5972600 -0.5182200
H 2.0522600 -2.6856700 4.0959400
H 2.4892300 -2.4738200 1.7106100
H -0.2985400 4.2356600 -4.3342700

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SUPPORTING INFORMATION

H	-0.6876500	0.1599300	-0.7467700
H	-0.8187400	0.3262100	1.3483200
H	-1.0212800	4.2208000	-6.7080400
H	-1.1249600	-0.9488800	7.1248800
H	-1.1779600	0.2434100	5.8108100
H	-1.2734100	0.1099600	3.7085900
H	-1.3058700	0.5293800	-6.3689600
H	-1.5766000	2.7103200	-7.5021400
H	-2.0431500	-1.3169700	5.6273100
H	-2.6052400	3.5156300	-6.2816500
N	0.0963600	-1.4075600	5.4989400
O	1.9027100	-0.0930700	-3.0798100
O	-0.2282300	-1.0116900	-4.6129100

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3_ADC2_SVP

C	0.0158711	-0.3640121	3.4976927
C	0.1562782	-0.2611107	2.1151016
C	0.5660310	-0.1226830	-0.9131748
C	0.8473909	0.0315263	-2.2330941
C	0.9367704	-1.0984427	4.2855984
C	1.2254318	-0.8803968	1.4231773
C	1.4102424	-0.8085555	0.0015285
C	1.5698699	-2.1998366	6.3634754
C	2.0144953	-1.7124477	3.6003492
C	2.1480752	-1.6049932	2.2179792
C	-0.0260611	0.8244178	-3.1644160
C	-0.3464279	2.1442476	-2.9501746
C	-0.4692667	-0.8271089	6.2574894
C	-0.4962659	0.1804309	-4.3658355
C	-1.2549789	2.8145642	-3.8200671
C	-1.4017652	0.8610911	-5.2280100
C	-1.7686191	2.1886582	-4.9608335
C	-3.1185333	2.3429439	-6.9006806
H	0.0357164	2.6706464	-2.0666649
H	1.3205188	-3.2330268	6.0365491
H	1.3732533	-2.1179420	7.4442153
H	1.7023445	-0.8437054	-3.6633794
H	2.3025165	-1.2912154	-0.4245667
H	2.6514966	-2.0428966	6.2169111
H	2.7646485	-2.2940628	4.1439310
H	2.9964264	-2.1026575	1.7274769
H	-0.3588259	0.3523125	-0.5572854
H	-0.3969970	-0.9270045	7.3522261
H	-0.5913945	0.3232100	1.5639111
H	-0.7179185	0.2258664	6.0433648
H	-0.8374407	0.1396714	3.9611702
H	-1.3089043	-1.4627003	5.8998478
H	-1.5614991	3.8472657	-3.6159130
H	-1.7484971	0.3031456	-6.1018473
H	-2.3067271	2.0737200	-7.6016623
H	-3.7177933	1.4428595	-6.6705291
H	-3.7642929	3.1022104	-7.3633147
N	0.8041145	-1.1860286	5.6697725
O	1.9940132	-0.4422159	-2.8102583
O	-0.0399466	-0.9810596	-4.6875381
O	-2.6033901	2.9353149	-5.7225124

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3_ADC2_SVP Negative Dihedral Angle

SUPPORTING INFORMATION

C 0.0399548 0.7867774 -4.3552370
 C 0.1476465 -0.1127981 6.3432452
 C 0.2420823 -0.6376937 -2.2807775
 C 0.2693877 -0.1752964 2.1106220
 C 0.3045291 -0.0994370 3.5020730
 C 0.3169166 -0.4146211 -0.9430235
 C 1.0539014 -1.2288050 -0.0402170
 C 1.0577187 -1.1055370 1.3908678
 C 1.1293328 -0.9543115 4.2740985
 C 1.7985001 -1.9371086 6.4039619
 C 1.8738267 -1.9634129 2.1691010
 C 1.9126784 -1.8941559 3.5600657
 C -0.5965103 0.2010736 -3.2029474
 C -0.6957499 1.6546880 -5.2098821
 C -1.9488788 0.3772538 -3.0320089
 C -2.0597433 1.8857992 -4.9755271
 C -2.2865226 3.3171754 -6.8515581
 C -2.6724848 1.2593540 -3.8860028
 H 0.1326188 0.9391736 6.0121549
 H 0.3600346 -0.1084660 7.4243431
 H 1.2509833 -1.3254457 -3.7137937
 H 1.2768459 -2.9092279 6.2675365
 H 1.6486139 -2.0385849 -0.4891401
 H 1.7893076 -1.6863774 7.4767758
 H 2.4954372 -2.7117364 1.6584068
 H 2.5616891 -2.5965774 4.0899521
 H 2.8535657 -2.0684772 6.1107818
 H -0.1433259 2.0857808 -6.0491449
 H -0.2639835 0.4351847 -0.5604659
 H -0.3414454 0.6373970 3.9869353
 H -0.4059383 0.5041303 1.5758888
 H -0.8669934 -0.5398600 6.1879967
 H -1.4546188 3.9859636 -6.5632395
 H -1.9215369 2.5750694 -7.5858360
 H -2.4660879 -0.1087127 -2.1962280
 H -3.0911764 3.9132562 -7.3048057
 H -3.7349179 1.4612095 -3.7075562
 N 1.1870004 -0.8550220 5.6626753
 O 0.8514215 -1.6992073 -2.8927971
 O 1.2547560 0.4663517 -4.6455930
 O -2.8588353 2.6851940 -5.7216906

41

3_ADC2_SVP_E

C 0.0068329 0.1042144 6.4567013
 C 0.1908104 -0.5075740 -2.1431508
 C 0.1991525 -0.3714845 -0.8294910
 C 0.2148248 -0.0541047 2.2234695
 C 0.2316946 0.0378785 3.6152649
 C 0.3157056 0.7254683 -4.3174228
 C 0.8035999 -1.2979679 0.1175726
 C 0.8147294 -1.1402682 1.5335000
 C 0.8511714 -0.9453640 4.4231433
 C 1.2711465 -2.0066432 6.5757304
 C 1.4291418 -2.1260711 2.3539195
 C 1.4498941 -2.0355835 3.7412104
 C -0.3092460 1.4814911 -5.3212401
 C -0.4450340 0.1834628 -3.2531402
 C -1.6573515 3.0542991 -7.2256669

SUPPORTING INFORMATION

C	-1.6834744	1.7410589	-5.2476267
C	-1.8467724	0.4043076	-3.2373880
C	-2.4558608	1.1980017	-4.1938151
H	0.1775787	0.0727368	7.5447787
H	0.2131333	1.1368955	6.1266812
H	0.3220093	1.8450782	-6.1346843
H	0.5792079	-2.8634700	6.4219452
H	1.2754381	-1.7512118	7.6475109
H	1.2781819	-2.1980488	-0.3055645
H	1.9021585	-2.9950797	1.8755198
H	1.9350143	-2.8406671	4.2993306
H	1.9385925	-0.1523210	-3.8183000
H	2.2915795	-2.3374205	6.3167510
H	-0.2625039	0.8995793	4.0719835
H	-0.2844159	0.7468817	1.6643219
H	-0.3304066	0.5204686	-0.4726541
H	-0.8603776	3.7366262	-6.8770998
H	-1.0666177	-0.1134508	6.2651721
H	-1.2154218	2.2710233	-7.8685984
H	-2.3996528	3.6232367	-7.8038247
H	-2.4332776	-0.0421586	-2.4264307
H	-3.5309143	1.4028469	-4.1783703
N	0.9011361	-0.8339696	5.8124632
O	0.8990446	-1.6384892	-2.8816982
O	1.6563712	0.5765301	-4.4120332
O	-2.3668530	2.4892931	-6.1387508

41

3_ADC2_TZVP

C	0.0192829	-0.3608081	3.4852585
C	0.1548709	-0.2589038	2.1082588
C	0.5616439	-0.1197762	-0.9041334
C	0.8290411	0.0288598	-2.2143983
C	0.9439826	-1.0768242	4.2692838
C	1.2175906	-0.8751165	1.4189897
C	1.4065463	-0.8049941	0.0072026
C	1.5679597	-2.1876464	6.3343065
C	2.0044504	-1.7019221	3.5852941
C	2.1366657	-1.5965915	2.2098093
C	-0.0439128	0.8130227	-3.1454111
C	-0.3647393	2.1224434	-2.9260721
C	-0.4585778	-0.8234640	6.2347836
C	-0.5130671	0.1782566	-4.3447098
C	-1.2501977	2.8008086	-3.8039804
C	-1.3804917	0.8746693	-5.2239909
C	-1.7570377	2.1857168	-4.9428620
C	-3.0963756	2.3288364	-6.8860926
H	0.0190078	2.6396128	-2.0526893
H	1.2874570	-3.1948564	5.9938727
H	1.3739629	-2.1145829	7.4037267
H	1.6838047	-0.8327050	-3.6456029
H	2.2913041	-1.2816707	-0.4088679
H	2.6410999	-2.0614599	6.1879590
H	2.7446187	-2.2772701	4.1272988
H	2.9697535	-2.0939769	1.7198604
H	-0.3502644	0.3515796	-0.5484505
H	-0.3903779	-0.9276515	7.3169563
H	-0.5884751	0.3131818	1.5622625
H	-0.7333453	0.2105076	6.0238545

SUPPORTING INFORMATION

H	-0.8225460	0.1369988	3.9501396
H	-1.2627482	-1.4779981	5.8688933
H	-1.5593871	3.8176792	-3.5876477
H	-1.7085509	0.3368790	-6.1043775
H	-2.2861457	2.0746051	-7.5744779
H	-3.6715014	1.4298901	-6.6493190
H	-3.7461627	3.0687776	-7.3442344
N	0.8299676	-1.1422074	5.6562203
O	1.9776736	-0.4459878	-2.7969561
O	-0.0872412	-0.9967556	-4.6551075
O	-2.5895386	2.9408441	-5.7048300

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3_ADC2_TZVP Negative Dihedral Angle

C	0.0338962	0.7878504	-4.3516786
C	0.1489647	-0.1138338	6.3391341
C	0.2357260	-0.6350755	-2.2765257
C	0.2747343	-0.1792717	2.1120392
C	0.3064777	-0.1085579	3.4984168
C	0.3140546	-0.4202641	-0.9407183
C	1.0517241	-1.2261078	-0.0369620
C	1.0565646	-1.1036862	1.3904618
C	1.1292881	-0.9540288	4.2697269
C	1.7977611	-1.9360835	6.3996691
C	1.8679948	-1.9572058	2.1699792
C	1.9042384	-1.8902962	3.5557991
C	-0.5959480	0.2011990	-3.1997222
C	-0.7025982	1.6487509	-5.2093132
C	-1.9416517	0.3876651	-3.0307044
C	-2.0521241	1.8862233	-4.9710317
C	-2.2813128	3.3165206	-6.8520122
C	-2.6630144	1.2522316	-3.8926660
H	0.1326018	0.9265648	6.0126647
H	0.3592143	-0.1114215	7.4083324
H	1.2398863	-1.3208540	-3.7035208
H	1.2813298	-2.8968347	6.2659382
H	1.6427737	-2.0282458	-0.4758663
H	1.7869656	-1.6875517	7.4606215
H	2.4838761	-2.6974377	1.6663627
H	2.5486363	-2.5829913	4.0826652
H	2.8410131	-2.0675246	6.1105996
H	-0.1583944	2.0833137	-6.0386860
H	-0.2587087	0.4234055	-0.5664103
H	-0.3292232	0.6228308	3.9812097
H	-0.3933746	0.4930917	1.5841540
H	-0.8539195	-0.5366719	6.1867448
H	-1.4605579	3.9777859	-6.5635988
H	-1.9225325	2.5806194	-7.5762239
H	-2.4571301	-0.0981765	-2.2086698
H	-3.0787855	3.9043501	-7.2987333
H	-3.7135156	1.4525844	-3.7117215
N	1.1892297	-0.8532900	5.6553465
O	0.8515544	-1.6964018	-2.8860860
O	1.2452418	0.4732133	-4.6421436
O	-2.8609561	2.6835423	-5.7168612

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3_ADC2_TZVP_E

C	0.0144478	0.1019758	6.4184554
C	0.1710985	-0.4871411	-2.1103990

SUPPORTING INFORMATION

C	0.2091010	-0.0548869	2.2137327
C	0.2152753	-0.3488677	-0.8103604
C	0.2359365	0.0372106	3.5983506
C	0.3132152	0.7442834	-4.2743855
C	0.8060829	-1.1367147	1.5276878
C	0.8105948	-1.2897880	0.1219918
C	0.8690435	-0.9328453	4.3972011
C	1.2708522	-1.9993200	6.5397457
C	1.4180159	-2.1204065	2.3410267
C	1.4452514	-2.0285192	3.7194834
C	-0.3029584	1.4943680	-5.2770101
C	-0.4516340	0.2143028	-3.2152300
C	-1.6261272	3.0210169	-7.2009495
C	-1.6773006	1.7155585	-5.2252472
C	-1.8519856	0.4042226	-3.2198437
C	-2.4585841	1.1618465	-4.1909243
H	0.1761622	0.0822317	7.4957524
H	0.1850671	1.1259021	6.0838537
H	0.3197843	1.8762737	-6.0742636
H	0.5562106	-2.8184344	6.3744748
H	1.2792415	-1.7552451	7.6015315
H	1.2866984	-2.1717698	-0.3055167
H	1.8763778	-2.9793056	1.8577719
H	1.9149932	-0.1392758	-3.7750921
H	1.9231036	-2.8260094	4.2745673
H	2.2673319	-2.3602711	6.2822083
H	-0.2497901	0.8895121	4.0577926
H	-0.2504946	0.5606921	-0.4463576
H	-0.2936007	0.7333874	1.6629824
H	-0.8520357	3.6920812	-6.8220881
H	-1.0356115	-0.1542777	6.2168914
H	-1.1728560	2.2483778	-7.8263935
H	-2.3477494	3.5869503	-7.7838576
H	-2.4232153	-0.0390500	-2.4122090
H	-3.5269544	1.3390824	-4.1995953
N	0.9466884	-0.8070066	5.7841759
O	0.7218451	-1.6165340	-2.9069874
O	1.6537581	0.5956426	-4.3605177
O	-2.3653198	2.4408101	-6.1324392

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3_CC2_SVP

C	0.0022528	-0.4053834	3.4882524
C	0.1358201	-0.3200239	2.1074390
C	0.4164060	-0.3230107	-0.9065729
C	0.7595879	0.0734398	-2.1889347
C	0.9253721	-1.1443551	4.2779989
C	1.2017418	-0.9417630	1.4099406
C	1.3596973	-0.8613641	-0.0153171
C	1.5880712	-2.2041031	6.3779675
C	2.0183504	-1.7416907	3.5920883
C	2.1388873	-1.6436266	2.2086980
C	-0.0883843	0.8278081	-3.1102925
C	-0.2313080	2.2141285	-3.0489431
C	-0.4689797	-0.8196117	6.2540401
C	-0.5734738	0.1252606	-4.2981971
C	-1.0682118	2.8821022	-3.9603304
C	-1.5364905	0.7977634	-5.1327351
C	-1.7352930	2.1698176	-4.9914451

SUPPORTING INFORMATION

C -3.1348986 2.3144955 -6.9090545
 H 0.2113707 2.7728270 -2.2143539
 H 1.3623178 -2.1117155 7.4517117
 H 1.3938365 -3.2537827 6.0681457
 H 1.9453371 -0.2898226 -3.5968509
 H 2.3292892 -1.1620736 -0.4439732
 H 2.6645934 -1.9955903 6.2469946
 H 2.7792234 -2.3096758 4.1361536
 H 2.9902889 -2.1273285 1.7119374
 H -0.3900750 -0.9307862 7.3463410
 H -0.5889698 0.2862263 1.5525880
 H -0.6038783 -0.0949113 -0.5637325
 H -0.6664944 0.2463362 6.0444491
 H -0.8419296 0.1132675 3.9512980
 H -1.2455922 3.9595032 -3.8791488
 H -1.3411384 -1.4123146 5.9029035
 H -2.0303854 0.1944876 -5.9012093
 H -2.3470376 1.9940688 -7.6185795
 H -3.7551710 3.0989108 -7.3664853
 H -3.7712892 1.4448081 -6.6564830
 N 0.7807130 -1.2427258 5.6519025
 O 2.0453286 -0.0974950 -2.6367919
 O -0.0603425 -1.0018240 -4.5854619
 O -2.5691526 2.9196873 -5.7559373

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3_CC2_SVP_E

C 0.0070323 0.0822729 6.4552433
 C 0.0422427 -0.4810109 -2.0652088
 C 0.2100234 0.0105455 3.6226159
 C 0.2104797 -0.0667033 2.2337407
 C 0.2578189 -0.2528323 -0.7939487
 C 0.2629961 0.7180782 -4.2368751
 C 0.8629568 -1.1280686 1.5274406
 C 0.8664200 -0.9612300 4.4248465
 C 0.8971478 -1.2249468 0.1284231
 C 1.3224558 -2.0042479 6.5862462
 C 1.5004342 -2.1122215 2.3532790
 C 1.5017187 -2.0378255 3.7384015
 C -0.2819529 1.5339153 -5.2430680
 C -0.5756449 0.1900794 -3.2012591
 C -1.5359168 3.0753201 -7.2440752
 C -1.6713915 1.7148588 -5.2972788
 C -1.9922822 0.3406418 -3.3208522
 C -2.5307662 1.1118476 -4.3266916
 H 0.1929683 0.0688343 7.5416613
 H 0.1937525 1.1112424 6.1019970
 H 0.4028007 1.9301391 -5.9978221
 H 0.6549194 -2.8831171 6.4490495
 H 1.3275367 -1.7322522 7.6545532
 H 1.3746343 -2.1017509 -0.3404779
 H 1.7221102 -0.3190722 -3.6878645
 H 1.9999544 -2.9610660 1.8643791
 H 2.0027897 -2.8344212 4.2965617
 H 2.3497204 -2.3061316 6.3180397
 H -0.0781351 0.7201985 -0.4113738
 H -0.3201028 0.8480192 4.0856841
 H -0.3293556 0.7070951 1.6743332
 H -0.8032255 3.7752510 -6.8039520

SUPPORTING INFORMATION

H -1.0110424 2.3267802 -7.8647212
H -1.0648458 -0.1555539 6.2769954
H -2.2571533 3.6302520 -7.8613388
H -2.6287327 -0.1135221 -2.5525285
H -3.6094152 1.2761276 -4.4262681
N 0.9073134 -0.8526427 5.8116612
O 0.3483069 -1.5790281 -2.9973399
O 1.5803037 0.4949380 -4.2438081
O -2.3089041 2.4412081 -6.2284396

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3_CC2_TZVP

C 0.0021003 -0.4056499 3.4884071
C 0.1358252 -0.3197893 2.1072295
C 0.4163538 -0.3220917 -0.9078827
C 0.7586998 0.0728560 -2.1865687
C 0.9255391 -1.1441691 4.2771346
C 1.2014327 -0.9418499 1.4101423
C 1.3604368 -0.8617006 -0.0149658
C 1.5884726 -2.2045732 6.3784655
C 2.0181108 -1.7419359 3.5921952
C 2.1392046 -1.6435414 2.2084819
C -0.0879955 0.8288531 -3.1109315
C -0.2314562 2.2135647 -3.0484595
C -0.4696036 -0.8193934 6.2544921
C -0.5749769 0.1260228 -4.2976996
C -1.0683244 2.8819381 -3.9610001
C -1.5359871 0.7979105 -5.1334262
C -1.7351366 2.1685530 -4.9905683
C -3.1355021 2.3138293 -6.9102430
H 0.2111756 2.7721538 -2.2153454
H 1.3625601 -2.1118253 7.4506169
H 1.3940343 -3.2526336 6.0683571
H 1.9455746 -0.2897689 -3.5959028
H 2.3282407 -1.1618563 -0.4433839
H 2.6634343 -1.9958008 6.2470316
H 2.7783557 -2.3091212 4.1357068
H 2.9894952 -2.1268887 1.7124764
H -0.3901348 -0.9307050 7.3452498
H -0.5883761 0.2856559 1.5531358
H -0.6026802 -0.0950047 -0.5643265
H -0.6662619 0.2452068 6.0446084
H -0.8410970 0.1126580 3.9509759
H -1.2455596 3.9584832 -3.8791063
H -1.3401816 -1.4117029 5.9031654
H -2.0297661 0.1952378 -5.9006514
H -2.3478610 1.9944061 -7.6176815
H -3.7544942 3.0979460 -7.3661247
H -3.7705602 1.4458226 -6.6565368
N 0.7807724 -1.2426472 5.6518323
O 2.0458343 -0.0972299 -2.6377398
O -0.0608504 -1.0014485 -4.5855028
O -2.5688370 2.9202299 -5.7556273

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3_CC2_TZVP_E

C 0.0070300 0.0822700 6.4552400
C 0.0422400 -0.4810100 -2.0652100
C 0.2100200 0.0105500 3.6226200
C 0.2104800 -0.0667000 2.2337400

SUPPORTING INFORMATION

C	0.2578200	-0.2528300	-0.7939500
C	0.2630000	0.7180800	-4.2368800
C	0.8629600	-1.1280700	1.5274400
C	0.8664200	-0.9612300	4.4248500
C	0.8971500	-1.2249500	0.1284200
C	1.3224600	-2.0042500	6.5862500
C	1.5004300	-2.1122200	2.3532800
C	1.5017200	-2.0378300	3.7384000
C	-0.2819500	1.5339200	-5.2430700
C	-0.5756400	0.1900800	-3.2012600
C	-1.5359200	3.0753200	-7.2440800
C	-1.6713900	1.7148600	-5.2972800
C	-1.9922800	0.3406400	-3.3208500
C	-2.5307700	1.1118500	-4.3266900
H	0.1929700	0.0688300	7.5416600
H	0.1937500	1.1112400	6.1020000
H	0.4028000	1.9301400	-5.9978200
H	0.6549200	-2.8831200	6.4490500
H	1.3275400	-1.7322500	7.6545500
H	1.3746300	-2.1017500	-0.3404800
H	1.7221100	-0.3190700	-3.6878600
H	1.9999500	-2.9610700	1.8643800
H	2.0027900	-2.8344200	4.2965600
H	2.3497200	-2.3061300	6.3180400
H	-0.0781400	0.7202000	-0.4113700
H	-0.3201000	0.8480200	4.0856800
H	-0.3293600	0.7071000	1.6743300
H	-0.8032300	3.7752500	-6.8039500
H	-1.0110400	2.3267800	-7.8647200
H	-1.0648500	-0.1555500	6.2770000
H	-2.2571500	3.6302500	-7.8613400
H	-2.6287300	-0.1135200	-2.5525300
H	-3.6094200	1.2761300	-4.4262700
N	0.9073100	-0.8526400	5.8116600
O	0.3483100	-1.5790300	-2.9973400
O	1.5803000	0.4949400	-4.2438100
O	-2.3089000	2.4412100	-6.2284400
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4_ADC2_SVP			
C	0.2970087	-1.3868763	-0.4284999
C	0.5466185	-2.4868873	-1.1929599
C	0.6857647	2.5645654	3.0849629
C	0.9479204	0.2114477	1.4370852
C	1.1203279	-0.9768295	0.6498437
C	1.6471104	4.0548364	4.7550165
C	1.7076274	1.6091446	3.3135480
C	1.8304453	0.4764826	2.5125130
C	-0.0643107	1.1745194	1.2069967
C	-0.1955423	2.3100013	2.0043920
C	-0.2859283	4.7766991	3.4145616
C	-0.3140633	-2.8682389	-2.3675678
C	-0.7001801	-1.9578660	-3.3093124
C	-0.7108512	-4.2494280	-2.5160238
C	-1.5639315	-4.6007255	-3.5809837
C	-1.6010741	-2.3201599	-4.3883974
C	-2.0112144	-3.6353047	-4.5124343
C	-2.0665001	-1.2370732	-5.3181090
H	0.0870657	5.2176588	2.4643064

H	1.3016187	-4.2111685	-1.1424184
H	1.3647022	4.9407448	5.3468866
H	1.8728784	3.2448958	5.4690164
H	1.9703068	-1.6341220	0.8916925
H	2.4309757	1.7460654	4.1228923
H	2.5756050	4.2891749	4.1899729
H	2.6433923	-0.2329857	2.7216482
H	-0.3154491	5.5696382	4.1798476
H	-0.3637814	-0.9148121	-3.2316902
H	-0.5861611	-0.7926097	-0.7031978
H	-0.7688815	1.0468387	0.3754721
H	-0.9991946	3.0123636	1.7627271
H	-1.2017966	-0.7364633	-5.7920213
H	-1.3244177	4.4403256	3.2550136
H	-1.8655719	-5.6517371	-3.6575178
H	-2.6281296	-0.4666803	-4.7573152
H	-2.6861555	-3.9316360	-5.3253880
H	-2.7198762	-1.6389896	-6.1101596
N	0.5401790	3.6890302	3.8960415
O	1.6322904	-3.2851693	-0.9998220
O	-0.2287964	-5.1586597	-1.7205881

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4_ADC2_SVP Negative Dihedral Angle

C	0.0804166	1.3365189	1.0484544
C	0.4442863	-3.1798426	-3.7491325
C	0.4946732	-1.1749521	-0.6707080
C	0.6985648	-2.3218434	-1.3800359
C	0.8431095	2.7031231	2.9394687
C	1.1113503	0.3856325	1.2414139
C	1.2991433	-0.7821869	0.4273235
C	1.7787610	4.1473124	4.6658389
C	1.8830513	1.7599894	3.1310627
C	2.0054701	0.6423212	2.3096551
C	-0.0495316	2.4576156	1.8662224
C	-0.1833699	-2.7345290	-2.5257708
C	-0.1902855	4.8712753	3.3601223
C	-0.3689791	-3.4874309	-4.8583533
C	-1.5456815	-2.7370390	-2.4355051
C	-1.7780885	-3.4152014	-4.7753722
C	-2.3766067	-3.0476472	-3.5836549
C	-3.8658790	-2.9428581	-3.4360986
H	0.1223064	5.3440527	2.4039672
H	0.1397963	-3.7925930	-5.7805250
H	1.4836973	5.0187328	5.2714470
H	1.9922405	3.3205455	5.3651028
H	2.0469416	-3.5051246	-1.9471258
H	2.1413054	-1.4452571	0.6758892
H	2.6190218	1.8938376	3.9284830
H	2.7182581	4.3963213	4.1266231
H	2.8274790	-0.0632018	2.4919450
H	-0.2069864	5.6467304	4.1421862
H	-0.3607176	-0.5569244	-0.9741153
H	-0.6426562	1.2070298	0.2335321
H	-0.8651901	3.1535151	1.6513109
H	-1.2249456	4.5055949	3.2411193
H	-2.0313868	-2.4490293	-1.4929401
H	-2.3915359	-3.6494955	-5.6541832
H	-4.1562205	-1.9079876	-3.1790597

SUPPORTING INFORMATION

H -4.2161917 -3.5984607 -2.6185471
H -4.3802047 -3.2311141 -4.3667241
N 0.6904373 3.8020838 3.7772641
O 1.6821597 -3.2121796 -1.0712615
O 1.7319876 -3.3573341 -3.7993385

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4_ADC2_SVP_E

C 0.6794449 1.4005554 0.7169797
C 0.9687437 -1.0902862 0.7439312
C 1.1153865 2.6730204 1.0829326
C 1.3827663 0.2271419 1.0932210
C 2.0980106 5.2836760 1.6131581
C 2.2841964 2.8677352 1.8574791
C 2.5598536 0.4319741 1.8626468
C 2.9985290 1.6997284 2.2295095
C 4.0361565 4.2935771 2.7709798
C -0.1174997 -1.3918947 -0.1794735
C -0.6473334 -2.5757559 -0.4010262
C -1.5184480 -4.0701665 -2.2057734
C -1.7453551 -3.0842467 -1.2154932
C -2.5871926 -4.4665627 -3.0273455
C -3.0391857 -2.5350277 -1.0606198
C -3.8452064 -3.8867197 -2.8761064
C -4.0947179 -2.9003919 -1.8959131
C -5.4522561 -2.2574108 -1.7719430
H 0.2870328 -4.4369195 -1.6812839
H 0.5195104 3.5288461 0.7533515
H 1.0061244 5.3004940 1.7687709
H 1.5072491 -1.9430283 1.1898302
H 2.2914216 5.3161799 0.5192782
H 2.5032311 6.2025679 2.0648899
H 3.1495451 -0.4420797 2.1721065
H 3.9222990 1.7742281 2.8105365
H 4.1873461 5.3433178 3.0680286
H 4.1895983 3.6764008 3.6723343
H 4.8187496 4.0231720 2.0296288
H -0.2495084 1.3252293 0.1381495
H -0.5736063 -0.5822146 -0.7623553
H -2.3965062 -5.2262374 -3.7938531
H -3.1864526 -1.7852316 -0.2735994
H -4.6625004 -4.2082434 -3.5350111
H -5.4848298 -1.5765248 -0.9045323
H -5.6925761 -1.6681122 -2.6754249
H -6.2453589 -3.0150200 -1.6422721
N 2.6916825 4.1361222 2.2621560
O -0.1161323 -3.8508610 0.2541766
O -0.3075209 -4.6272709 -2.4373292

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4_ADC2_TZVP

C 0.3100283 -1.3612714 -0.4392247
C 0.5378962 -2.4652568 -1.1836548
C 0.6786647 2.5512085 3.0784844
C 0.9456380 0.2211964 1.4258023
C 1.1222257 -0.9623722 0.6496461
C 1.6415960 4.0316181 4.7403678
C 1.7019190 1.6076645 3.2960903
C 1.8244273 0.4825259 2.4976817
C -0.0621063 1.1792291 1.1993031

SUPPORTING INFORMATION

C	-0.1888165	2.3081368	1.9957330
C	-0.2836472	4.7538162	3.4080475
C	-0.3236999	-2.8514227	-2.3526123
C	-0.7024416	-4.2287833	-2.5191505
C	-0.7230135	-1.9494720	-3.2811023
C	-1.5417312	-4.5864588	-3.5840899
C	-1.6052743	-2.3209318	-4.3670381
C	-2.0044166	-3.6266621	-4.5031283
C	-2.0613570	-1.2458817	-5.2996580
H	0.1100850	5.1761338	2.4721117
H	1.2580666	-4.1919466	-1.1190017
H	1.3678828	4.9088121	5.3250789
H	1.8839423	3.2331122	5.4427322
H	1.9526401	-1.6161834	0.9112040
H	2.4143218	1.7456525	4.0996610
H	2.5438288	4.2645987	4.1565353
H	2.6247375	-0.2240596	2.7002737
H	-0.3103146	5.5402415	4.1611131
H	-0.4060697	-0.9129877	-3.2015734
H	-0.5435958	-0.7528135	-0.7261630
H	-0.7631506	1.0496573	0.3809463
H	-0.9831175	3.0067754	1.7640996
H	-1.1991100	-0.7570459	-5.7608349
H	-1.3117743	4.4331356	3.2345067
H	-1.8240557	-5.6313942	-3.6648639
H	-2.6121577	-0.4791209	-4.7489600
H	-2.6681829	-3.9143126	-5.3113599
H	-2.7035918	-1.6450729	-6.0828277
N	0.5175990	3.6565052	3.9080553
O	1.6134865	-3.2829227	-0.9783003
O	-0.2273510	-5.1436771	-1.7239203

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4_ADC2_TZVP Negative Dihedral Angle

C	0.0812823	1.3379970	1.0443681
C	0.4367556	-3.1660051	-3.7372538
C	0.4889456	-1.1711686	-0.6598637
C	0.6846047	-2.3066942	-1.3681149
C	0.8408838	2.6905517	2.9299454
C	1.1076821	0.3911849	1.2377571
C	1.2945810	-0.7753856	0.4342256
C	1.7739020	4.1332338	4.6535083
C	1.8796932	1.7580406	3.1178487
C	2.0007617	0.6453873	2.3013680
C	-0.0440359	2.4541899	1.8594235
C	-0.1858959	4.8544447	3.3547525
C	-0.1872739	-2.7153740	-2.5181413
C	-0.3724437	-3.4844059	-4.8412623
C	-1.5413547	-2.7176791	-2.4352096
C	-1.7716594	-3.4116011	-4.7626730
C	-2.3631156	-3.0437730	-3.5770187
C	-3.8467633	-2.9451722	-3.4338399
H	0.1244736	-3.7892867	-5.7561995
H	0.1372233	5.3175442	2.4120834
H	1.4776470	4.9966559	5.2475795
H	1.9961123	3.3197462	5.3455461
H	2.0034599	-3.4969936	-1.9488078
H	2.1308070	-1.4246768	0.6858069
H	2.6036408	1.8925899	3.9118588

SUPPORTING INFORMATION

H	2.6948458	4.3835717	4.1087079
H	2.8124210	-0.0553863	2.4813252
H	-0.1961104	5.6186631	4.1304470
H	-0.3521744	-0.5555684	-0.9673707
H	-0.6351228	1.2096983	0.2382397
H	-0.8514589	3.1467949	1.6562509
H	-1.2103003	4.5010322	3.2291163
H	-2.0295256	-2.4415660	-1.5047158
H	-2.3810514	-3.6474906	-5.6286099
H	-4.1314553	-1.9220231	-3.1776768
H	-4.1924471	-3.5921346	-2.6243019
H	-4.3520921	-3.2309880	-4.3545074
N	0.6788384	3.7763253	3.7788689
O	1.6730427	-3.2023974	-1.0695733
O	1.7226668	-3.3318712	-3.7939376

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4_ADC2_TZVP_E

C	0.6880160	1.4011923	0.6932306
C	0.9730983	-1.0788456	0.7433276
C	1.1172751	2.6658081	1.0731217
C	1.3831741	0.2329616	1.0779438
C	2.0947305	5.2584697	1.6139447
C	2.2645823	2.8518944	1.8663055
C	2.5508487	0.4319477	1.8526656
C	2.9823854	1.6916797	2.2266633
C	4.0189653	4.2680173	2.7643871
C	-0.1226801	-1.3748864	-0.1631160
C	-0.6558001	-2.5441437	-0.3944066
C	-1.5104244	-4.0405058	-2.1950253
C	-1.7388746	-3.0535405	-1.2166079
C	-2.5705887	-4.4476908	-3.0074873
C	-3.0317958	-2.5141517	-1.0612671
C	-3.8234033	-3.8729219	-2.8599274
C	-4.0779016	-2.8889801	-1.8890153
C	-5.4414178	-2.2710078	-1.7626286
H	0.3001875	-4.3727503	-1.6978544
H	0.5327321	3.5181647	0.7478888
H	1.0111678	5.2890794	1.7389915
H	1.5109834	-1.9187153	1.1829540
H	2.3176317	5.2581784	0.5369329
H	2.5013232	6.1685449	2.0542269
H	3.1315737	-0.4367341	2.1533908
H	3.8917483	1.7672643	2.8102754
H	4.1776527	5.3061194	3.0549677
H	4.1992293	3.6503087	3.6453703
H	4.7603967	4.0001559	1.9977226
H	-0.2202609	1.3285363	0.1023947
H	-0.5725114	-0.5743955	-0.7445175
H	-2.3850942	-5.2084396	-3.7566391
H	-3.1773699	-1.7750180	-0.2797479
H	-4.6287876	-4.1947765	-3.5135157
H	-5.4877648	-1.6026567	-0.9020245
H	-5.6905285	-1.6923616	-2.6553802
H	-6.2102575	-3.0372814	-1.6430448
N	2.6549616	4.1159270	2.3036324
O	-0.1856847	-3.8243694	0.2685564
O	-0.2968482	-4.5962971	-2.4319387

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4_CC2_SVP

C	0.1736732	-1.4002056	-0.3095401
C	0.4999323	-2.3244535	-1.2966022
C	0.7178979	2.5663470	3.1270936
C	0.9180187	0.1948570	1.5028539
C	1.0761411	-0.9687857	0.6723978
C	1.6994392	4.0203568	4.8245161
C	1.7629019	1.6211216	3.3213227
C	1.8545042	0.4791804	2.5310142
C	-0.1127384	1.1524977	1.3055988
C	-0.2158226	2.2989135	2.0868699
C	-0.2962468	4.7601368	3.5361925
C	-0.3971175	-2.7268114	-2.3860083
C	-0.5930792	-1.9861640	-3.5465169
C	-0.8564208	-4.1135941	-2.3208605
C	-1.5247612	-2.4230577	-4.5333496
C	-1.8337954	-4.5100258	-3.2846743
C	-1.9204802	-1.4825376	-5.6427951
C	-2.1344352	-3.6848622	-4.3763431
H	1.4249419	4.9185598	5.4040270
H	1.5764428	-3.8069019	-1.6209587
H	1.8682717	3.1948217	5.5398495
H	2.0131245	-1.5425916	0.7740020
H	2.5332240	1.7873988	4.0788890
H	2.6536490	4.2175446	4.2886389
H	2.6801654	-0.2241597	2.7100779
H	-0.0415268	5.2052462	2.5500236
H	-0.1354089	-0.9873827	-3.6405107
H	-0.2515124	5.5544614	4.3010948
H	-0.8175353	-0.9332879	-0.3984765
H	-0.8354358	1.0107886	0.4919024
H	-1.0177422	3.0069751	1.8578046
H	-1.0340289	-0.9771158	-6.0714343
H	-1.3392920	4.3959157	3.4924447
H	-2.2901347	-5.5010429	-3.1724843
H	-2.4456541	-2.0185037	-6.4537265
H	-2.6034832	-0.6929200	-5.2677483
H	-2.8678007	-4.0184476	-5.1250074
N	0.6150603	3.6960255	3.9164313
O	1.7455560	-2.8617388	-1.3604792
O	-0.2484920	-4.8965484	-1.5055092

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4_CC2_SVP_E

C	0.1089700	-1.3338710	-0.4675810
C	0.7846120	1.4161960	0.6119900
C	1.1805620	2.6915230	1.0042100
C	1.2276010	-1.0360780	0.4845260
C	1.5296560	0.2412050	0.9664000
C	2.1604650	5.3305130	1.5036450
C	2.3572030	2.9057180	1.7780220
C	2.6771080	0.4712940	1.8009250
C	3.0757770	1.7412860	2.1874740
C	4.1105490	4.3604970	2.6731080
C	-0.6266330	-2.4185150	-0.4669290
C	-1.4497730	-3.9305570	-2.2545100
C	-1.7323300	-2.9239090	-1.2882270
C	-2.4731710	-4.3336240	-3.1397700
C	-3.0675300	-2.4584210	-1.1285670

SUPPORTING INFORMATION

C -3.7597270 -3.8223090 -2.9894280
 C -4.0847950 -2.8765480 -1.9765730
 C -5.4812880 -2.3200290 -1.8818010
 H 0.2818200 -4.3023720 -1.5851230
 H 0.5701720 3.5379000 0.6773440
 H 1.0697690 5.3416020 1.6734690
 H 1.8564480 -1.8925860 0.7911290
 H 2.3431190 5.3639370 0.4069930
 H 2.5722840 6.2493910 1.9530300
 H 3.2691890 -0.3925860 2.1328840
 H 3.9721100 1.8350720 2.8068000
 H 4.2468410 5.4199710 2.9454450
 H 4.2551740 3.7649270 3.5907830
 H 4.9035940 4.0798970 1.9459760
 H -0.1297500 -0.6011840 -1.2541080
 H -0.1315540 1.3104480 0.0178340
 H -2.2357550 -5.0703110 -3.9138130
 H -3.2516460 -1.7070070 -0.3500070
 H -4.5447230 -4.1484680 -3.6834440
 H -5.5806410 -1.6475630 -1.0130390
 H -5.7287170 -1.7402050 -2.7888930
 H -6.2338980 -3.1221860 -1.7822610
 N 2.7703460 4.1798340 2.1446500
 O -0.2268390 -4.4671220 -2.4152660
 O -0.5845590 -3.6957410 0.2827300

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4_CC2_TZVP

C 0.4795093 -1.1665455 -0.4636959
 C 1.8037907 -0.6802229 -0.2392541
 C 2.0944632 0.5364522 0.4152123
 C 2.9092243 -1.4394512 -0.6799816
 C 3.3962287 0.9606427 0.6190535
 C 4.2156315 -1.0241991 -0.4844429
 C 4.4994110 0.1902479 0.1803830
 C 6.0370304 1.9592280 0.8549549
 C 6.8721153 -0.0626021 -0.3098560
 C -0.7031346 -0.5235605 -0.0972785
 C -1.9668544 -1.0077523 -0.3569156
 C -3.1922940 -0.2959333 0.0023307
 C -3.7536467 0.6401524 -0.8553308
 C -3.8336277 -0.6227371 1.2711728
 C -4.9100655 1.3627374 -0.5075823
 C -5.0106539 0.1385941 1.5925030
 C -5.4652041 2.4272619 -1.4070029
 C -5.5226976 1.0865784 0.7299630
 H 0.3867079 -2.1260477 -0.9695869
 H 1.2872891 1.1671152 0.7745337
 H 2.7270195 -2.3807963 -1.1923216
 H 3.5551861 1.9051876 1.1235468
 H 5.0188214 -1.6504149 -0.8512230
 H 5.5482932 2.1375911 1.8148078
 H 5.6805695 2.7110590 0.1380699
 H 6.7604442 0.0124854 -1.3997059
 H 6.9200312 -1.1196019 -0.0398489
 H 7.1081115 2.0952343 0.9984671
 H 7.8175254 0.3964624 -0.0242932
 H -0.6785866 0.4395360 0.4053556
 H -3.0139764 -2.5017779 -0.8758417

SUPPORTING INFORMATION

H -3.2547405 0.8583863 -1.7984725
H -4.9519256 2.4463571 -2.3683826
H -5.3670499 3.4200781 -0.9557488
H -5.4854977 -0.0692274 2.5474377
H -6.4151366 1.6407128 1.0058699
H -6.5292781 2.2661650 -1.5917632
N 5.7976295 0.6025974 0.4020742
O -2.0968822 -2.2068937 -1.0105039
O -3.3984108 -1.5580691 2.0133569
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4_CC2_TZVP_E

C 0.0410900 -1.3888300 -0.3616000
C 0.7157700 1.3636300 0.7281300
C 1.1132800 2.6389600 1.1117300
C 1.1594000 -1.0932900 0.5886900
C 1.4600500 0.1860100 1.0771200
C 2.0921100 5.2797500 1.6117200
C 2.2894100 2.8576000 1.8838500
C 2.6046700 0.4208000 1.9140300
C 3.0040000 1.6914400 2.2962700
C 4.0424700 4.3090400 2.7813500
C -0.7011100 -2.4715000 -0.3537100
C -1.5197800 -3.9884800 -2.1477400
C -1.8043100 -2.9886400 -1.1737500
C -2.5459900 -4.3889600 -3.0289600
C -3.1330300 -2.5194900 -1.0135300
C -3.8272500 -3.8782300 -2.8770700
C -4.1562900 -2.9363900 -1.8618200
C -5.5511500 -2.3722100 -1.7723200
H 0.2061200 -4.3641900 -1.4802100
H 0.5011500 3.4879200 0.7871400
H 1.0022400 5.2917400 1.7818300
H 1.7841800 -1.9495000 0.8994200
H 2.2751800 5.3134600 0.5163000
H 2.5037500 6.1973100 2.0619300
H 3.1991400 -0.4443700 2.2427500
H 3.9015600 1.7850800 2.9157600
H 4.1783600 5.3678300 3.0543800
H 4.1885200 3.7139800 3.6987700
H 4.8354500 4.0293500 2.0549500
H -0.1932000 -0.6509200 -1.1463200
H -0.1978800 1.2579700 0.1291100
H -2.3050900 -5.1220500 -3.8100600
H -3.3148900 -1.7570900 -0.2457100
H -4.6104800 -4.1969100 -3.5811000
H -5.6514100 -1.6989600 -0.9030900
H -5.7932800 -1.7945800 -2.6846100
H -6.3084000 -3.1725700 -1.6743500
N 2.7044300 4.1308400 2.2501400
O -0.2924200 -4.5101600 -2.3196100
O -0.6617200 -3.7516000 0.3849800
41

5_ADC2_SVP

C 0.0216923 -0.6880721 -1.5878534
C 0.2640155 0.1046015 6.0989232
C 0.4000979 -1.2082473 -2.8220149
C 0.5970852 0.7616151 3.7532359
C 1.1291926 0.3844405 5.0403887

C 1.3910349 -2.0542573 -5.3468404
 C 3.3722455 0.5807422 4.2489192
 C -0.2300801 -0.8012699 -4.0257223
 C -0.3161135 -0.6645224 -6.4561670
 C -0.7574214 0.7890543 3.5608968
 C -0.9257628 0.5090640 1.0618478
 C -1.0161408 0.2682914 -1.4639716
 C -1.1191833 0.1944357 5.9065003
 C -1.2671556 0.1588073 -3.9085734
 C -1.3458589 1.1148907 2.2107001
 C -1.4443961 0.8279888 -0.2171354
 C -1.6403377 0.6728008 -2.6706242
 C -1.6714193 0.5709181 4.6571552
 H 0.0290189 -1.2318632 -7.3347044
 H 0.0617726 0.3773781 -6.5388012
 H 0.5569666 -1.0361219 -0.6963604
 H 0.6935100 -0.1788996 7.0655050
 H 1.2123685 -1.9395760 -2.8387321
 H 1.2619538 0.9793444 2.9121518
 H 1.3936187 -2.9281296 -4.6741474
 H 1.5104727 -2.4347067 -6.3735963
 H 2.2720311 -1.4224125 -5.1011037
 H 3.2569282 1.6233136 3.9045090
 H 3.2614875 -0.1094091 3.3939778
 H 4.3658700 0.4504603 4.6983699
 H -0.1360539 -0.2462989 1.1668885
 H -1.4175202 -0.6373372 -6.4981474
 H -1.7915658 0.5243999 -4.7951896
 H -1.8171630 -0.0087235 6.7268945
 H -2.2484381 1.5780945 -0.2405552
 H -2.4441760 1.4196627 -2.6282871
 H -2.8189391 1.8935358 3.0600046
 N 0.1367408 -1.3352396 -5.2548261
 O 2.4433834 0.2739542 5.2833963
 O -2.2869010 2.0842820 2.2320383
 O -2.9368802 0.7830311 4.4910607
 41
 5_ADC2_SVP_E
 C 0.2751658 -0.0668749 -1.6861476
 C 0.4387992 0.8522948 6.0880354
 C 0.6267542 -0.2448552 5.2161999
 C 0.7723877 -0.4644700 -2.9254854
 C 1.6919474 -2.3185425 4.8080844
 C 1.8443302 -1.0100329 -5.4948414
 C -0.0152726 -0.2452804 3.9788539
 C -0.0772194 -0.6709415 -4.0377059
 C -0.3339001 1.9419828 5.7079416
 C -0.4374003 -0.9817279 -6.4259194
 C -0.7810438 0.8764160 3.5745720
 C -0.8813134 0.6541039 1.0246963
 C -0.9534470 1.9778755 4.4439717
 C -1.1088116 0.1484302 -1.4620233
 C -1.3501003 0.8760296 2.2340845
 C -1.4618023 -0.4457240 -3.8270021
 C -1.6564640 0.5312888 -0.2026695
 C -1.9534276 -0.0488804 -2.5879300
 H 0.0629056 -1.0791278 3.2781038
 H 0.0947731 -1.3727771 -7.3082123

SUPPORTING INFORMATION

H	0.2068891	0.5165150	0.9990014
H	0.7768829	-2.9001520	4.5872245
H	0.9259909	0.8200804	7.0686181
H	0.9941450	0.0804058	-0.8718502
H	1.8526347	-0.6046488	-3.0161573
H	2.0740396	-1.4051126	-6.4977677
H	2.1354618	-1.9668746	3.8576445
H	2.2327365	0.0301087	-5.4291456
H	2.3984696	-1.6281490	-4.7678079
H	2.4157227	-2.9612195	5.3313290
H	-0.4757206	2.7977082	6.3770037
H	-0.7439645	0.0662976	-6.6360329
H	-1.3511133	-1.5877680	-6.3022355
H	-2.1783682	-0.5757120	-4.6429796
H	-2.2041319	2.9114813	3.3330940
H	-2.7466669	0.6735080	-0.1248281
H	-3.0347662	0.1096456	-2.4741588
N	0.4187326	-1.1008258	-5.2661255
O	1.4243606	-1.2388224	5.6796103
O	-1.6405372	3.0970277	4.1136856
O	-2.8304474	1.1453199	2.5195922

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5_ADC2_TZVP

C	0.0258848	-0.6856335	-1.5837121
C	0.2579588	0.1064323	6.0856404
C	0.4005956	-1.2008381	-2.8140465
C	0.6026949	0.7341710	3.7397417
C	1.1193417	0.3806988	5.0320371
C	1.3778365	-2.0466689	-5.3270755
C	3.3512020	0.5865933	4.2330490
C	-0.2385153	-0.8063691	-4.0073045
C	-0.3221084	-0.6624553	-6.4283334
C	-0.7432559	0.7725585	3.5392839
C	-0.9102661	0.5119661	1.0475050
C	-1.0073455	0.2660569	-1.4620299
C	-1.1144204	0.2055378	5.8847180
C	-1.2591341	0.1594700	-3.8935294
C	-1.3197264	1.1072467	2.1944517
C	-1.4379269	0.8257175	-0.2252355
C	-1.6300848	0.6708876	-2.6621464
C	-1.6553534	0.5639191	4.6319460
H	0.0195295	-1.2196055	-7.2994435
H	0.0738905	0.3612514	-6.4874875
H	0.5552328	-1.0304110	-0.7013227
H	0.6766836	-0.1648163	7.0480180
H	1.2045709	-1.9252848	-2.8390327
H	1.2689592	0.9501155	2.9137820
H	1.4024905	-2.9064757	-4.6566981
H	1.4987880	-2.4207647	-6.3426415
H	2.2308958	-1.3957348	-5.0881636
H	3.2209247	1.6161563	3.8951820
H	3.2251448	-0.1019087	3.3956624
H	4.3380997	0.4618964	4.6681972
H	-0.1255863	-0.2327778	1.1451807
H	-1.4103807	-0.6137535	-6.4767302
H	-1.7753509	0.5189779	-4.7742274
H	-1.8107007	0.0147764	6.6947057
H	-2.2393397	1.5622339	-0.2563544

SUPPORTING INFORMATION

H -2.4233117 1.4118921 -2.6142720
H -2.7816755 1.8657421 3.0503465
N 0.1067869 -1.3587493 -5.2326421
O 2.4330053 0.2779407 5.2866111
O -2.2654198 2.0770284 2.2269999
O -2.9206141 0.7629801 4.4593706

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5_ADC2_TZVP Negative Dihedral Angle

C 0.3081060 -0.0876322 -1.6811898
C 0.3573772 0.0570695 3.8646581
C 0.7561954 1.4097582 5.8714761
C 0.7996574 -0.3337305 -2.9529544
C 1.1093922 0.3450725 5.0536151
C 1.8096795 -0.5365599 -5.5843712
C 2.5564167 -1.4944182 4.6239595
C -0.0575474 -0.6181609 -4.0356244
C -0.3539801 2.1799751 5.5427780
C -0.4787425 -0.8305516 -6.4157990
C -0.6928051 0.8526016 3.5221059
C -0.9051925 0.4097462 1.0597273
C -1.0748151 -0.0962415 -1.4064341
C -1.1230648 1.9161886 4.3898399
C -1.4420061 -0.6113989 -3.7700210
C -1.4829777 0.6009232 2.2710254
C -1.6366881 0.1548093 -0.1219639
C -1.9283354 -0.3637786 -2.4981117
H 0.0566964 -1.0899576 -7.3279443
H 0.1801649 0.4448143 1.0335391
H 0.6268585 -0.7724322 3.2227194
H 1.0189373 0.1307868 -0.8908023
H 1.3467070 1.6076068 6.7587356
H 1.7470909 -2.2254821 4.5833252
H 1.8718400 -0.3029036 -3.0988820
H 1.9849632 0.5435921 -5.4801715
H 2.0466534 -0.8312215 -6.6056471
H 2.4996295 -1.0626483 -4.9237437
H 2.8280536 -1.1789457 3.6150936
H 3.4200387 -1.9255528 5.1210913
H -0.6642738 3.0066390 6.1733494
H -0.9139578 0.1716530 -6.5357597
H -1.2921088 -1.5472233 -6.2982481
H -2.1539719 -0.8019203 -4.5625653
H -2.7219220 0.1399035 -0.0342156
H -2.9842130 1.2790775 3.1261202
H -3.0021634 -0.3674770 -2.3323078
N 0.4396688 -0.9102706 -5.2981357
O 2.1836882 -0.3683311 5.4249322
O -2.2162989 2.5545896 4.1297325
O -2.8227504 0.5520315 2.4670688

41

5_ADC2_TZVP_E

C 0.0002354 -0.2511647 3.9750373
C 0.2871968 -0.0557011 -1.6840083
C 0.4320526 0.8644593 6.0661232
C 0.6233735 -0.2368259 5.2118635
C 0.7742519 -0.4527083 -2.9216802
C 1.6678325 -2.3094156 4.8022267
C 1.8256915 -1.0098653 -5.4780139

SUPPORTING INFORMATION

C	-0.0790811	-0.6805365	-4.0161981
C	-0.3459118	1.9387236	5.6774531
C	-0.4460157	-0.9773868	-6.3949258
C	-0.7640688	0.8590453	3.5558872
C	-0.8728688	0.6281956	1.0134539
C	-0.9467658	1.9594477	4.4126602
C	-1.0921496	0.1520481	-1.4581493
C	-1.3272754	0.8373140	2.2193035
C	-1.4527697	-0.4325279	-3.8110601
C	-1.6485525	0.5113501	-0.2076621
C	-1.9375359	-0.0350929	-2.5784617
H	0.0696713	-1.3635689	-7.2734218
H	0.0838747	-1.0834959	3.2906385
H	0.2065647	0.5170775	0.9778920
H	0.7463098	-2.8513546	4.5734551
H	0.9116592	0.8503355	7.0386474
H	1.0049225	0.1034573	-0.8851147
H	1.8440618	-0.5878203	-3.0239209
H	2.0561844	-1.3952070	-6.4706414
H	2.1211933	-1.9524715	3.8736147
H	2.1651554	0.0340852	-5.4181084
H	2.3606685	-2.9679522	5.3186674
H	2.3984922	-1.5967193	-4.7588009
H	-0.4949821	2.7875191	6.3345735
H	-0.7085451	0.0745826	-6.5755563
H	-1.3701282	-1.5456646	-6.2831818
H	-2.1599239	2.8913496	3.2762222
H	-2.1599572	-0.5548851	-4.6220339
H	-2.7275623	0.6418776	-0.1373015
H	-3.0047219	0.1365169	-2.4596279
N	0.4048655	-1.1512957	-5.2358642
O	1.4206628	-1.2283327	5.6912896
O	-1.6275141	3.0804894	4.0678300
O	-2.7913805	1.0401482	2.5511643

41

5_CC2_SVP

C	0.0333363	-0.7131179	-1.6602927
C	0.1692829	0.1582809	6.1625324
C	0.4213954	-1.1913082	-2.9074987
C	0.6833076	0.8597491	3.8666810
C	1.1139372	0.5213549	5.1951698
C	1.3085922	-2.0917410	-5.4583056
C	3.4037408	0.7248650	4.5713694
C	-0.2282858	-0.7584074	-4.0981207
C	-0.4399942	-0.6695715	-6.5298891
C	-0.6316151	0.6386781	3.5244346
C	-1.0030005	0.2871468	1.0182873
C	-1.0186122	0.2292517	-1.5079540
C	-1.1962000	0.1044000	5.8401467
C	-1.2084972	0.9962881	2.1843718
C	-1.2637572	0.2080487	-3.9577842
C	-1.4312550	0.7491522	-0.2397104
C	-1.6364408	0.6827497	-2.7036571
C	-1.6404402	0.4192473	4.5378979
H	0.5308243	-0.0996486	7.1650393
H	0.5887494	-1.0531338	-0.7774716
H	1.2269648	-2.9907616	-4.8215352
H	1.2599910	-1.8926496	-2.9521199

SUPPORTING INFORMATION

H	1.3946973	-2.4308505	-6.5021730
H	1.4056351	1.1423815	3.0928695
H	2.2414385	-1.5550562	-5.1867173
H	3.3009115	0.0228064	3.7222013
H	3.3533017	1.7646824	4.1971807
H	4.3731237	0.5614209	5.0647534
H	-0.0808025	-1.2284430	-7.4075892
H	-0.1605812	0.3972255	-6.6541487
H	-0.3839195	-0.6175252	1.0968207
H	-1.5423450	-0.7404192	-6.5161493
H	-1.7773075	0.6074536	-4.8373676
H	-1.9426002	-0.1582962	6.6008371
H	-2.1078547	1.6185089	-0.2361178
H	-2.4380559	1.4314373	-2.6365909
H	-2.4797688	1.9723282	3.0771300
N	0.1299361	-1.2570898	-5.3340050
O	2.4166666	0.4739105	5.5613613
O	-1.8760118	2.1541995	2.2480155
O	-2.8684965	0.7224322	4.1981081
41			
5_CC2_SVP_E			
C	0.2401440	-0.0196750	-1.7022800
C	0.2504930	-0.3388800	3.9651820
C	0.4367660	0.9308420	6.0283950
C	0.7181030	-0.4913040	-2.9165370
C	0.7637440	-0.2192610	5.2557650
C	1.6807410	-2.4043610	5.2538810
C	1.7799600	-1.0550210	-5.4948860
C	-0.1380650	-0.6396440	-4.0452220
C	-0.4156900	1.9109430	5.5389960
C	-0.5093750	-0.9917300	-6.4307780
C	-0.5939680	0.6778000	3.4460490
C	-0.7704670	1.0380940	0.9195400
C	-1.0025400	1.7625380	4.2623970
C	-1.1357310	0.3441020	-1.5135500
C	-1.1727120	0.6108990	2.0987510
C	-1.5194710	-0.3266490	-3.8605490
C	-1.6042490	0.9059740	-0.3211330
C	-1.9895850	0.1618490	-2.6538850
H	0.0271460	-1.4085630	-7.2988360
H	0.2356300	1.4850590	0.8625680
H	0.5056980	-1.1757030	3.3073420
H	0.6819820	-2.8353210	5.0438020
H	0.8749970	1.0163610	7.0304930
H	0.9409570	0.0969180	-0.8652440
H	1.7864520	-0.7162640	-2.9984910
H	1.9838290	-1.4411840	-6.5061930
H	2.2022810	-0.0301970	-5.4169740
H	2.2107380	-3.0427860	5.9769630
H	2.2655210	-2.3591900	4.3136080
H	2.3107660	-1.7059580	-4.7791840
H	-0.6920600	2.7845310	6.1418250
H	-0.8017420	0.0551820	-6.6661330
H	-1.4284110	-1.5879390	-6.2904860
H	-2.2284260	-0.4356040	-4.6860930
H	-2.3162150	2.3672340	3.0374590
H	-2.6579460	1.2431690	-0.2640660
H	-3.0545790	0.4152350	-2.5567210

SUPPORTING INFORMATION

N 0.3472470 -1.0829500 -5.2634530
O 1.5646530 -1.1310110 5.8717160
O -1.8745140 2.7034260 3.8509500
O -2.4548940 0.1170700 2.5592820

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5_CC2_TZVP

C 0.2972249 0.1299276 -1.8011688
C 0.4229856 -0.0966366 4.0173987
C 0.7071587 1.5067542 5.8436228
C 0.7648864 -0.0884286 -3.0831492
C 1.0830855 0.3223701 5.2035628
C 1.7676457 -0.6026094 -5.6754190
C 2.5608228 -1.5360856 5.1043412
C -0.1258978 -0.3920801 -4.1455770
C -0.3526829 2.2678926 5.3610997
C -0.5154716 0.7473207 3.4609984
C -0.5841357 -0.8895446 -6.4937694
C -0.8474320 0.5424021 0.9606664
C -1.0448847 1.8668805 4.1964878
C -1.0823862 0.0616280 -1.4892836
C -1.3134112 0.4302675 2.2539757
C -1.5125373 -0.4257987 -3.8515750
C -1.5993830 0.2143967 -0.1721006
C -1.9639479 -0.2158879 -2.5612631
H 0.1951102 0.8303630 0.8634710
H 0.7070613 -1.0033122 3.4928813
H 1.0180702 0.3368322 -1.0175568
H 1.2626874 1.8050349 6.7264104
H 1.7541478 -2.2749546 5.0808839
H 1.8320506 -0.0336018 -3.2636394
H 1.9369362 -0.9101875 -6.7057016
H 2.1686944 0.4091753 -5.5421403
H 2.3181055 -1.2839735 -5.0192227
H 2.9022886 -1.3319318 4.0845849
H 3.3882030 -1.9124633 5.7013126
H -0.0139989 -1.1239254 -7.3905873
H -0.6766807 3.1670224 5.8781288
H -1.2019656 -0.0062623 -6.6939459
H -1.2455588 -1.7342272 -6.2777886
H -2.2325633 -0.6295270 -4.6354490
H -2.6595606 0.0097415 -0.0220751
H -2.8022107 0.7646147 3.2349313
H -3.0306999 -0.2619585 -2.3611654
N 0.3441449 -0.6614234 -5.4033281
O 2.1441990 -0.3366876 5.7528573
O -2.2107095 2.3092095 3.8215261
O -2.5593505 0.0296439 2.5667451

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5_CC2_TZVP_E

C 0.2495179 -0.3395319 3.9528821
C 0.2534725 -0.0054813 -1.7069665
C 0.4216770 0.9245748 6.0144670
C 0.7228718 -0.4717204 -2.9194320
C 0.7423684 -0.2162978 5.2410421
C 1.6742298 -2.3843824 5.2363992
C 1.7682793 -1.0611756 -5.4807418
C -0.1365341 -0.6258831 -4.0341899
C -0.4261475 1.8997707 5.5355976

C	-0.5148468	-0.9904527	-6.4122851
C	-0.5953213	0.6736163	3.4385795
C	-0.7802384	1.0146379	0.9053156
C	-0.9906406	1.7576906	4.2554813
C	-1.1128481	0.3614109	-1.5226684
C	-1.1638226	0.6056876	2.0929325
C	-1.5059571	-0.2936956	-3.8565937
C	-1.6023763	0.8756600	-0.3252057
C	-1.9699685	0.1846511	-2.6515198
H	0.0120273	-1.4071564	-7.2702220
H	0.2199893	1.4415156	0.8496655
H	0.4917046	-1.1733118	3.3035323
H	0.6888598	-2.8147834	5.0271675
H	0.8572274	0.9917009	7.0061331
H	0.9422475	0.0808203	-0.8718858
H	1.7732419	-0.7256926	-3.0027802
H	1.9702360	-1.4428339	-6.4811307
H	2.1716230	-0.0416716	-5.4006106
H	2.2139794	-3.0119764	5.9421091
H	2.2421384	-2.2994093	4.3042955
H	2.2975458	-1.6978177	-4.7699385
H	-0.6986010	2.7575191	6.1417613
H	-0.7866357	0.0509991	-6.6360459
H	-1.4328545	-1.5647590	-6.2762249
H	-2.2077313	-0.4147494	-4.6737029
H	-2.2636815	2.4054777	3.0124881
H	-2.6569245	1.1524752	-0.2592708
H	-3.0249923	0.4274674	-2.5450318
N	0.3370278	-1.1050348	-5.2436634
O	1.5400388	-1.1182756	5.8804531
O	-1.8597491	2.7064556	3.8503826
O	-2.4132228	0.0820017	2.5837055

SECTION 10: REFERENCES

- 1 X. Cheng, K. Wang, S. Huang, H. Zhang, H. Zhang and Y. Wang, *Angew. Chemie Int. Ed.*, 2015, **54**, 8369–8373.
- 2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revis. D.01, Gaussian, Inc., Wallingford CT*, 2009.