

# Chemistry–A European Journal

Supporting Information

## **Bifunctional Hydrogen Bond Donor-Catalyzed Diels–Alder Reactions: Origin of Stereoselectivity and Rate Enhancement**

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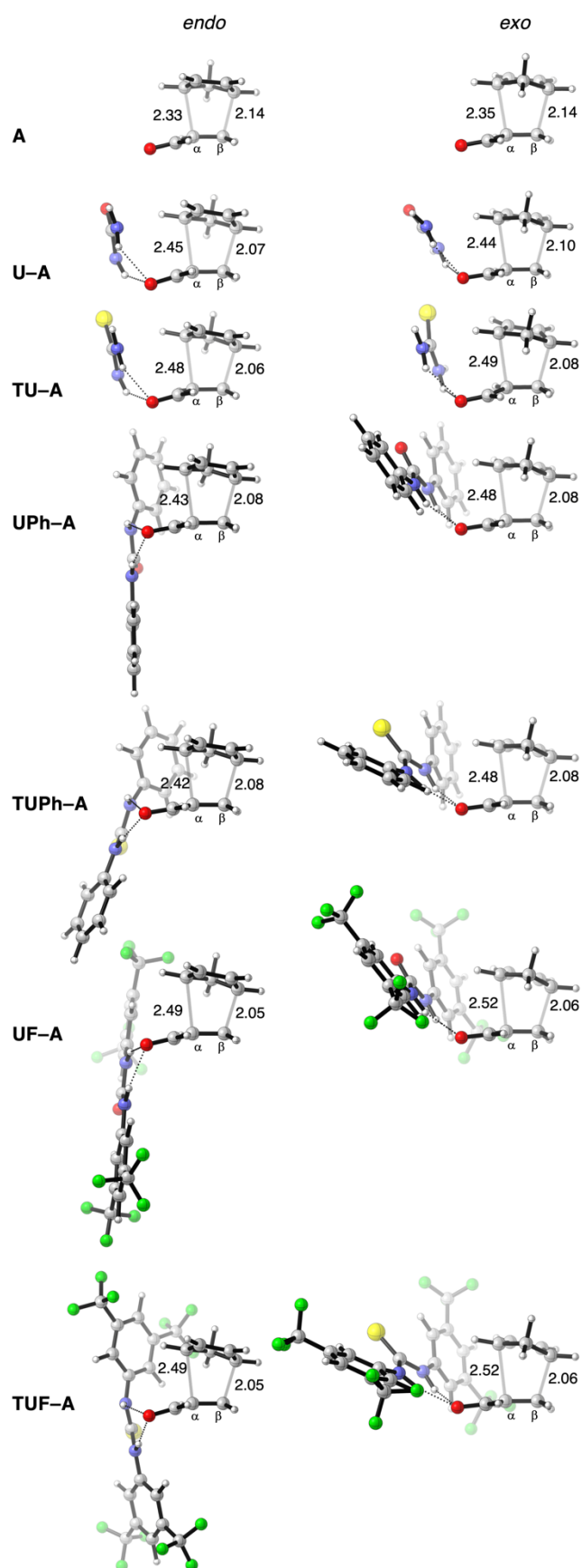
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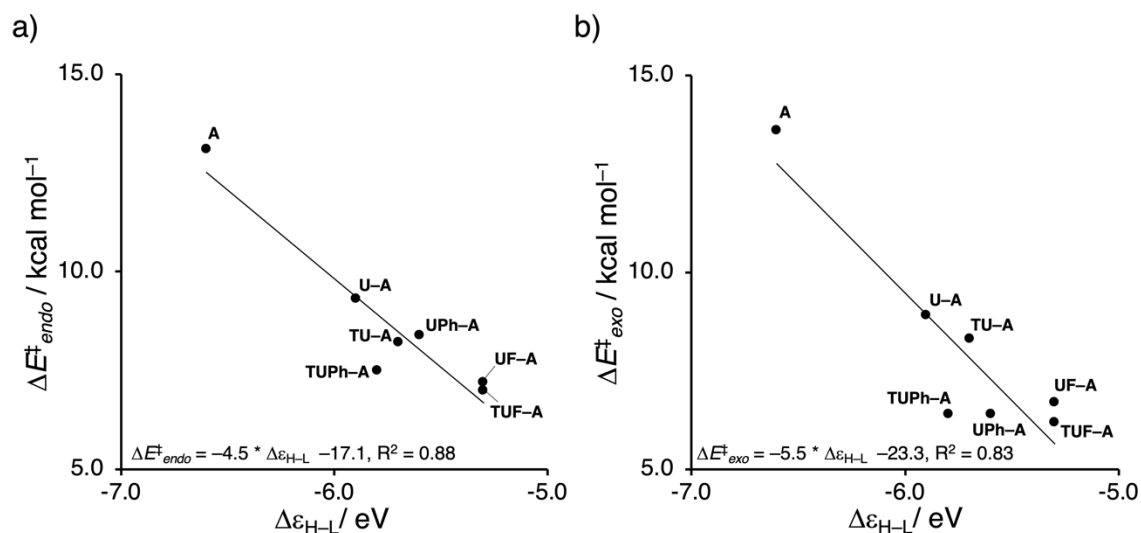
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**Figure S14.** Key occupied orbitals (isovalue = 0.03 au) computed at the equilibrium structures of **A**, **U-A**, and **UPh-A**, where the MO coefficients of the carbon  $2p_z$  atomic orbitals, contributing to the occupied orbitals, are shown. Computed at the ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP level.

**Table S2.** Cartesian coordinates (in Å), energies (in kcal mol<sup>-1</sup>), and number of imaginary frequencies of all stationary points, computed at M06-2X/def2-SVPP.



**Figure S1.** Transition state structures for the uncatalyzed and hydrogen bond donor-catalyzed Diels–Alder reaction between **CP** and **A** forming an *endo* (left) or *exo* (right) cycloadduct, computed at M06-2X/def2-def2-SVPP.

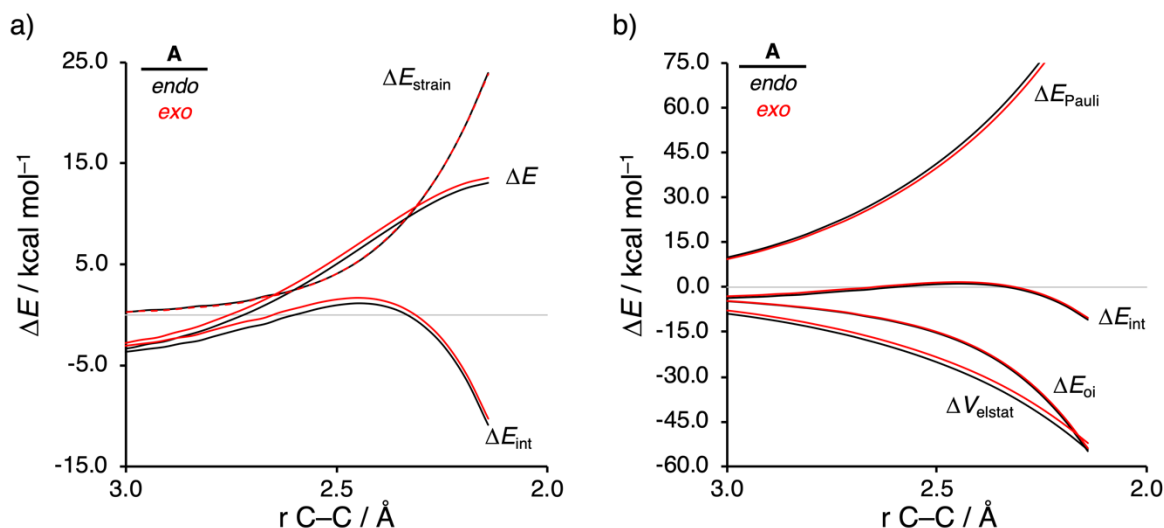


**Figure S2.** Activation barriers ( $\Delta E^{\ddagger}$ ) for the uncatalyzed and HB-catalyzed Diels-Alder reactions versus the HOMO<sub>CP</sub>-LUMO<sub>HB-A</sub> energy gap ( $\Delta \epsilon_{H-L}$ ) of the reactants for the a) *endo* and b) *exo* pathway, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.

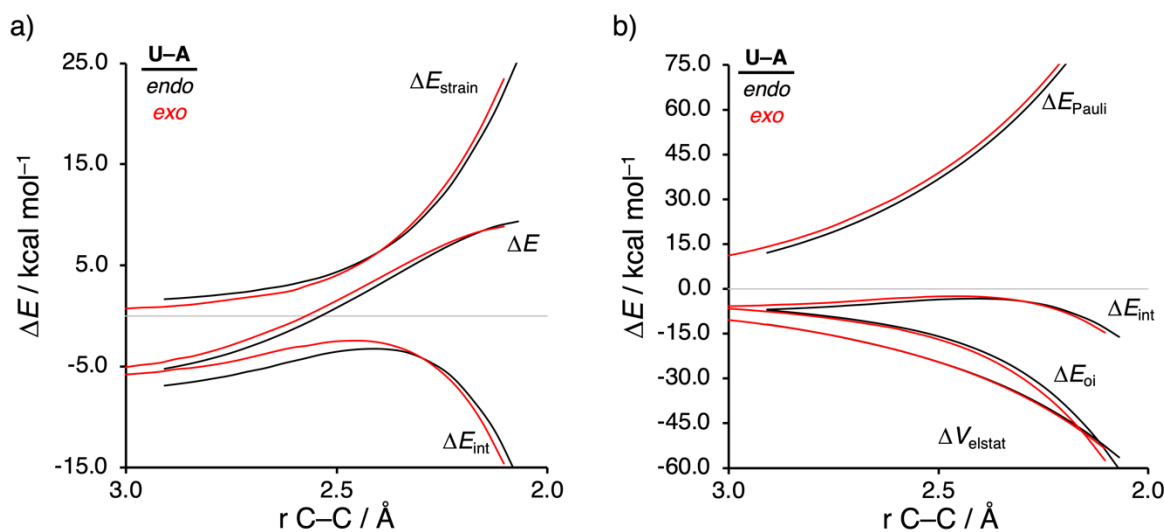
**Table S1.** Energy decomposition analyses (in kcal mol<sup>-1</sup>) of the interaction between CP and the HB at the transition states structures of the *endo* and *exo* pathway for the hydrogen bond donor-catalyzed Diels-Alder reaction.

HB	cycloadduct	$\Delta E_{int}$	$\Delta V_{elstat}$	$\Delta E_{Pauli}$	$\Delta E_{oi}$
<b>U</b>	<i>endo</i>	-1.4	-2.7	2.5	-1.2
	<i>exo</i>	-1.1	-2.9	3.0	-1.2
<b>TU</b>	<i>endo</i>	-2.2	-3.2	2.7	-1.7
	<i>exo</i>	-2.4	-3.9	3.2	-1.8
<b>UPh</b>	<i>endo</i>	-2.7	-2.7	1.3	-1.3
	<i>exo</i>	-3.3	-3.5	2.1	-1.8
<b>TUPh</b>	<i>endo</i>	-3.1	-3.0	1.6	-1.6
	<i>exo</i>	-3.5	-3.7	2.2	-1.9
<b>UF</b>	<i>endo</i>	-2.1	-2.3	1.3	-1.1
	<i>exo</i>	-3.6	-3.0	1.4	-2.0
<b>TUF</b>	<i>endo</i>	-3.7	-3.9	2.3	-2.0
	<i>exo</i>	-3.7	-3.0	1.4	-2.0

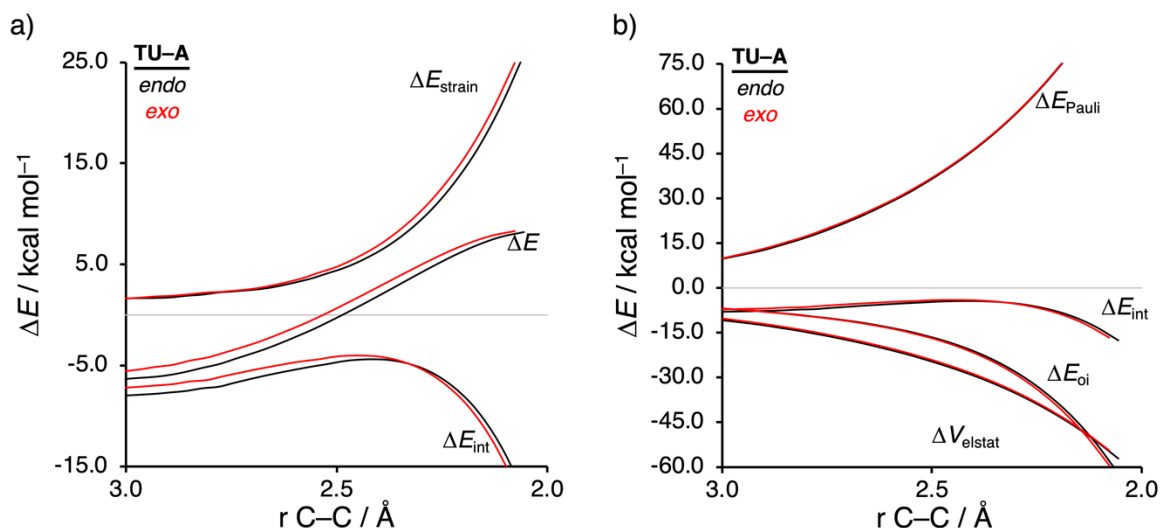
[a] Computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP



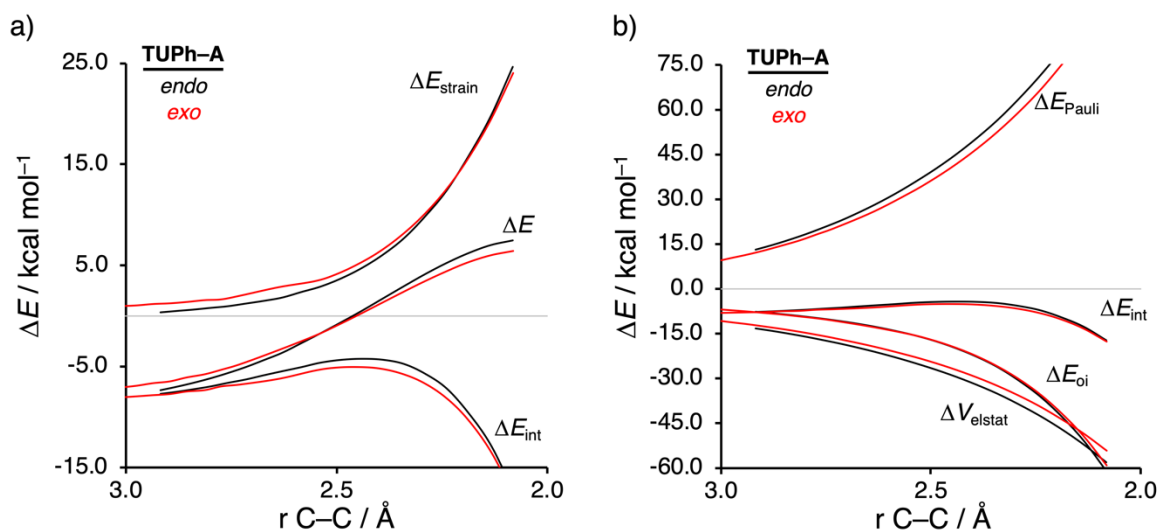
**Figure S3.** a) Activation strain analyses and b) energy decomposition analyses of the catalyzed *endo* and *exo* Diels-Alder reactions between **CP** and **A**, where the energy values are projected onto the shorter newly forming  $C_{CP}\cdots C_{\beta}$  bond between **CP** and **A**, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



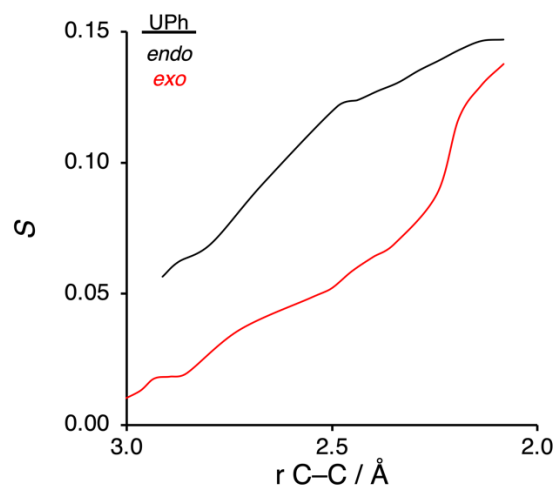
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**Figure S5.** a) Activation strain analyses and b) energy decomposition analyses of the catalyzed *endo* and *exo* Diels-Alder reactions between CP and TU-A, where the energy values are projected onto the shorter newly forming  $C_{CP}\cdots C_{\beta}$  bond between CP and TU-A, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



**Figure S6.** a) Activation strain analyses and b) energy decomposition analyses of the catalyzed *endo* and *exo* Diels-Alder reactions between CP and TUPh-A, where the energy values are projected onto the shorter newly forming  $C_{CP}\cdots C_{\beta}$  bond between CP and TUPh-A, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



**Figure S7.** Occupied-occupied orbital overlap between HOMO-6<sub>CP</sub> and HOMO-6<sub>UPh-A</sub> for the *endo* and *exo* Diels-Alder reactions between **CP** and **UPh-A** going from the reactants to the transition state, where the orbital overlap value is projected onto the shorter newly forming C<sub>CP</sub>•••C<sub>β</sub> bond between **CP** and the **UPh-A**, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



**Table S2.** Occupied-occupied orbital overlap for the *endo* Diels-Alder reactions between **CP** and **UPh-A** in the transition state.<sup>[a]</sup>

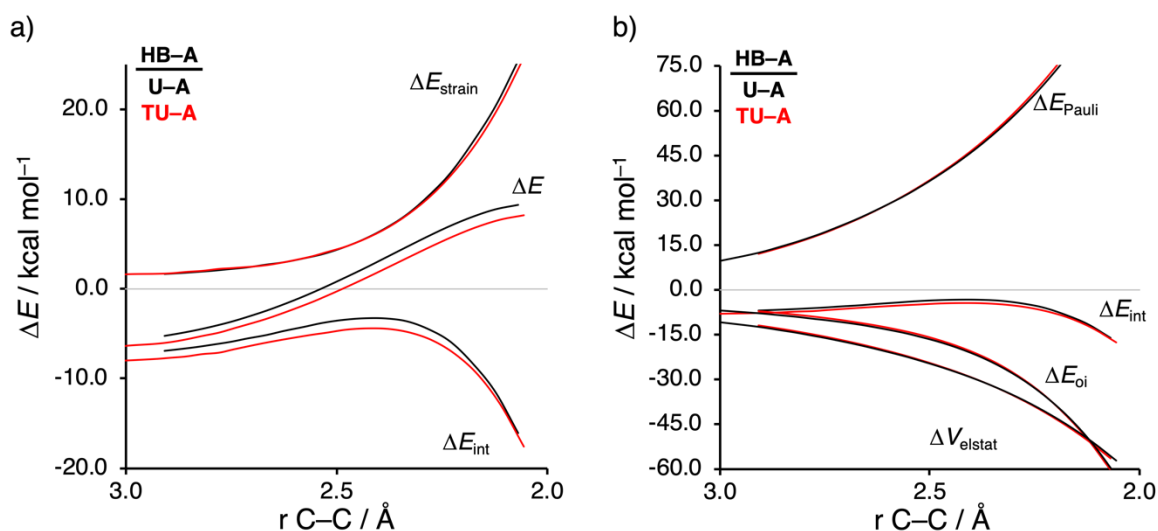
		UPh-A										
		HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4	HOMO-5	HOMO-6	HOMO-7	HOMO-8	HOMO-9	HOMO-10
<b>CP</b>	HOMO	0.01	0.01	0.00	0.00	0.01	0.00	0.05	0.01	0.00	0.00	0.00
	HOMO-1	0.01	0.01	0.00	0.01	0.01	0.03	0.10	0.03	0.01	0.01	0.00
	HOMO-2	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01
	HOMO-3	0.00	0.00	0.00	0.01	0.00	0.02	0.00	0.00	0.02	0.00	0.01
	HOMO-4	0.01	0.01	0.00	0.02	0.00	0.00	0.02	0.01	0.01	0.00	0.00
	HOMO-5	0.01	0.01	0.00	0.03	0.00	0.01	0.01	0.01	0.00	0.00	0.01
	HOMO-6	0.01	0.01	0.00	0.01	0.01	0.04	0.15	0.04	0.00	0.01	0.00
	HOMO-7	0.01	0.01	0.00	0.02	0.00	0.00	0.03	0.01	0.01	0.00	0.00
	HOMO-8	0.01	0.01	0.00	0.03	0.00	0.00	0.00	0.00	0.01	0.00	0.00
	HOMO-9	0.00	0.00	0.00	0.02	0.01	0.03	0.05	0.00	0.01	0.00	0.00
HOMO-10	0.01	0.01	0.00	0.02	0.00	0.01	0.04	0.01	0.01	0.00	0.00	

[a] Computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP

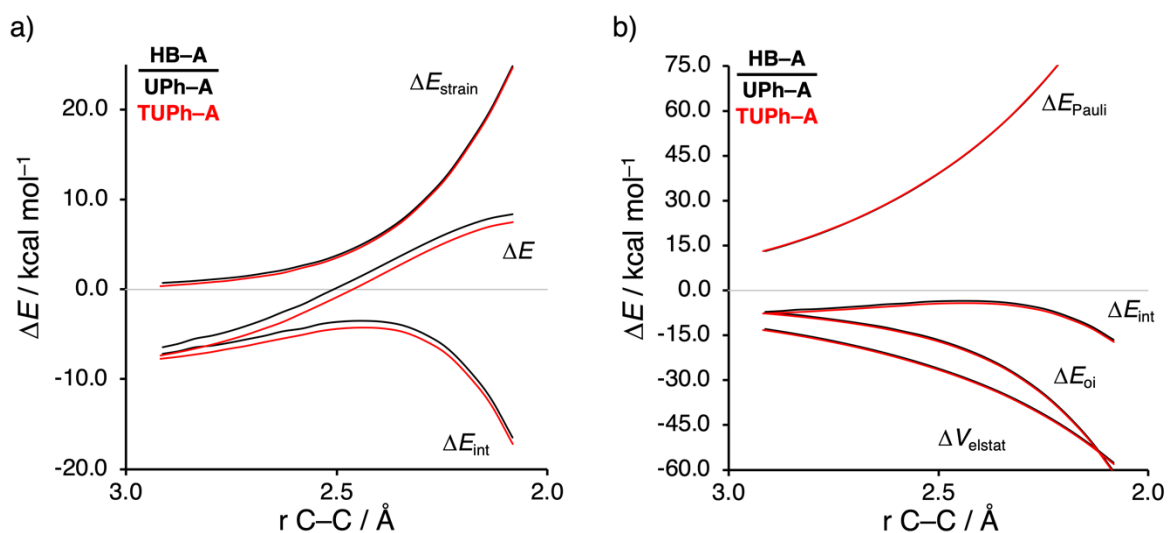
**Table S3.** Occupied-occupied orbital overlap for the *exo* Diels-Alder reactions between **CP** and **UPh-A** in the transition state.<sup>[a]</sup>

		UPh-A										
		HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4	HOMO-5	HOMO-6	HOMO-7	HOMO-8	HOMO-9	HOMO-10
<b>CP</b>	HOMO	0.00	0.00	0.00	0.03	0.00	0.00	0.05	0.00	0.01	0.00	0.00
	HOMO-1	0.00	0.00	0.00	0.02	0.00	0.02	0.10	0.00	0.03	0.01	0.00
	HOMO-2	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.02	0.01	0.00	0.00
	HOMO-3	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.01	0.02	0.00	0.01
	HOMO-4	0.01	0.01	0.00	0.00	0.00	0.01	0.02	0.02	0.00	0.00	0.00
	HOMO-5	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.00
	HOMO-6	0.00	0.01	0.00	0.00	0.00	0.02	0.14	0.01	0.00	0.01	0.00
	HOMO-7	0.01	0.00	0.00	0.01	0.00	0.01	0.02	0.00	0.01	0.00	0.00
	HOMO-8	0.01	0.01	0.00	0.00	0.00	0.01	0.01	0.02	0.00	0.00	0.00
	HOMO-9	0.00	0.00	0.00	0.01	0.00	0.02	0.05	0.02	0.01	0.00	0.00
HOMO-10	0.01	0.01	0.00	0.00	0.00	0.00	0.04	0.01	0.01	0.00	0.00	

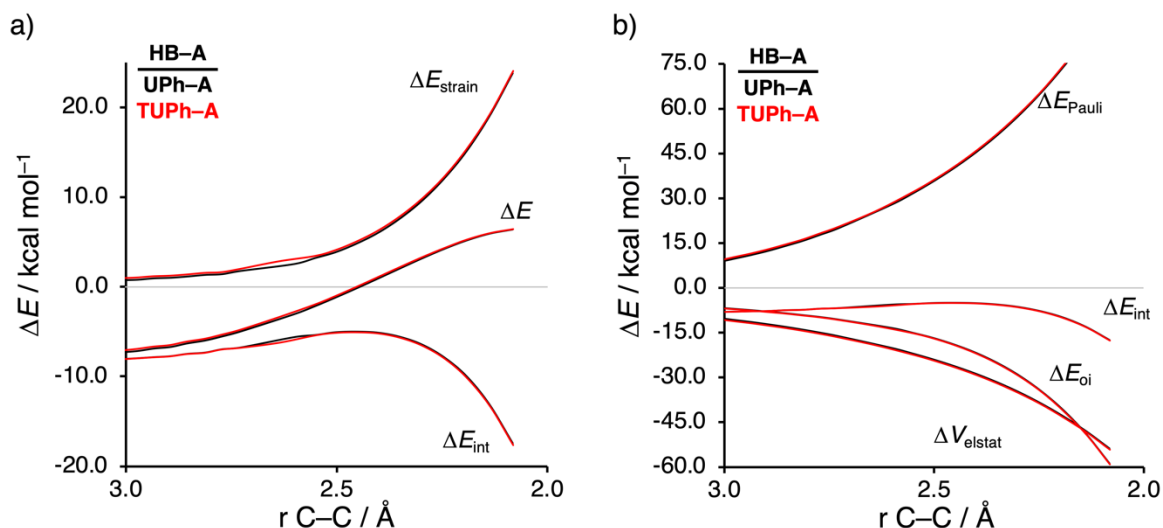
[a] Computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP



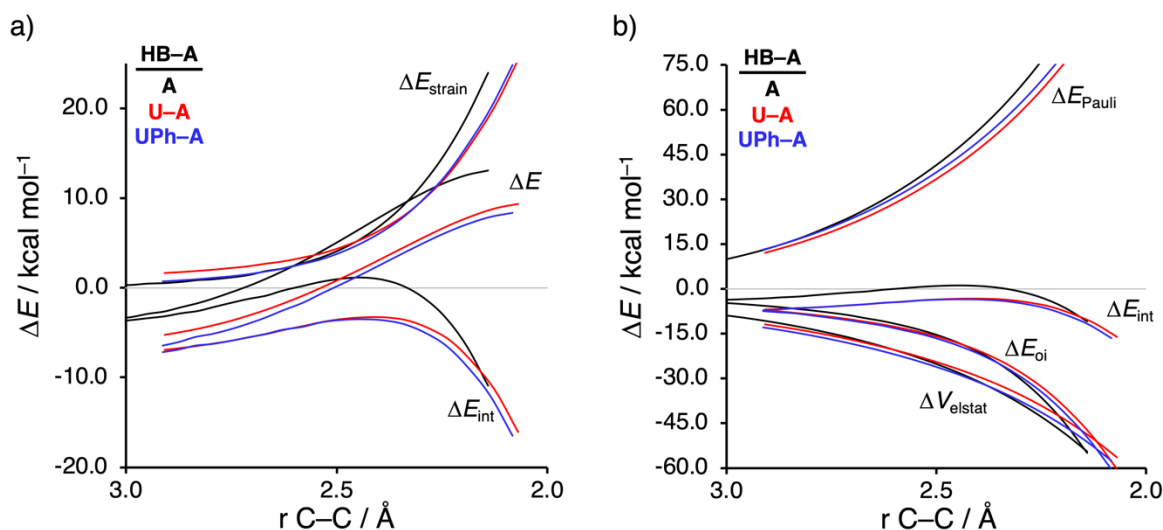
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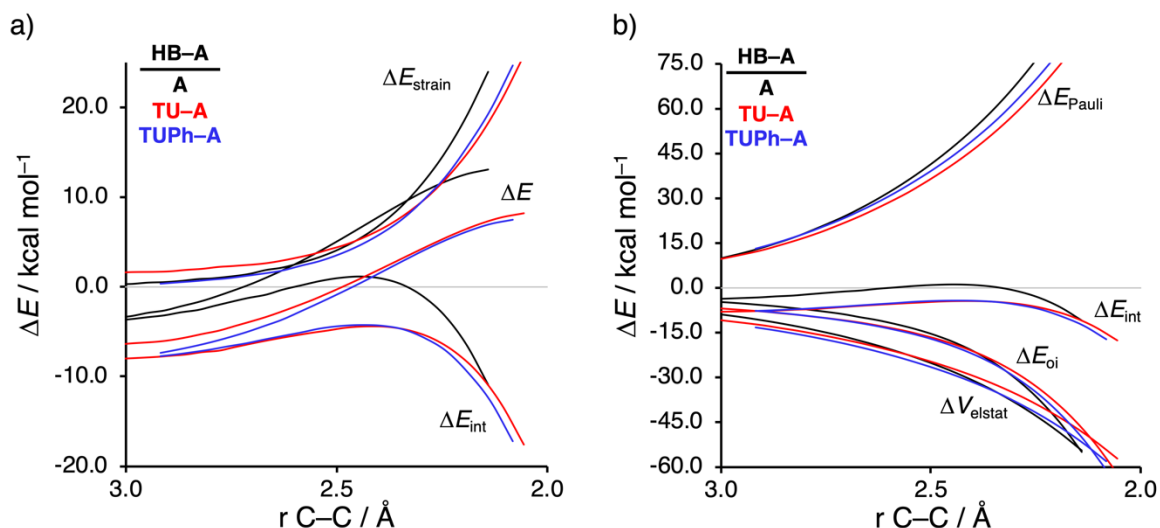
**Figure S9.** a) Activation strain analyses and b) energy decomposition analyses of the *endo* Diels-Alder reactions between CP and UPh-A and TUPh-A, where the energy values are projected onto the shorter newly forming  $C_{CP}\cdots C_{\beta}$  bond between CP and HB-A, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



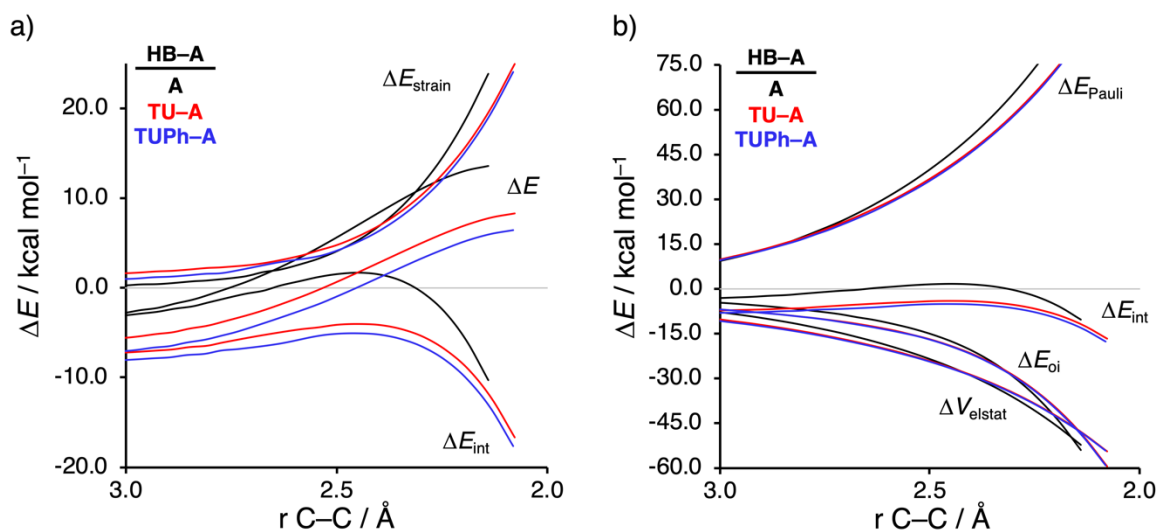
**Figure S10.** a) Activation strain analyses and b) energy decomposition analyses of the *endo* Diels-Alder reactions between CP and UPh-A and TUPh-A, where the energy values are projected onto the shorter newly forming  $C_{CP}\cdots C_{\beta}$  bond between CP and HB-A, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



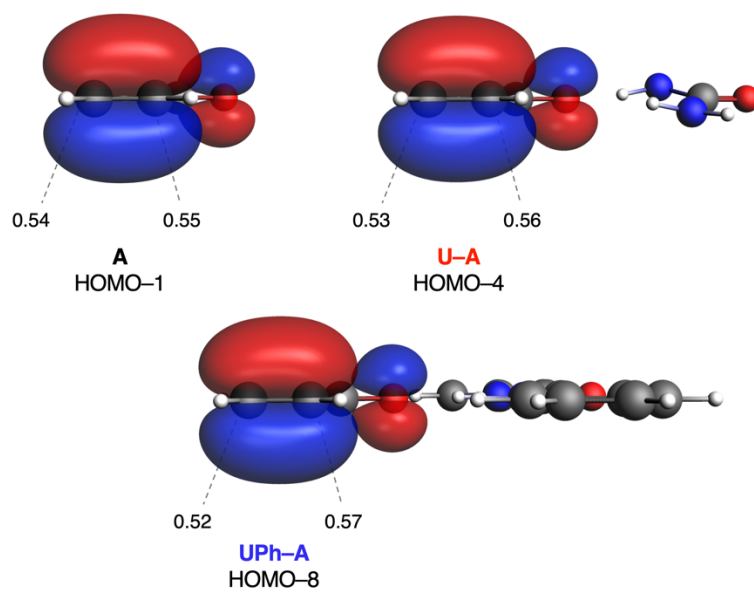
**Figure S11.** a) Activation strain analyses and b) energy decomposition analyses of the *endo* Diels-Alder reactions between CP and A, U-A, and UPh-A, where the energy values are projected onto the shorter newly forming  $C_{CP}\cdots C_{\beta}$  bond between CP and HB-A, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



**Figure S12.** a) Activation strain analyses and b) energy decomposition analyses of the *endo* Diels-Alder reactions between **CP** and **A**, **TU-A**, and **TUPh-A**, where the energy values are projected onto the shorter newly forming  $\text{C}_{\text{CP}} \cdots \text{C}_{\beta}$  bond between **CP** and **HB-A**, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



**Figure S13.** a) Activation strain analyses and b) energy decomposition analyses of the *exo* Diels-Alder reactions between **CP** and **A**, **TU-A**, and **TUPh-A**, where the energy values are projected onto the shorter newly forming  $\text{C}_{\text{CP}} \cdots \text{C}_{\beta}$  bond between **CP** and **HB-A**, computed at ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP.



**Figure S14.** Key occupied orbitals (isovalue = 0.03 au) computed at the equilibrium structures of **A**, **U-A**, and **UPh-A**, where the MO coefficients of the carbon  $2p_z$  atomic orbitals, contributing to the occupied orbitals, are shown. Computed at the ZORA-M06-2X/TZ2P//M06-2X/def2-SVPP level.

**Table S4.** Cartesian coordinates (in Å), energies (in Hartree), and number of imaginary frequencies of all stationary points, computed at M06-2X/def2-SVPP.

**cyclopentadiene (CP)**

**E** = -193.757376

**H** = -193.752288

**G** = -193.783979

**N<sub>imag</sub>** = 0

C	1.17779	0.28251	0.00000
C	0.73558	-0.99032	-0.00000
C	-0.73557	-0.99032	-0.00000
C	-1.17779	0.28250	0.00000
C	-0.00000	1.21499	0.00000
H	2.21842	0.61047	0.00000
H	1.35660	-1.88803	-0.00000
H	-1.35659	-1.88804	-0.00000
H	-2.21842	0.61047	0.00000
H	-0.00000	1.87948	-0.88521
H	-0.00000	1.87948	0.88521

**Acrolein (A)**

**E** = -191.606101

**H** = -191.60080

**G** = -191.632382

**N<sub>imag</sub>** = 0

O	1.78657	-0.12203	0.00002
C	0.68162	0.34839	-0.00017
H	0.52268	1.45788	0.00023
C	-0.56388	-0.45242	-0.00004
C	-1.75805	0.14461	0.00010
H	-0.44503	-1.54099	-0.00008
H	-2.69320	-0.42352	0.00018
H	-1.83515	1.23938	0.00014

**Acrolein + Urea (U-A)**

**E** = -416.538391

**H** = -416.526644

**G** = -416.577863

**N<sub>imag</sub>** = 0

O	-0.89256	0.39083	-0.06114
C	-2.08490	0.57332	-0.09185
H	-2.49728	1.59630	-0.26567
C	-3.09062	-0.48904	0.08894
C	-4.39410	-0.19840	0.03941
H	-2.71636	-1.50313	0.26109
H	-5.16404	-0.96461	0.16926
H	-4.73346	0.83006	-0.13540
H	1.06611	1.26981	-0.09567
H	0.75135	-0.98067	0.04750
N	1.73896	-1.12761	-0.13099
C	2.63730	-0.09522	0.01045

H	2.12530	-2.05750	-0.03242
N	2.04906	1.14291	0.12085
H	2.67692	1.93271	0.04571
O	3.83871	-0.26258	0.03550

**Acrolein + 1,3-diphenylurea (UPh-A)**

**E** = -877.943360

**H** = -877.923144

**G** = -877.996.417

**N<sub>imag</sub>** = 0

O	0.24256	2.41639	0.00045
C	0.38533	3.61675	-0.00017
H	-0.50506	4.28855	-0.00112
C	1.69161	4.29393	0.00027
C	1.75451	5.62937	-0.00037
H	2.58368	3.65954	0.00118
H	2.70914	6.16354	-0.00003
H	0.83994	6.23505	-0.00128
H	-1.02094	0.79968	-0.00042
H	0.98751	0.50314	0.00118
N	0.96579	-0.51305	0.00084
C	-0.27864	-1.11705	-0.00031
N	-1.29461	-0.17945	-0.00081
O	-0.45478	-2.31561	-0.00087
C	2.21888	-1.13545	0.00043
C	2.41080	-2.52627	0.00116
C	3.34549	-0.29519	-0.00054
C	3.70723	-3.03978	0.00087
C	4.63123	-0.82365	-0.00080
C	4.82372	-2.20526	-0.00011
H	1.54825	-3.18781	0.00195
H	3.19900	0.78972	-0.00115
H	3.84017	-4.12482	0.00145
H	5.48985	-0.14727	-0.00156
H	5.83185	-2.62506	-0.00029
C	-2.67463	-0.41225	-0.00039
C	-3.50962	0.71824	0.00064
C	-3.26032	-1.68818	-0.00105
C	-4.89328	0.58361	0.00101
C	-4.64978	-1.80510	-0.00061
C	-5.47711	-0.68329	0.00041
H	-3.05677	1.71479	0.00121
H	-2.62605	-2.57090	-0.00191
H	-5.51936	1.47956	0.00180
H	-5.09082	-2.80536	-0.00112
H	-6.56356	-0.79370	0.00071

**Acrolein + 1,3-bis(3,5-bis(trifluoromethyl)phenyl)urea (UF-A)****E** = -2224.693060**H** = -2224.685437**G** = -2224.769955**N<sub>imag</sub>** = 0

O	0.17154	3.12409	-0.01228
C	0.36437	4.31114	-0.15950
H	-0.49910	5.01517	-0.18834
C	1.69012	4.92676	-0.30968
C	1.79385	6.25196	-0.46003
H	2.56608	4.26978	-0.29573
H	2.76357	6.74500	-0.57494
H	0.90102	6.88908	-0.47243
H	-1.05293	1.44027	0.06882
H	0.96855	1.34129	0.07791
N	1.04841	0.32615	0.06554
C	-0.12763	-0.39942	0.04717
N	-1.23017	0.43785	0.05911
O	-0.18496	-1.60720	0.02475
C	2.34979	-0.16697	0.04985
C	2.68604	-1.52901	-0.03243
C	3.37892	0.78211	0.10968
C	4.02867	-1.89331	-0.06036
C	4.71163	0.39109	0.07960
C	5.05764	-0.95308	-0.01078
H	1.90333	-2.28298	-0.07980
H	3.12590	1.84293	0.17591
H	6.10394	-1.26306	-0.04886
C	-2.57272	0.06201	0.04405
C	-3.52309	1.09838	0.03469
C	-3.02020	-1.26541	0.03866
C	-4.87952	0.81243	0.02001
C	-4.39181	-1.52369	0.01905
C	-5.33676	-0.50609	0.00872
H	-3.19015	2.13921	0.03506
H	-2.30286	-2.08419	0.04837
H	-6.40419	-0.73075	-0.00967
C	5.78202	1.44410	0.19495
F	5.37840	2.61117	-0.32361
F	6.10321	1.67910	1.46837
F	6.89795	1.08554	-0.43507
C	4.41115	-3.35086	-0.13833
F	5.25525	-3.57092	-1.14915
F	5.03214	-3.74349	0.97629
F	3.35561	-4.14054	-0.31161
C	-4.82731	-2.96761	-0.01689
F	-6.14811	-3.09060	0.11730
F	-4.48607	-3.54638	-1.16908
F	-4.25353	-3.67111	0.95891
C	-5.88656	1.93211	0.05787
F	-5.33872	3.10520	-0.26954



F	-6.89572	1.70718	-0.78304
F	-6.41543	2.06991	1.27509

**Acrolein + Thioruea (TU-A)**

**E** = -739.441708

**H** = -739.429644

**G** = -739.481619

**N<sub>imag</sub>** = 0

O	-1.42544	0.42971	-0.00186
C	-2.62416	0.57790	-0.00013
H	-3.06616	1.60261	0.00238
C	-3.59504	-0.52945	-0.00100
C	-4.90704	-0.27382	0.00131
H	-3.19049	-1.54650	-0.00354
H	-5.65278	-1.07420	0.00078
H	-5.27819	0.75845	0.00388
H	0.48485	1.33653	0.00085
H	0.19843	-0.90372	-0.00100
N	1.20474	-1.04489	0.00117
C	2.06907	-0.00479	0.00037
H	1.60153	-1.97472	-0.00035
N	1.49439	1.21904	0.00003
H	2.11170	2.01974	0.00001
S	3.72773	-0.21837	0.00001

**Acrolein + 1,3-diphenylthiourea (TUPh-A)**

**E** = -1200.835995

**H** = -1200.815480

**G** = -1200.889366

**N<sub>imag</sub>** = 0

O	0.18236	2.57663	0.77899
C	0.87430	3.28903	0.08679
H	0.54819	4.33202	-0.13970
C	2.15905	2.88561	-0.50741
C	2.84921	3.75699	-1.25101
H	2.51383	1.86487	-0.32169
H	3.80538	3.49047	-1.71069
H	2.47219	4.77256	-1.42437
H	-1.10303	0.96237	0.65760
H	0.77561	0.58920	0.90162
N	0.81989	-0.30210	0.40914
C	-0.39529	-0.84427	0.06827
N	-1.40361	0.03130	0.37330
S	-0.60114	-2.34687	-0.61009
C	2.12545	-0.80863	0.28165
C	2.54815	-1.65445	-0.75298
C	3.06591	-0.36108	1.22387
C	3.88375	-2.04846	-0.81728
C	4.39936	-0.75064	1.14027
C	4.81631	-1.60515	0.12007
H	1.83152	-1.99806	-1.49525

H	2.73597	0.29266	2.03742
H	4.19842	-2.71212	-1.62655
H	5.11204	-0.39285	1.88741
H	5.85930	-1.92285	0.05645
C	-2.79681	-0.06157	0.19023
C	-3.48401	1.15217	0.03121
C	-3.52340	-1.25876	0.21533
C	-4.86707	1.17308	-0.11163
C	-4.90879	-1.22457	0.06069
C	-5.58990	-0.01990	-0.10577
H	-2.91631	2.08774	0.02041
H	-3.00529	-2.20423	0.35493
H	-5.38074	2.12976	-0.23424
H	-5.46343	-2.16604	0.07984
H	-6.67556	-0.00943	-0.22462

**Acrolein + 1,3-bis(3,5-bis(trifluoromethyl)phenyl)thiourea  
(TUF-A)**

**E** = -2547.583708

**H** = -2547.548708

**G** = -2547.661712

**N<sub>imag</sub>** = 0

O	0.20219	2.90405	0.01650
C	0.51667	4.05735	-0.18509
H	-0.27352	4.82978	-0.32918
C	1.90103	4.54283	-0.25849
C	2.13665	5.84221	-0.47351
H	2.71117	3.81645	-0.13455
H	3.15396	6.23995	-0.53345
H	1.31003	6.55269	-0.59668
H	-0.99808	1.21075	0.06492
H	0.90147	1.10672	0.17248
N	1.01627	0.09644	0.08370
C	-0.14541	-0.63439	0.08368
N	-1.22333	0.21762	0.12343
S	-0.22607	-2.28872	0.04561
C	2.35961	-0.28582	0.04919
C	2.85609	-1.49825	-0.45267
C	3.27188	0.67818	0.50108
C	4.23263	-1.71022	-0.48462
C	4.64126	0.45386	0.43644
C	5.14357	-0.74703	-0.05445
H	2.17371	-2.25915	-0.82530
H	2.89514	1.62110	0.90832
H	6.21820	-0.92466	-0.11221
C	-2.60163	-0.02612	0.10241
C	-3.40711	1.06111	-0.28363
C	-3.22106	-1.22531	0.46957
C	-4.78744	0.94585	-0.31024
C	-4.61370	-1.32063	0.41964
C	-5.41331	-0.25382	0.03347

H	-2.93881	2.00674	-0.56786
H	-2.62666	-2.07606	0.79552
H	-6.50035	-0.34792	0.00600
C	5.55869	1.53928	0.93253
F	5.20241	2.73360	0.43378
F	5.51178	1.65444	2.25999
F	6.82414	1.32249	0.58923
C	4.74740	-3.04013	-0.97915
F	5.96998	-2.92491	-1.50100
F	4.82465	-3.92723	0.01329
F	3.95299	-3.55850	-1.91362
C	-5.24010	-2.64516	0.77972
F	-6.55307	-2.53050	0.98263
F	-5.06280	-3.54355	-0.18895
F	-4.70020	-3.15131	1.88832
C	-5.64458	2.12341	-0.69449
F	-4.91504	3.14496	-1.14893
F	-6.51968	1.79656	-1.64501
F	-6.34896	2.56943	0.34716

**TS: endo\_CP + A**

**E** = -385.343710

**H** = -385.334897

**G** = -385.376146

**N<sub>imag</sub>** = 1, -465.2270i cm<sup>-1</sup>

C	-0.93989	0.85934	0.31751
C	-0.02044	1.62617	-0.38808
H	0.40658	2.52090	0.07372
C	-1.93786	0.04076	-0.38664
O	-2.92096	-0.44529	0.11168
H	-1.70530	-0.11704	-1.47432
H	-1.15302	1.05641	1.37226
H	-0.08099	1.65468	-1.48033
C	0.41253	-0.96327	0.84893
C	0.67006	-1.43195	-0.43610
C	1.53831	-0.53232	-1.07979
C	1.81182	0.53305	-0.21592
C	1.46148	0.06046	1.17240
H	-0.19488	-1.48019	1.59481
H	0.18486	-2.29068	-0.90335
H	1.84259	-0.58722	-2.12687
H	2.57302	1.29220	-0.41138
H	1.17423	0.83759	1.89319
H	2.34460	-0.47773	1.57490

**TS: exo\_CP + A**

$E = -385.342776$

$H = -385.333980$

$G = -385.375205$

$N_{\text{imag}} = 1, -460.6969i \text{ cm}^{-1}$

C	-2.13339	-0.02150	-0.55796
C	-1.35122	-1.17642	-0.74380
C	-0.37188	-1.21782	0.24116
C	-1.62822	0.70006	0.52839
C	-0.78119	-0.26026	1.32206
H	-2.92182	0.32276	-1.23016
H	-1.42557	-1.86254	-1.58911
H	0.35784	-2.01919	0.37511
H	-2.13608	1.55727	0.97709
H	0.03009	0.18232	1.91565
H	-1.45553	-0.80385	2.01553
C	0.92384	0.51741	-0.67600
C	0.09087	1.59123	-0.38301
C	2.07833	0.20735	0.17911
H	2.09740	0.77285	1.15072
O	2.95716	-0.57275	-0.08837
H	0.95078	0.07381	-1.67355
H	0.32600	2.21249	0.48975
H	-0.44326	2.10586	-1.18369

**PC: endo\_CP + A**

$E = -385.405568$

$H = -385.397453$

$G = -385.437502$

$N_{\text{imag}} = 0$

C	-0.73696	0.50900	0.30359
C	0.17875	1.23460	-0.72383
H	0.16873	2.32190	-0.55178
C	-1.91522	-0.18990	-0.32300
O	-3.05049	-0.07939	0.04873
H	-1.65999	-0.85279	-1.19098
H	-1.13786	1.20526	1.05557
H	-0.13172	1.05890	-1.76699
C	0.26510	-0.48320	1.00226
C	0.73005	-1.47697	-0.04917
C	1.52321	-0.81488	-0.90186
C	1.58805	0.62798	-0.43578
C	1.50336	0.42888	1.08855
H	-0.12287	-0.90418	1.93889
H	0.38944	-2.51108	-0.13371
H	1.95865	-1.19575	-1.82822
H	2.42282	1.22798	-0.82143
H	1.31757	1.36377	1.64355
H	2.38108	-0.09204	1.50070

**PC: exo\_CP + A**

**E** = -385.405056

**H** = -385.396891

**G** = -385.437131

**N<sub>imag</sub>** = 0

C	-2.11705	-0.17308	-0.59131
C	-1.41473	-1.29196	-0.37026
C	-0.22938	-0.91815	0.50048
C	-1.40768	0.95868	0.12931
C	-0.85193	0.20553	1.35104
H	-2.97699	-0.05437	-1.25372
H	-1.57464	-2.27535	-0.81691
H	0.26907	-1.74314	1.02761
H	-2.00070	1.86266	0.32138
H	-0.11775	0.79227	1.92896
H	-1.64195	-0.16714	2.02040
C	0.72176	-0.09403	-0.44848
C	-0.08508	1.21955	-0.65560
C	2.06390	0.14033	0.19804
H	2.04119	0.75551	1.13729
O	3.10358	-0.29150	-0.21469
H	0.90889	-0.63850	-1.38467
H	0.44534	2.08586	-0.22243
H	-0.25998	1.43301	-1.71980

**TS: endo\_CP + U**

**E** = -610.284702

**H** = -610.269952

**G** = -610.326211

**N<sub>imag</sub>** = 1, -460.6106i cm<sup>-1</sup>

C	-0.91176	1.22063	-0.71766
C	-2.30622	1.18570	-0.76039
C	-0.25509	1.84509	0.42030
O	0.89253	2.24661	0.46668
H	-0.91442	1.95952	1.31812
C	-0.58311	-1.10186	-0.00712
C	-1.13907	-0.94221	1.25670
C	-2.52733	-0.76201	1.12499
C	-2.85941	-0.73834	-0.23746
C	-1.70090	-1.37246	-0.96542
H	2.10073	1.34618	-0.82028
H	-0.30376	1.03791	-1.60756
H	-2.80434	1.14001	-1.73334
H	-2.86613	1.72910	0.00681
H	0.46213	-1.34364	-0.21100
H	-0.56622	-0.88135	2.18337
H	-3.21856	-0.54658	1.94254
H	-3.88817	-0.79085	-0.60274
H	-1.53608	-1.05020	-2.00270
H	-1.86580	-2.46979	-0.97021
H	2.31497	0.85298	1.39557

N	2.40792	-0.13225	1.16993
C	2.67055	-0.53102	-0.12283
H	2.72078	-0.77224	1.88970
N	2.53130	0.45498	-1.06062
H	2.62228	0.16882	-2.02652
O	2.96272	-1.67913	-0.40089

**TS: exo\_CP + U-A**

**E** = -610.284689

**H** = -610.270159

**G** = -610.325662

**N<sub>imag</sub>** = 1, -438.5839i cm<sup>-1</sup>

C	-2.36474	1.69462	0.51789
C	-0.96571	1.67867	0.35966
C	-0.63820	0.78051	-0.64562
C	-2.93593	0.75070	-0.34511
C	-1.89459	0.45500	-1.39431
H	-2.90877	2.25908	1.27813
H	-0.24110	2.20152	0.98545
H	0.37416	0.57290	-1.00561
H	-4.00968	0.68252	-0.53738
H	-1.94026	-0.53761	-1.86336
H	-2.00893	1.21305	-2.19627
C	-1.16951	-1.13152	0.77617
C	-2.55690	-1.02656	0.71336
C	-0.43370	-2.00457	-0.11867
H	-1.03877	-2.45249	-0.94759
O	0.75092	-2.27887	-0.03092
H	-0.61451	-0.73640	1.62989
H	-3.09698	-1.66860	0.00712
H	-3.11890	-0.76374	1.61157
H	1.72472	-0.89966	1.11393
H	2.24130	-1.18501	-1.03303
N	2.65511	-0.25663	-1.09079
H	3.31187	-0.07654	-1.84162
C	2.91242	0.44290	0.07379
N	2.16120	0.02100	1.14781
H	2.45594	0.38929	2.04431
O	3.67870	1.38045	0.12249

**PC: endo\_CP + U-A**

**E** = -610.338571

**H** = -610.323908

**G** = -610.383489

**N<sub>imag</sub>** = 0

C	1.29455	-0.49279	0.08806
C	2.32851	-0.72705	1.22965
C	0.25087	0.52620	0.43391
O	-0.93745	0.35319	0.32884
H	0.64175	1.50385	0.80835
C	2.21437	-0.04479	-1.11066

C	2.85394	1.27900	-0.72675
C	3.74072	1.02722	0.24521
C	3.69674	-0.46327	0.52720
C	3.39914	-1.00271	-0.88358
H	-2.55749	-0.96082	-0.12335
H	0.77279	-1.42267	-0.18392
H	2.26071	-1.76048	1.60219
H	2.17625	-0.05289	2.08831
H	1.70802	-0.08362	-2.08375
H	2.56340	2.25633	-1.11787
H	4.31914	1.75750	0.81510
H	4.56013	-0.88499	1.05802
H	3.10922	-2.06673	-0.89552
H	4.22205	-0.82386	-1.59196
H	-2.89013	1.22887	0.39600
N	-3.85280	1.15520	0.08387
C	-4.44392	-0.07587	-0.07918
H	-4.48761	1.92430	0.25466
N	-3.55630	-1.12640	-0.05843
H	-3.93053	-2.01956	-0.35117
O	-5.63925	-0.22227	-0.22838

**PC: exo\_CP + U-A**

**E** = -610.337904

**H** = -610.323185

**G** = -601.383006

**N<sub>imag</sub>** = 0

C	-3.95623	1.05467	0.10592
C	-3.02352	1.41864	-0.78367
C	-2.12443	0.21782	-1.01328
C	-3.68955	-0.39162	0.47978
C	-3.14158	-0.92790	-0.85443
H	-4.71010	1.69420	0.56937
H	-2.84872	2.41486	-1.19453
H	-1.50842	0.23569	-1.92267
H	-4.52269	-0.93915	0.93936
H	-2.68630	-1.92949	-0.76963
H	-3.89381	-0.92892	-1.65731
C	-1.29638	0.08137	0.32439
C	-2.38375	-0.39135	1.33311
C	-0.18551	-0.91449	0.16443
H	-0.49959	-1.96585	-0.05348
O	0.98750	-0.64879	0.23718
H	-0.83965	1.04187	0.60148
H	-2.17304	-1.41031	1.70231
H	-2.44717	0.27307	2.20642
H	2.99379	-1.28534	-0.20030
H	2.50344	0.82827	0.48734
N	3.49458	1.03083	0.56358
H	3.79446	1.97901	0.74913
C	4.42546	0.22033	-0.04228

N	3.91352	-0.97405	-0.49454
H	4.60008	-1.66306	-0.77340
O	5.59175	0.53039	-0.16858

**TS: endo\_CP + UPh-A**

**E** = -1071.688596

**H** = -1071.665058

**G** = -1071.744236

**N<sub>imag</sub>** = 1, -453.6662i cm<sup>-1</sup>

C	-0.92225	-1.53658	0.45082
C	-1.37265	-2.24688	1.56251
C	-0.41362	-2.18959	-0.73989
O	0.18909	-1.64323	-1.65230
H	-0.61023	-3.28910	-0.79338
C	-3.07844	-1.27345	-0.63734
C	-3.43307	-2.61325	-0.73957
C	-3.69412	-3.10778	0.55014
C	-3.44824	-2.09426	1.48792
C	-3.46929	-0.79085	0.72542
H	0.00691	0.52631	-1.54901
H	-0.74688	-0.46134	0.53028
H	-1.31328	-1.76889	2.54457
H	-1.25958	-3.33523	1.57925
H	-2.84769	-0.61309	-1.47437
H	-3.41558	-3.20605	-1.65562
H	-3.92255	-4.14701	0.79580
H	-3.74019	-2.16940	2.53833
H	-2.87899	0.04304	1.13230
H	-4.52719	-0.45889	0.66934
H	1.72994	-0.44144	-1.17619
N	2.16622	0.28425	-0.60859
C	1.35575	1.32780	-0.22201
N	0.13190	1.28510	-0.88067
O	1.65342	2.18053	0.58500
C	3.48096	0.02480	-0.19984
C	4.24352	0.89594	0.59279
C	4.05182	-1.18386	-0.63166
C	5.54962	0.54526	0.93351
C	5.35557	-1.51741	-0.28282
C	6.11701	-0.65349	0.50498
H	3.80954	1.83182	0.93644
H	3.45666	-1.86333	-1.24954
H	6.13344	1.23312	1.55076
H	5.77843	-2.46286	-0.63186
H	7.14152	-0.91252	0.78060
C	-1.03983	1.94834	-0.49748
C	-2.11822	1.93063	-1.39669
C	-1.20667	2.57232	0.75006
C	-3.34590	2.48682	-1.04979
C	-2.43940	3.13487	1.07955
C	-3.51784	3.09145	0.19581



H	-1.97864	1.47538	-2.38203
H	-0.36933	2.61931	1.44366
H	-4.17072	2.45661	-1.76653
H	-2.55371	3.61784	2.05355
H	-4.47700	3.53687	0.46821

**TS: exo\_CP + UPh-A**

$E = -1071.691932$

$H = -1071.668590$

$G = -1071.746104$

$N_{\text{imag}} = 1, -436.4597i \text{ cm}^{-1}$

C	-3.41909	-2.12893	-1.20430
C	-2.76144	-0.96423	-1.12593
C	-1.31293	-1.28596	-0.80335
C	-2.42181	-3.23879	-0.92762
C	-1.14837	-2.62901	-1.53793
H	-4.49429	-2.26999	-1.33187
H	-3.17590	0.04677	-1.16564
H	-0.58319	-0.49234	-1.01883
H	-2.70685	-4.24716	-1.25588
H	-0.22799	-3.17795	-1.27326
H	-1.20944	-2.51128	-2.62998
C	-1.35597	-1.76574	0.70557
C	-2.06942	-3.14434	0.58857
C	0.01803	-1.87882	1.29025
H	0.68311	-2.65773	0.84050
O	0.44144	-1.17954	2.18142
H	-1.91822	-1.04563	1.31659
H	-1.39429	-3.97071	0.87321
H	-2.95696	-3.19963	1.23482
H	1.81632	0.31437	1.64763
H	-0.15513	0.87885	1.76984
N	-0.18504	1.39985	0.89715
C	0.96166	1.38152	0.11866
N	2.02074	0.78247	0.76991
O	1.02296	1.83386	-1.00431
C	3.28078	0.47905	0.22927
C	3.80120	1.08197	-0.92486
C	4.05148	-0.47502	0.91277
C	5.07225	0.72108	-1.37070
C	5.32013	-0.81836	0.45837
C	5.84031	-0.22302	-0.69100
H	3.21021	1.81944	-1.46259
H	3.64082	-0.95058	1.80906
H	5.46771	1.19726	-2.27157
H	5.90372	-1.56141	1.00758
H	6.83524	-0.49202	-1.05204
C	-1.46139	1.82984	0.51095
C	-2.51442	1.58578	1.40979
C	-1.74305	2.46993	-0.70667
C	-3.81940	1.94939	1.09624

C	-3.05752	2.83088	-1.00405
C	-4.10373	2.57228	-0.11945
H	-2.29861	1.10634	2.36988
H	-0.93805	2.67446	-1.40749
H	-4.61908	1.74457	1.81222
H	-3.26101	3.32692	-1.95657
H	-5.12703	2.85984	-0.36945

**PC: endo\_CP + UPh-A**

**E** = -1071.745927

**H** = -1071.722943

**G** = -1071.802435

**N<sub>imag</sub>** = 0

C	-1.77412	-1.38812	0.01310
C	-1.82911	-2.14106	1.37471
C	-0.89847	-2.05024	-1.00483
O	-0.05716	-1.48649	-1.66685
H	-1.06592	-3.14573	-1.14685
C	-3.29145	-1.35348	-0.41472
C	-3.74393	-2.78706	-0.63192
C	-3.79188	-3.37626	0.57038
C	-3.35954	-2.34827	1.59951
C	-3.91815	-1.06275	0.96133
H	0.05464	0.55320	-1.34038
H	-1.42452	-0.35452	0.14904
H	-1.38451	-1.52266	2.16896
H	-1.28790	-3.10122	1.35536
H	-3.49776	-0.63954	-1.22265
H	-3.90632	-3.25792	-1.60387
H	-3.99526	-4.42848	0.78092
H	-3.63334	-2.55622	2.64199
H	-3.53839	-0.13505	1.42119
H	-5.01792	-1.04891	0.92287
H	1.76415	-0.48446	-1.14972
N	2.24594	0.16819	-0.53758
C	1.53349	1.27465	-0.11711
N	0.28523	1.32319	-0.71573
O	1.94301	2.09815	0.67042
C	3.54441	-0.20776	-0.16708
C	4.38180	0.56455	0.65242
C	4.01677	-1.43422	-0.66304
C	5.66093	0.09951	0.95597
C	5.29540	-1.88214	-0.35111
C	6.13016	-1.11712	0.46382
H	4.02640	1.51460	1.04351
H	3.36572	-2.03888	-1.30216
H	6.30289	0.71149	1.59494
H	5.64002	-2.83929	-0.75057
H	7.13503	-1.46592	0.71104
C	-0.77270	2.19155	-0.42562
C	-1.96461	1.99913	-1.14634

C	-0.71996	3.20689	0.54189
C	-3.08422	2.78584	-0.89775
C	-1.85070	3.98916	0.77586
C	-3.03689	3.78850	0.07128
H	-1.99972	1.22360	-1.91886
H	0.20006	3.37221	1.09745
H	-3.99808	2.61608	-1.47312
H	-1.79534	4.77617	1.53245
H	-3.91217	4.41089	0.26846

**PC: exo\_CP + UPh-A**

**E** = -1071.691932

**H** = -1071.668590

**G** = -1070.746104

**N<sub>imag</sub>** = 0

C	-3.41909	-2.12893	-1.20430
C	-2.76144	-0.96423	-1.12593
C	-1.31293	-1.28596	-0.80335
C	-2.42181	-3.23879	-0.92762
C	-1.14837	-2.62901	-1.53793
H	-4.49429	-2.26999	-1.33187
H	-3.17590	0.04677	-1.16564
H	-0.58319	-0.49234	-1.01883
H	-2.70685	-4.24716	-1.25588
H	-0.22799	-3.17795	-1.27326
H	-1.20944	-2.51128	-2.62998
C	-1.35597	-1.76574	0.70557
C	-2.06942	-3.14434	0.58857
C	0.01803	-1.87882	1.29025
H	0.68311	-2.65773	0.84050
O	0.44144	-1.17954	2.18142
H	-1.91822	-1.04563	1.31659
H	-1.39429	-3.97071	0.87321
H	-2.95696	-3.19963	1.23482
H	1.81632	0.31437	1.64763
H	-0.15513	0.87885	1.76984
N	-0.18504	1.39985	0.89715
C	0.96166	1.38152	0.11866
N	2.02074	0.78247	0.76991
O	1.02296	1.83386	-1.00431
C	3.28078	0.47905	0.22927
C	3.80120	1.08197	-0.92486
C	4.05148	-0.47502	0.91277
C	5.07225	0.72108	-1.37070
C	5.32013	-0.81836	0.45837
C	5.84031	-0.22302	-0.69100
H	3.21021	1.81944	-1.46259
H	3.64082	-0.95058	1.80906
H	5.46771	1.19726	-2.27157
H	5.90372	-1.56141	1.00758
H	6.83524	-0.49202	-1.05204

C	-1.46139	1.82984	0.51095
C	-2.51442	1.58578	1.40979
C	-1.74305	2.46993	-0.70667
C	-3.81940	1.94939	1.09624
C	-3.05752	2.83088	-1.00405
C	-4.10373	2.57228	-0.11945
H	-2.29861	1.10634	2.36988
H	-0.93805	2.67446	-1.40749
H	-4.61908	1.74457	1.81222
H	-3.26101	3.32692	-1.95657
H	-5.12703	2.85984	-0.36945

**TS: endo\_CP + UF-A**

**E** = -2418.440410

**H** = -2418.403313

**G** = -2418.517151

**N<sub>imag</sub>** = 1, -444.7589i cm<sup>-1</sup>

C	-1.52576	-2.53082	1.08387
C	-1.69065	-3.19287	2.30328
C	-0.67638	-3.08168	0.05367
O	-0.24418	-2.48284	-0.92483
H	-0.39790	-4.15355	0.19749
C	-3.60590	-3.41411	0.02728
C	-3.25566	-4.75647	0.07223
C	-3.25428	-5.17742	1.41435
C	-3.53828	-4.08017	2.24113
C	-4.17266	-3.03411	1.35867
H	-0.63660	-0.66782	-0.94802
H	-1.84279	-1.48912	0.97255
H	-1.93382	-2.59689	3.18794
H	-1.07176	-4.07096	2.51069
H	-3.74545	-2.83217	-0.88658
H	-2.95567	-5.36198	-0.78455
H	-2.96059	-6.16859	1.76619
H	-3.78243	-4.18365	3.30127
H	-4.04540	-1.98541	1.65811
H	-5.26252	-3.23913	1.32068
H	1.31650	-1.04845	-0.86380
N	1.62796	-0.12105	-0.57885
C	0.64838	0.84171	-0.40755
N	-0.60025	0.32753	-0.70170
O	0.85554	1.97878	-0.05008
C	2.99890	0.02462	-0.37160
C	3.61195	1.22307	0.01725
C	3.79865	-1.11461	-0.56921
C	4.99460	1.25360	0.20359
C	5.17156	-1.05335	-0.38229
C	5.79223	0.13275	0.01133
H	3.01206	2.11803	0.17365
H	3.33451	-2.05782	-0.86871
H	6.87102	0.17759	0.16644

C	-1.82771	0.96279	-0.57416
C	-2.96024	0.20490	-0.91841
C	-2.00825	2.27867	-0.12266
C	-4.23547	0.73718	-0.79419
C	-3.30106	2.79244	-0.02060
C	-4.42784	2.04290	-0.34444
H	-2.82305	-0.81084	-1.29972
H	-1.14377	2.88593	0.14260
H	-5.42872	2.46668	-0.25677
C	6.01862	-2.27018	-0.65068
F	6.56398	-2.22435	-1.86771
F	7.02032	-2.36884	0.22339
F	5.30585	-3.39639	-0.58067
C	5.60743	2.55585	0.65458
F	6.93982	2.50377	0.65456
F	5.24165	3.56493	-0.13580
F	5.21908	2.86872	1.89201
C	-5.41806	-0.14056	-1.10209
F	-6.48521	0.56154	-1.46544
F	-5.14537	-1.01246	-2.07818
F	-5.77243	-0.87096	-0.03236
C	-3.45064	4.22043	0.44415
F	-4.72823	4.54198	0.65150
F	-2.79112	4.43017	1.58333
F	-2.96268	5.07499	-0.45479

**TS: exo\_CP + UF-A**

**E** = -2418.441687

**H** = -2418.403739

**G** = -2418.520680

**N<sub>imag</sub>** = 1, -433.6023i cm<sup>-1</sup>

C	3.70378	-2.07810	2.53218
C	2.97649	-1.05341	1.89417
C	1.63588	-1.40304	1.88415
C	2.83236	-3.12003	2.87786
C	1.44213	-2.53513	2.84458
H	4.79042	-2.10625	2.63462
H	3.40807	-0.16676	1.42462
H	0.82357	-0.79951	1.47092
H	3.11469	-3.93477	3.54940
H	0.62260	-3.23206	2.62241
H	1.24794	-2.09408	3.84388
C	2.03467	-3.22500	0.19536
C	2.65566	-4.11154	1.07627
C	0.62389	-3.31001	-0.08885
H	0.05361	-4.04299	0.53211
O	0.02220	-2.66698	-0.94220
H	2.63832	-2.57903	-0.44487
H	2.06151	-4.93708	1.48671
H	3.71466	-4.33896	0.93824
H	-1.33900	-1.21826	-0.97078

H	0.61085	-0.91629	-1.37730
N	0.64678	0.07849	-1.13628
C	-0.55029	0.66958	-0.76480
N	-1.58631	-0.24421	-0.79216
O	-0.66463	1.83264	-0.45077
C	-2.93315	0.00455	-0.52790
C	-3.46278	1.27405	-0.26471
C	-3.79693	-1.10532	-0.53423
C	-4.82977	1.40522	-0.01369
C	-5.15105	-0.94471	-0.28392
C	-5.68971	0.31501	-0.01622
H	-2.81192	2.14673	-0.25208
H	-3.39615	-2.10231	-0.73449
H	-6.75418	0.43877	0.18803
C	1.92182	0.60471	-0.96785
C	2.99063	-0.15071	-1.47136
C	2.20255	1.79883	-0.28066
C	4.30521	0.22931	-1.22812
C	3.52851	2.16831	-0.07400
C	4.59733	1.39524	-0.52826
H	2.78552	-1.05805	-2.04651
H	1.38846	2.41890	0.09079
H	5.62907	1.69862	-0.34504
C	-6.07373	-2.13461	-0.33849
F	-6.75671	-2.16841	-1.48391
F	-5.40610	-3.28593	-0.24116
F	-6.96896	-2.09995	0.64913
C	-5.35159	2.78879	0.28345
F	-6.67772	2.80144	0.41889
F	-4.82810	3.27104	1.41178
F	-5.03616	3.64428	-0.68922
C	3.82416	3.38839	0.76168
F	3.98985	3.04967	2.04511
F	4.94716	3.99028	0.36933
F	2.84018	4.28061	0.71105
C	5.40025	-0.70610	-1.66508
F	6.60408	-0.14893	-1.57775
F	5.41135	-1.80400	-0.89214
F	5.22672	-1.12204	-2.91861

**PC: endo\_CP + UF-A**

**E** = -2418.469001

**H** = -2418.458745

**G** = -2418.573998

**N<sub>imag</sub>** = 0

C	-2.00634	2.72940	-0.70540
C	-1.98143	3.25743	-2.17121
C	-0.88693	3.25535	0.13614
O	-0.17548	2.57445	0.84204
H	-0.72330	4.35827	0.09535
C	-3.42880	3.19801	-0.20425

C	-3.43592	4.71705	-0.20426
C	-3.43029	5.11599	-1.48301
C	-3.40538	3.87021	-2.34886
C	-4.23843	2.90929	-1.48148
H	-0.62168	0.66479	0.96255
H	-1.96353	1.62923	-0.68546
H	-1.81055	2.42571	-2.87116
H	-1.19112	4.00650	-2.34228
H	-3.75987	2.70873	0.72166
H	-3.37119	5.34734	0.68517
H	-3.35333	6.14043	-1.85350
H	-3.70686	3.99738	-3.39655
H	-4.18256	1.85585	-1.80232
H	-5.28986	3.21665	-1.38090
H	1.34062	1.07257	0.82680
N	1.65045	0.14028	0.56212
C	0.67487	-0.82917	0.41138
N	-0.57773	-0.32337	0.71194
O	0.88480	-1.96815	0.06470
C	3.02288	-0.00206	0.35139
C	3.63889	-1.20870	-0.01713
C	3.81574	1.14310	0.51446
C	5.01776	-1.23765	-0.20904
C	5.19034	1.08479	0.31692
C	5.81209	-0.10451	-0.05186
H	3.04079	-2.10614	-0.16071
H	3.34910	2.09328	0.78941
H	6.88853	-0.14459	-0.22458
C	-1.80339	-0.97216	0.59313
C	-2.93850	-0.24944	0.99809
C	-1.97375	-2.26857	0.08849
C	-4.20922	-0.78907	0.86361
C	-3.26190	-2.79464	-0.01714
C	-4.39198	-2.07482	0.35517
H	-2.81508	0.74542	1.43463
H	-1.10681	-2.85418	-0.21463
H	-5.38890	-2.50698	0.26262
C	6.00981	2.32813	0.54820
F	7.16717	2.28554	-0.10873
F	5.35588	3.42358	0.15294
F	6.29274	2.49079	1.84218
C	5.67575	-2.55069	-0.55501
F	4.85619	-3.35201	-1.23229
F	6.77033	-2.36589	-1.29522
F	6.05225	-3.20677	0.54456
C	-5.40151	0.05841	1.22059
F	-6.43494	-0.67654	1.61848
F	-5.11486	0.92819	2.19396
F	-5.81193	0.78160	0.17000
C	-3.39685	-4.19247	-0.56986
F	-4.66563	-4.60107	-0.58089

F	-2.94082	-4.26062	-1.82135
F	-2.69561	-5.06660	0.15051

**PC: exo\_CP + UF-A**

**E** = -2418.496735

**H** = -2418.459436

**G** = -2418.575471

**N<sub>imag</sub>** = 0

C	3.92482	1.97032	-2.43273
C	3.12250	1.03726	-1.90357
C	1.74748	1.66158	-1.75557
C	3.09610	3.22366	-2.64618
C	1.72847	2.59868	-2.97788
H	5.00132	1.89411	-2.59713
H	3.39715	0.03840	-1.55598
H	0.90514	0.96727	-1.62179
H	3.49904	3.95902	-3.35460
H	0.90007	3.32859	-2.97468
H	1.73041	2.04123	-3.92611
C	1.90495	2.71825	-0.58010
C	2.79949	3.80560	-1.22972
C	0.55101	3.19710	-0.15603
H	0.06659	3.97273	-0.79735
O	-0.05309	2.76174	0.79928
H	2.38402	2.24219	0.28516
H	2.26483	4.76774	-1.31515
H	3.71496	3.97734	-0.64599
H	-1.39728	1.23033	1.07056
H	0.58658	0.93037	1.43076
N	0.62041	-0.04963	1.15186
C	-0.57741	-0.63329	0.76882
N	-1.62619	0.26270	0.85422
O	-0.68409	-1.78169	0.40641
C	-2.97130	0.01149	0.57355
C	-3.48723	-1.25500	0.26946
C	-3.84569	1.11006	0.61852
C	-4.85279	-1.39286	0.01924
C	-5.19964	0.94362	0.36484
C	-5.72574	-0.31260	0.06408
H	-2.82851	-2.12086	0.23271
H	-3.45831	2.10308	0.86201
H	-6.79250	-0.44445	-0.12158
C	1.89780	-0.57996	0.98441
C	2.96589	0.15274	1.52042
C	2.17733	-1.76025	0.27534
C	4.28074	-0.23190	1.28609
C	3.50319	-2.13835	0.08151
C	4.57202	-1.38496	0.56602
H	2.76489	1.04717	2.11736
H	1.36416	-2.36440	-0.12314
H	5.60347	-1.69186	0.38832



C	-6.10819	2.14599	0.36445
F	-7.32670	1.83802	0.80559
F	-5.62993	3.12563	1.13392
F	-6.24955	2.64655	-0.86508
C	-5.36350	-2.76823	-0.33231
F	-4.90412	-3.68828	0.51538
F	-6.69517	-2.82289	-0.30915
F	-4.96941	-3.13061	-1.55429
C	3.79029	-3.34025	-0.78300
F	4.94968	-3.91264	-0.46002
F	2.83628	-4.26161	-0.68893
F	3.87258	-2.98292	-2.06931
C	5.37483	0.68069	1.77315
F	6.57863	0.12915	1.65701
F	5.38422	1.82050	1.06910
F	5.19783	1.02063	3.05041

**TS: endo\_CP + TU-A**

**E** = -933.189032

**H** = -993.174058

**G** = -993.230977

**N<sub>imag</sub>** = 1, -457.0710i cm<sup>-1</sup>

C	1.38030	-1.12111	-0.81266
C	2.74234	-0.82342	-0.89472
C	0.89067	-1.92230	0.29259
O	-0.18391	-2.49554	0.35669
H	1.60551	-2.00256	1.15004
C	0.67582	1.05522	0.13302
C	1.33331	0.89658	1.34739
C	2.72024	0.97506	1.13037
C	2.96270	1.11435	-0.24477
C	1.66653	1.58677	-0.85457
H	-1.57769	-1.77851	-0.85886
H	0.70891	-0.97451	-1.66277
H	3.17718	-0.61873	-1.87759
H	3.42625	-1.31442	-0.19569
H	-0.40772	1.12461	-0.00299
H	0.84623	0.66992	2.29737
H	3.48983	0.82636	1.89082
H	3.94047	1.38467	-0.65162
H	1.48969	1.32100	-1.90564
H	1.63969	2.69320	-0.77380
H	-1.71148	-1.48337	1.37331
N	-2.14858	-0.57495	1.23472
C	-2.48397	-0.13298	0.00125
H	-2.45328	-0.01791	2.02239
N	-2.14680	-0.94629	-1.02059
H	-2.36787	-0.62863	-1.95515
S	-3.22465	1.35268	-0.23686

**TS: exo\_CP + TU-A** $E = -933.189032$  $H = -993.174058$  $G = -993.230977$  $N_{\text{imag}} = 1, -457.0710i \text{ cm}^{-1}$ 

C	-2.09395	1.90203	0.55844
C	-0.74598	1.65955	0.22871
C	-0.70293	0.72365	-0.79345
C	-2.91764	1.06543	-0.20815
C	-2.07811	0.59983	-1.37134
H	-2.43984	2.55246	1.36461
H	0.13985	2.06424	0.72446
H	0.21030	0.36763	-1.27515
H	-4.00186	1.18860	-0.27278
H	-2.34026	-0.37490	-1.80579
H	-2.17107	1.36285	-2.17128
C	-1.40759	-1.09303	0.75822
C	-2.75348	-0.73496	0.81527
C	-0.92303	-2.09917	-0.16429
H	-1.65552	-2.41126	-0.95156
O	0.17916	-2.62374	-0.13804
H	-0.71965	-0.78747	1.54901
H	-3.46261	-1.27559	0.17664
H	-3.17282	-0.38378	1.76024
H	1.92841	-1.81392	-1.05123
H	1.43032	-1.63140	1.12354
N	1.93837	-0.74884	1.19519
H	1.91033	-0.19854	2.04380
C	2.39777	-0.14008	0.08191
N	2.36052	-0.89230	-1.04218
H	2.71669	-0.47635	-1.89290
S	2.96574	1.43724	0.07998

**PC: endo\_CP + TU-A** $E = -933.241919$  $H = -933.226980$  $G = -933.286917$  $N_{\text{imag}} = 0$ 

C	1.77608	-0.46386	0.21310
C	2.83883	-0.44815	1.35245
C	0.74514	0.61379	0.35100
O	-0.44714	0.43185	0.31366
H	1.14613	1.64660	0.49206
C	2.66558	-0.29565	-1.07768
C	3.31587	1.07606	-1.01007
C	4.22649	1.03832	-0.02828
C	4.18855	-0.35346	0.57539
C	3.85472	-1.18793	-0.67447
H	-2.04715	-0.90215	0.06513
H	1.24664	-1.42732	0.16502
H	2.77943	-1.37454	1.94368

H	2.70905	0.39844	2.04625
H	2.13443	-0.54448	-2.00547
H	3.01751	1.94502	-1.60040
H	4.82072	1.87188	0.35214
H	5.06482	-0.65352	1.16453
H	3.56405	-2.22681	-0.44519
H	4.65918	-1.17407	-1.42512
H	-2.35209	1.32156	0.30935
N	-3.35642	1.20815	0.20017
C	-3.91780	-0.00534	0.00068
H	-3.97812	2.00453	0.23572
N	-3.04882	-1.04074	-0.03769
H	-3.43561	-1.96223	-0.19009
S	-5.56724	-0.21202	-0.18544

**PC: exo\_CP + TU-A**

**E** = -933.241150

**H** = -933.226153

**G** = -933.286543

**N<sub>imag</sub>** = 0

C	-4.42651	1.08667	0.24288
C	-3.59254	1.41113	-0.75364
C	-2.73021	0.19451	-1.03547
C	-4.13035	-0.34865	0.63623
C	-3.73096	-0.93540	-0.72905
H	-5.12314	1.74877	0.76093
H	-3.45753	2.39079	-1.21600
H	-2.21557	0.17537	-2.00588
H	-4.91275	-0.87222	1.20081
H	-3.27573	-1.93813	-0.65814
H	-4.56432	-0.95668	-1.44695
C	-1.76504	0.09805	0.21029
C	-2.74120	-0.33360	1.34518
C	-0.68271	-0.91177	-0.02542
H	-1.02418	-1.95899	-0.21727
O	0.49740	-0.66272	-0.03446
H	-1.27930	1.06414	0.40697
H	-2.49862	-1.34245	1.72244
H	-2.70544	0.35859	2.19818
H	2.46382	-1.37621	-0.27425
H	2.00193	0.77385	0.23862
N	2.99364	0.99589	0.25593
H	3.31581	1.93148	0.46269
C	3.93634	0.06057	0.00119
N	3.46027	-1.17542	-0.27009
H	4.13856	-1.89950	-0.46454
S	5.57244	0.40817	0.01963

**TS: endo\_CP + TUPh-A**

**E** = -1394.582257

**H** = -1394.558425

**G** = -1394.637765

**N<sub>imag</sub>** = 1, -454.6219i cm<sup>-1</sup>

C	-1.35946	-1.61120	0.71717
C	-2.14800	-2.16219	1.72648
C	-0.68690	-2.42918	-0.27331
O	0.16525	-2.04512	-1.06044
H	-1.00611	-3.50050	-0.29331
C	-3.14481	-1.19185	-0.87297
C	-3.62638	-2.48993	-0.99814
C	-4.24656	-2.85603	0.20880
C	-4.11083	-1.80699	1.13016
C	-3.78904	-0.56975	0.32683
H	0.00283	0.18604	-1.26424
H	-1.05673	-0.56208	0.77225
H	-2.26434	-1.60390	2.65993
H	-2.18099	-3.25001	1.84045
H	-2.64333	-0.62527	-1.65951
H	-3.46279	-3.14750	-1.85359
H	-4.65259	-3.84354	0.43788
H	-4.65326	-1.77149	2.07818
H	-3.21582	0.22302	0.82877
H	-4.75326	-0.13001	-0.00424
H	1.61541	-0.78317	-0.75364
N	2.16823	0.01728	-0.43529
C	1.44031	1.13945	-0.17272
N	0.16414	1.00550	-0.67891
S	1.96717	2.49866	0.62540
C	3.51589	-0.30080	-0.19074
C	4.54398	0.63525	-0.01816
C	3.82803	-1.67055	-0.17308
C	5.85005	0.19039	0.18578
C	5.13535	-2.09880	0.02575
C	6.15809	-1.16833	0.21371
H	4.32033	1.69874	-0.04208
H	3.02579	-2.39972	-0.32254
H	6.64197	0.93153	0.32048
H	5.35389	-3.16947	0.03632
H	7.18593	-1.50051	0.37534
C	-0.97656	1.78802	-0.42307
C	-1.90277	1.95619	-1.46016
C	-1.26273	2.32158	0.84224
C	-3.10399	2.62730	-1.23792
C	-2.45667	3.00877	1.04976
C	-3.38581	3.16176	0.01862
H	-1.66595	1.55975	-2.45187
H	-0.54282	2.19819	1.65084
H	-3.81437	2.74696	-2.05976
H	-2.66488	3.42575	2.03831

H	-4.31940	3.70151	0.19218
<b>TS: exo_CP + TUPh-A</b>			
<b>E</b> = -1394.584275			
<b>H</b> = -1394.560571			
<b>G</b> = -1394.639468			
<b>N<sub>imag</sub></b> = 1, -436.1877i cm <sup>-1</sup>			
C	-4.27604	-1.39970	-1.08854
C	-3.25893	-0.42798	-1.00880
C	-2.03274	-1.05985	-1.14881
C	-3.69745	-2.66981	-1.20836
C	-2.27815	-2.44441	-1.66533
H	-5.34245	-1.20660	-0.95471
H	-3.40254	0.63151	-0.78351
H	-1.06026	-0.56037	-1.14802
H	-4.26706	-3.56660	-1.46528
H	-1.54426	-3.21048	-1.37978
H	-2.29440	-2.38983	-2.77322
C	-2.20806	-2.09247	1.10282
C	-3.18109	-3.03643	0.77426
C	-0.80649	-2.44406	1.10364
H	-0.56830	-3.45860	0.69845
O	0.10625	-1.74156	1.51330
H	-2.47591	-1.14231	1.57221
H	-2.85874	-4.06871	0.59132
H	-4.18394	-2.94409	1.19547
H	1.64410	-0.68090	0.90881
H	-0.03630	0.19731	1.24884
N	0.08571	0.99755	0.62318
C	1.34977	1.15352	0.10264
N	2.13423	0.08934	0.45054
S	1.83418	2.45402	-0.81443
C	3.47637	-0.21683	0.16108
C	4.47197	0.72327	-0.13581
C	3.82252	-1.57678	0.23376
C	5.77669	0.29065	-0.37251
C	5.12858	-1.99278	0.00343
C	6.11706	-1.05913	-0.30972
H	4.22434	1.78059	-0.17940
H	3.04675	-2.30907	0.47805
H	6.54234	1.03526	-0.60466
H	5.37292	-3.05610	0.06594
H	7.14368	-1.38137	-0.49708
C	-1.06722	1.78633	0.49174
C	-1.99375	1.72189	1.54597
C	-1.37962	2.55346	-0.64004
C	-3.20571	2.40192	1.47434
C	-2.59119	3.24205	-0.69390
C	-3.51199	3.17276	0.35201
H	-1.74440	1.13586	2.43576
H	-0.67577	2.60599	-1.46752

H	-3.90838	2.33810	2.30885
H	-2.81869	3.83849	-1.58104
H	-4.45652	3.71827	0.29572

**PC: endo\_CP + TUPh-A**

**E** = -1394.638937

**H** = -1394.615562

**G** = -1394.695157

**N<sub>imag</sub>** = 0

C	1.79932	-1.50893	-0.33852
C	2.58512	-1.95213	-1.59892
C	0.83130	-2.50286	0.22567
O	-0.19072	-2.20115	0.79682
H	1.11570	-3.57987	0.13752
C	2.95469	-1.20324	0.69420
C	3.68249	-2.50891	0.96481
C	4.35888	-2.82443	-0.14769
C	4.07450	-1.74477	-1.17549
C	3.94342	-0.51127	-0.25927
H	-0.05475	0.21291	1.29621
H	1.24844	-0.57549	-0.52175
H	2.32251	-1.31493	-2.45706
H	2.38435	-2.99849	-1.88225
H	2.61258	-0.63565	1.56932
H	3.58522	-3.10995	1.87156
H	4.92347	-3.73982	-0.33811
H	4.77473	-1.67687	-2.01810
H	3.51333	0.37624	-0.75536
H	4.88835	-0.24837	0.24062
H	-1.64564	-0.83628	0.71288
N	-2.21059	-0.03159	0.43767
C	-1.49859	1.09994	0.15958
N	-0.21926	0.99125	0.66142
S	-2.05404	2.43523	-0.65515
C	-3.55778	-0.35618	0.19112
C	-4.59751	0.57932	0.11798
C	-3.85440	-1.72284	0.07059
C	-5.90334	0.13844	-0.09263
C	-5.16261	-2.14890	-0.13178
C	-6.19759	-1.21795	-0.22214
H	-4.38265	1.64007	0.22335
H	-3.04120	-2.45182	0.14055
H	-6.70570	0.87822	-0.15033
H	-5.37149	-3.21756	-0.22357
H	-7.22553	-1.54804	-0.38726
C	0.90558	1.80379	0.41710
C	1.81548	1.99736	1.46357
C	1.18765	2.34387	-0.84530
C	2.99472	2.71025	1.25501
C	2.35945	3.07169	-1.03916
C	3.26994	3.25737	0.00282

H	1.58603	1.58788	2.45167
H	0.48196	2.19613	-1.66216
H	3.69331	2.85001	2.08351
H	2.56513	3.49440	-2.02571
H	4.18702	3.82758	-0.16060

**PC: exo\_CP + TUPh-A**

**E** = -1394.640778

**H** = -1394.617708

**G** = -1394.695413

**N<sub>imag</sub>** = 0

C	-4.56703	-1.21432	-0.70490
C	-3.53579	-0.36294	-0.78810
C	-2.27039	-1.19645	-0.86259
C	-4.00216	-2.62260	-0.71203
C	-2.78365	-2.42829	-1.63167
H	-5.61761	-0.96126	-0.54896
H	-3.55450	0.72690	-0.70944
H	-1.37114	-0.68511	-1.23396
H	-4.70180	-3.42998	-0.96532
H	-2.08903	-3.28635	-1.62816
H	-3.06400	-2.18158	-2.66643
C	-2.11033	-1.80034	0.59474
C	-3.28588	-2.81324	0.66109
C	-0.76393	-2.44082	0.73737
H	-0.62597	-3.42804	0.23194
O	0.16824	-1.94289	1.32450
H	-2.18500	-0.99727	1.34307
H	-2.91573	-3.84906	0.75843
H	-3.95072	-2.61453	1.51354
H	1.72594	-0.74392	0.92511
H	0.02869	0.16373	1.25430
N	0.14670	0.92239	0.58340
C	1.41740	1.06984	0.07342
N	2.21007	0.02742	0.46755
S	1.90334	2.33914	-0.88180
C	3.55717	-0.26904	0.18076
C	4.55025	0.69093	-0.05042
C	3.90742	-1.62828	0.19296
C	5.86165	0.27874	-0.28439
C	5.22101	-2.02520	-0.03209
C	6.20811	-1.07138	-0.28061
H	4.29484	1.74768	-0.04554
H	3.13073	-2.37545	0.38308
H	6.62725	1.03730	-0.46548
H	5.47151	-3.08875	-0.01810
H	7.23999	-1.37850	-0.46443
C	-0.98560	1.74615	0.45431
C	-1.87017	1.78606	1.54329
C	-1.30449	2.46210	-0.70812
C	-3.04624	2.52854	1.47996

C	-2.47650	3.21576	-0.75388
C	-3.35325	3.25706	0.33112
H	-1.61700	1.23815	2.45613
H	-0.63354	2.42846	-1.56363
H	-3.71808	2.54631	2.34144
H	-2.70912	3.77430	-1.66393
H	-4.26801	3.85157	0.28102

**TS: endo\_CP + TUF-A**

*E* = -2741.331283

*H* = -2741.292980

*G* = -2741.410154

*N*<sub>imag</sub> = 1, -449.0877i cm<sup>-1</sup>

C	0.62944	2.23628	0.54856
C	0.62719	3.12454	1.62829
C	0.41229	2.71716	-0.79888
O	0.08097	2.04596	-1.76879
H	0.55646	3.81788	-0.92719
C	3.10101	2.17762	0.27424
C	3.27302	3.52486	-0.01383
C	3.00030	4.27314	1.14524
C	2.58853	3.40491	2.16743
C	3.04330	2.02438	1.76241
H	0.58227	0.05184	-1.78788
H	0.56593	1.15683	0.71907
H	0.34106	2.74229	2.61272
H	0.33766	4.16446	1.44997
H	3.28586	1.35684	-0.42282
H	3.50119	3.93703	-0.99807
H	2.99127	5.36339	1.20706
H	2.50399	3.71435	3.21206
H	2.45052	1.18270	2.14532
H	4.08498	1.89061	2.12287
H	-1.22450	0.61323	-1.35699
N	-1.53842	-0.25739	-0.91728
C	-0.52878	-1.09367	-0.52166
N	0.65194	-0.71716	-1.11860
S	-0.67504	-2.37445	0.52017
C	-2.90100	-0.28546	-0.59382
C	-3.62736	-1.46126	-0.36238
C	-3.56661	0.94607	-0.55416
C	-4.98674	-1.37851	-0.07434
C	-4.92967	1.00249	-0.28236
C	-5.65586	-0.15712	-0.02959
H	-3.13515	-2.43055	-0.41073
H	-3.00862	1.86953	-0.73345
H	-6.72307	-0.11149	0.19268
C	1.96546	-0.99876	-0.72593
C	2.95970	-0.92111	-1.70619
C	2.33887	-1.21504	0.60942
C	4.30479	-1.01771	-1.35385



C	3.68535	-1.30892	0.93737
C	4.68608	-1.21085	-0.03153
H	2.67707	-0.76184	-2.74990
H	1.57687	-1.27463	1.38572
H	5.74094	-1.27412	0.24269
C	-5.74462	-2.64508	0.23681
F	-7.03201	-2.53587	-0.09599
F	-5.24241	-3.69212	-0.41575
F	-5.69840	-2.93011	1.53899
C	-5.62030	2.34126	-0.30639
F	-5.92331	2.71069	-1.55244
F	-6.75527	2.32383	0.38977
F	-4.84248	3.29935	0.20414
C	5.34690	-0.80374	-2.42042
F	4.99253	-1.36810	-3.57361
F	5.51484	0.50170	-2.65873
F	6.52986	-1.29805	-2.06488
C	4.09580	-1.48553	2.37738
F	4.52972	-2.71804	2.62412
F	5.09161	-0.64807	2.69092
F	3.08759	-1.23436	3.21398

**TS: exo\_CP + TUF-A**

**E** = -2741.333035

**H** = -2741.294756

**G** = -2741.412138

**N<sub>imag</sub>** = 1, -432.9042i cm<sup>-1</sup>

C	4.12686	2.52319	-1.98704
C	3.35552	1.38864	-1.66505
C	2.01505	1.71365	-1.79213
C	3.27433	3.60149	-2.26071
C	1.91782	3.00474	-2.54423
H	5.21492	2.58272	-1.91898
H	3.74859	0.43460	-1.30782
H	1.17740	1.03197	-1.62171
H	3.61847	4.53148	-2.72023
H	1.04817	3.63803	-2.32226
H	1.88800	2.75873	-3.62562
C	2.09206	3.18992	0.24380
C	2.80657	4.23052	-0.35174
C	0.65337	3.21202	0.31423
H	0.15817	4.05114	-0.23136
O	-0.04881	2.40917	0.92024
H	2.61318	2.43608	0.83741
H	2.25229	5.11639	-0.68475
H	3.82554	4.43259	-0.01539
H	-1.32892	0.94329	0.75471
H	0.51638	0.62171	1.11237
N	0.57749	-0.34229	0.76531
C	-0.62349	-0.93456	0.44950
N	-1.63414	-0.01742	0.58094

S	-0.79933	-2.51755	-0.01090
C	-3.01564	-0.12389	0.38552
C	-3.74919	-1.31688	0.39937
C	-3.70013	1.08957	0.20237
C	-5.12979	-1.27325	0.20591
C	-5.07684	1.10723	0.02794
C	-5.81248	-0.07676	0.01749
H	-3.25018	-2.26957	0.56159
H	-3.13973	2.02876	0.19572
H	-6.89333	-0.06412	-0.13032
C	1.88813	-0.80731	0.66122
C	2.83626	-0.15692	1.46383
C	2.32847	-1.79186	-0.23857
C	4.19106	-0.44482	1.34180
C	3.68663	-2.08567	-0.31733
C	4.63693	-1.42326	0.46013
H	2.50427	0.59377	2.18676
H	1.61538	-2.31334	-0.87397
H	5.69831	-1.66223	0.37454
C	-5.78680	2.42961	-0.10303
F	-5.00539	3.35277	-0.66889
F	-6.89049	2.32232	-0.84152
F	-6.15377	2.90594	1.08822
C	-5.88346	-2.57933	0.16116
F	-5.41060	-3.44764	1.05422
F	-7.18229	-2.40566	0.40999
F	-5.78391	-3.15445	-1.03826
C	4.16896	-3.06139	-1.36100
F	5.21527	-3.76388	-0.92714
F	3.22038	-3.91674	-1.72638
F	4.56516	-2.41003	-2.46130
C	5.16812	0.39383	2.12077
F	6.38238	-0.14645	2.15155
F	5.28643	1.60916	1.56239
F	4.76787	0.58605	3.37629

**PC: endo\_CP + TUF-A**

**E** = -2741.386038

**H** = -2741.348555

**G** = -2741.463184

**N<sub>imag</sub>** = 0

C	-2.04398	2.60318	-0.75085
C	-2.26364	3.10670	-2.20789
C	-0.78392	3.10526	-0.12198
O	0.00375	2.41304	0.48560
H	-0.58500	4.19775	-0.22560
C	-3.34362	3.11944	-0.01603
C	-3.31195	4.63782	-0.04631
C	-3.52089	5.01561	-1.31439
C	-3.68078	3.75620	-2.14501
C	-4.37245	2.83386	-1.12503

H	-0.49947	0.50117	0.67113
H	-2.03003	1.50281	-0.71528
H	-2.23957	2.25913	-2.90946
H	-1.49728	3.83009	-2.53112
H	-3.51444	2.65296	0.96352
H	-3.07328	5.27990	0.80431
H	-3.48205	6.03124	-1.71420
H	-4.15895	3.87577	-3.12584
H	-4.40029	1.77386	-1.42947
H	-5.38161	3.17248	-0.84743
H	1.33803	0.84459	0.48318
N	1.68952	-0.10338	0.35092
C	0.72079	-1.07078	0.25541
N	-0.51510	-0.49460	0.44133
S	0.97564	-2.68354	-0.01802
C	3.08355	-0.13822	0.23020
C	3.87683	-1.29169	0.15047
C	3.71321	1.11683	0.19985
C	5.25959	-1.16192	0.03543
C	5.09329	1.21811	0.08979
C	5.88855	0.07886	-0.00177
H	3.41904	-2.27790	0.16826
H	3.10819	2.02716	0.25358
H	6.97167	0.15814	-0.10766
C	-1.80560	-1.03070	0.42117
C	-2.78166	-0.28925	1.10792
C	-2.19784	-2.18271	-0.27280
C	-4.11486	-0.67313	1.08264
C	-3.54045	-2.55963	-0.26619
C	-4.51297	-1.82301	0.40306
H	-2.48371	0.59464	1.67847
H	-1.46210	-2.77786	-0.80987
H	-5.55723	-2.14227	0.40217
C	5.72464	2.58573	0.11529
F	6.92544	2.58620	-0.45908
F	4.96729	3.48439	-0.51866
F	5.88182	3.02299	1.36662
C	6.10613	-2.41077	0.00507
F	5.44742	-3.44503	-0.51190
F	7.21339	-2.22873	-0.71627
F	6.49217	-2.76081	1.23427
C	-5.15287	0.17908	1.76376
F	-6.05048	-0.55818	2.41031
F	-4.60412	1.02313	2.64261
F	-5.82250	0.92403	0.87555
C	-3.96286	-3.76311	-1.07329
F	-5.02137	-4.36493	-0.52955
F	-4.30828	-3.40747	-2.31392
F	-2.98638	-4.65960	-1.17575

**PC: exo\_CP + TUF-A**

**E** = -2741.388007

**H** = -2741.350284

**G** = -2741.467823

**N<sub>imag</sub>** = 0

C	4.47262	2.54562	-1.57662
C	3.60630	1.52768	-1.49005
C	2.21425	2.12717	-1.43676
C	3.66995	3.83361	-1.58368
C	2.40537	3.36790	-2.32939
H	5.56226	2.48515	-1.54992
H	3.83251	0.46361	-1.39129
H	1.37951	1.44741	-1.66066
H	4.18228	4.72470	-1.96888
H	1.57455	4.09345	-2.27993
H	2.60148	3.09709	-3.37728
C	2.11841	2.81103	-0.00615
C	3.09724	4.00544	-0.14291
C	0.69595	3.19707	0.25715
H	0.33508	4.14659	-0.20640
O	-0.08189	2.52029	0.89267
H	2.42904	2.09693	0.76853
H	2.56851	4.97037	-0.05273
H	3.88152	3.97597	0.62667
H	-1.37686	0.96798	0.81882
H	0.49149	0.59230	1.14915
N	0.53400	-0.33438	0.72121
C	-0.67882	-0.89045	0.38461
N	-1.68253	0.01875	0.60367
S	-0.87889	-2.43005	-0.19163
C	-3.06616	-0.08011	0.40096
C	-3.79832	-1.27228	0.45450
C	-3.74811	1.12764	0.18922
C	-5.17988	-1.23460	0.27139
C	-5.12651	1.14068	0.01954
C	-5.86226	-0.04204	0.05396
H	-3.29777	-2.21863	0.64764
H	-3.18937	2.06759	0.16664
H	-6.94626	-0.03095	-0.06911
C	1.83501	-0.82938	0.58770
C	2.79074	-0.31424	1.47174
C	2.25179	-1.72225	-0.41273
C	4.13695	-0.63894	1.33529
C	3.59729	-2.06374	-0.50313
C	4.55848	-1.53009	0.35684
H	2.47701	0.35953	2.27454
H	1.53051	-2.13731	-1.11398
H	5.61155	-1.79846	0.25756
C	-5.82040	2.44898	-0.25906
F	-7.08240	2.43552	0.16599
F	-5.19867	3.46910	0.33641

F	-5.84600	2.71718	-1.56632
C	-5.93787	-2.53911	0.28880
F	-5.45261	-3.37294	1.20807
F	-7.23160	-2.35090	0.55169
F	-5.85863	-3.16065	-0.88816
C	4.06079	-2.93872	-1.64053
F	5.06328	-3.73342	-1.26770
F	3.08333	-3.70254	-2.11677
F	4.51187	-2.18900	-2.65335
C	5.12306	0.05724	2.23496
F	6.34429	-0.45772	2.13482
F	5.20644	1.35743	1.92140
F	4.75122	-0.00543	3.51362