

Electronic Supporting Information of the article entitled

**“Efficient Energy Decomposition Analysis of Field-Induced Reactivity and Selectivity”**

by

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## Construction of the FDB-EDA method

The FDB method follows as central equation the Eq. 3 on the manuscript, which is

$$\Delta E(F) = \Delta E(0) - \Delta\mu F - \frac{1}{2}\Delta\alpha F^2 - \frac{1}{6}\Delta\beta F^3 + \dots \quad \text{Eq. 1}$$

where  $\Delta\mu$  corresponds to the change on dipole moment,  $\Delta\alpha$  change in polarizability, and  $\Delta\beta$  change in the first hyperpolarizability from the reactants to the TS (or from any chemical species to another). These are tensorial quantities. The dipole moment, polarizability and 1<sup>st</sup> hyperpolarizability are, respectively, the negative of the first, second and third derivatives of the energy with respect to the electric field. Therefore, in a more general sense, we can rewrite the FDB equation for any type of difference as the Taylor expansion

$$\Delta E(F) = \Delta E(0) + \frac{1}{1!} \frac{\partial E}{\partial F} \Big|_{F=0} F + \frac{1}{2!} \frac{\partial^2 E}{\partial F^2} \Big|_{F=0} F^2 + \frac{1}{3!} \frac{\partial^3 E}{\partial F^3} \Big|_{F=0} F^3 + \dots \quad \text{Eq. 2}$$

On the other hand, the activation strain model / energy decomposition analysis (ASM/EDA) method, stems from the seminal equations

$$\begin{aligned} \Delta E(\xi) &= \Delta E_{Strain}(\xi) + \Delta E_{int}(\xi) \\ \Delta E_{int}(\xi) &= \Delta V_{elstat}(\xi) + \Delta E_{Pauli}(\xi) + \Delta E_{oi}(\xi) + \Delta E_{disp}(\xi) \end{aligned} \quad \text{Eq. 3}$$

This way, we were able to plug Eq. 3 and 4 into Eq. 2 and get an expression for the dependence of each term on the ASM/EDA with respect to the EF. At this point it is important to note that we considered only Grimme-type dispersion corrections to the energies, therefore upon derivative the constant added to the energy to account for dispersion vanishes, and this term does not need to be expanded in a Taylor series. The final equations (at a fixed value of  $\zeta$ ) for this work are Eq. 4 to Eq. 8

$$\Delta E_{Strain}(F) = \Delta E_{Strain R1}(F) + \Delta E_{Strain R1}(F) \quad \text{Eq. 4}$$

$$\Delta E_{Strain Ri}(F) = \Delta E_{Strain Ri}(0) - \Delta\mu F - \frac{1}{2}\Delta\alpha F^2 - \frac{1}{6}\Delta\beta F^3, i = 1,2 \quad \text{Eq. 5}$$

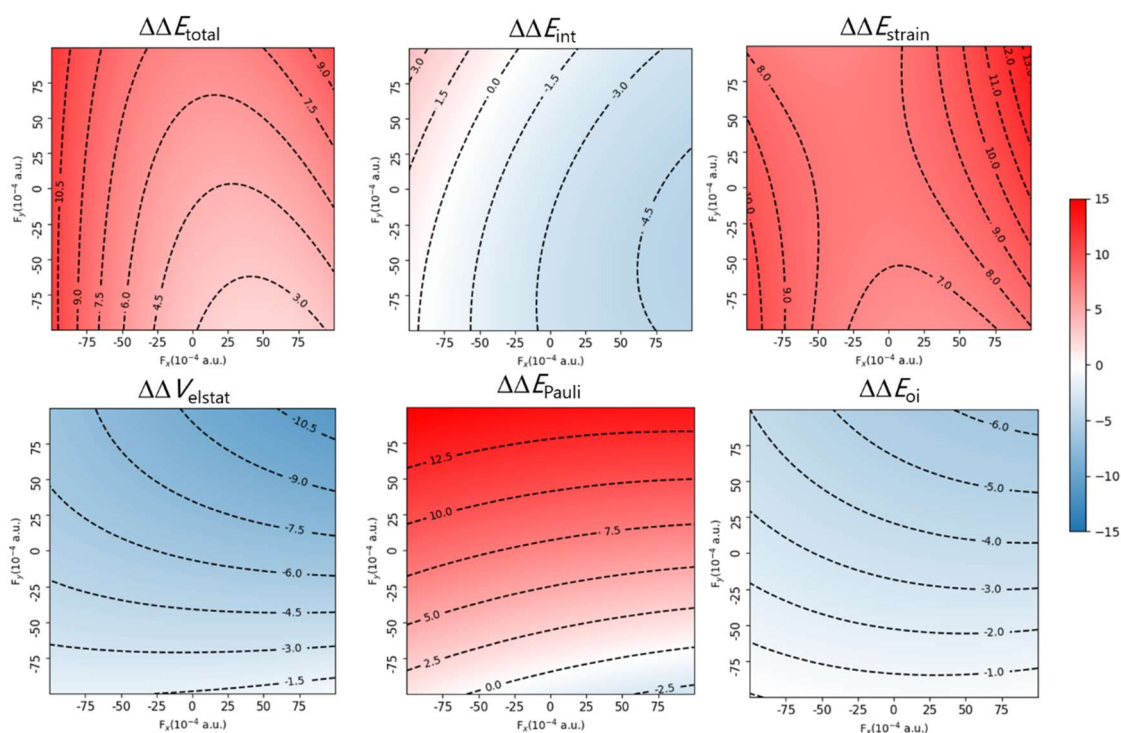
$$\Delta V_{elstat}(F) = \Delta V_{elstat}(0) + \frac{\partial V_{elstat}}{\partial F} \Big|_{F=0} F + \frac{1}{2} \frac{\partial^2 V_{elstat}}{\partial F^2} \Big|_{F=0} F^2 + \frac{1}{6} \frac{\partial^3 V_{elstat}}{\partial F^3} \Big|_{F=0} F^3 \quad \text{Eq. 6}$$

$$\Delta E_{Pauli}(F) = \Delta E_{Pauli}(0) + \frac{\partial E_{Pauli}}{\partial F} \Big|_{F=0} F + \frac{1}{2} \frac{\partial^2 E_{Pauli}}{\partial F^2} \Big|_{F=0} F^2 + \frac{1}{6} \frac{\partial^3 E_{Pauli}}{\partial F^3} \Big|_{F=0} F^3 \quad \text{Eq. 7}$$

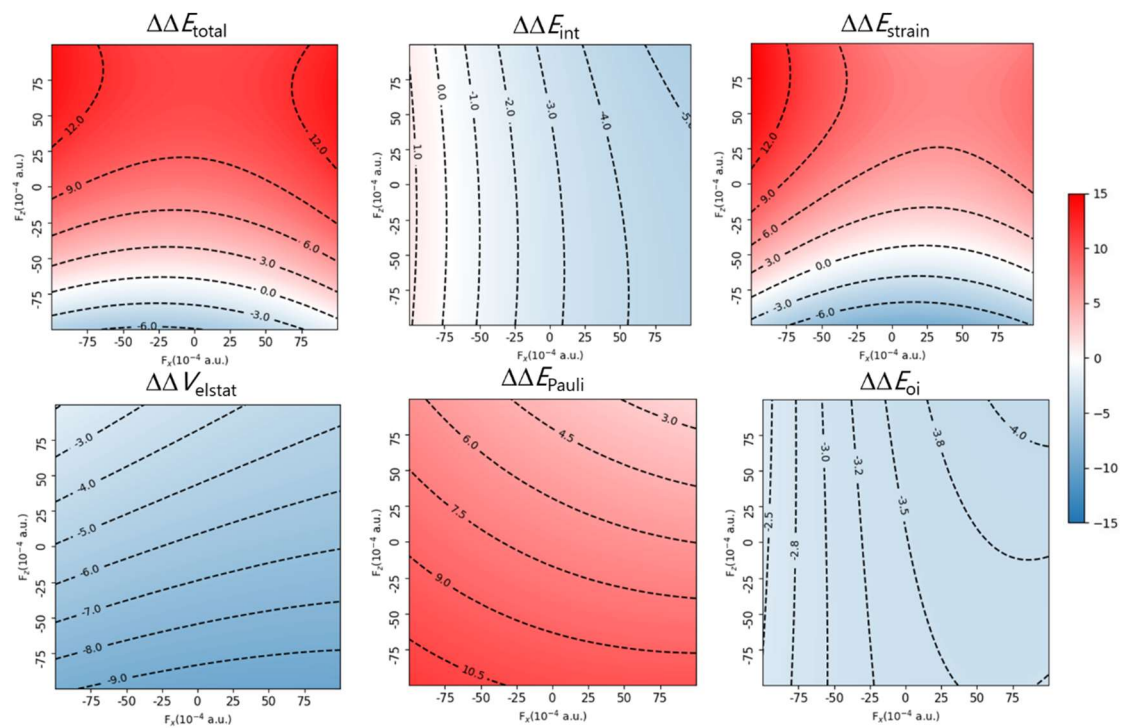
$$\Delta E_{oi}(F) = \Delta E_{oi}(0) + \frac{\partial E_{oi}}{\partial F} \Big|_{F=0} F + \frac{1}{2} \frac{\partial^2 E_{oi}}{\partial F^2} \Big|_{F=0} F^2 + \frac{1}{6} \frac{\partial^3 E_{oi}}{\partial F^3} \Big|_{F=0} F^3 \quad \text{Eq. 8}$$

In which the derivatives in Eq. 5 can be computed analytically, and the derivatives in Eq. 6 to 8 are computed numerically by using the finite-field and the Romberg-Rutishauser method (see Besalú-Sala, et al., *PCCP*, 2020, 22, 11871). Our experience gained during this research showed us that it suffices to use a total of eight fields in the FF calculation (i.e.  $0, \pm 10^{-4}, \pm 2 \cdot 10^{-4}, \pm 4 \cdot 10^{-4}, \pm 8 \cdot 10^{-4}$ ). Furthermore, all derivatives from Eq. 6 to 8 for a given field are obtained in a single calculation, therefore the numerical derivatives were computed very efficiently.

## Natural product FDB-EDA 2D plots for the XY and XZ vector fields



**S11.** FDB-ASM/EDA analysis of the **cmc** versus **mgIF** selectivity in the ( $F_x, F_y$ ) plane. The red (blue) color indicates the favoring of **mgIF** (**cmc**) selectivity. Energy differences in kcal/mol.



**S12.** FDB-ASM/EDA analysis of the **cmc** versus **mgIF** selectivity in the ( $F_x, F_z$ ) plane. The red (blue) color indicates the favoring of **mgIF** (**cmc**) selectivity. Energy differences in kcal/mol.

## Ratio index to account for the nuclear relaxation contribution in the polarizability

**SI3.** R indicator computed as the ratio of change in nuclear and electronic polarizability for each axis, and for the isotropic case.

System	R indicator ( $\Delta\alpha_i^{nr}/\Delta\alpha_i^{el}$ )			
	$i = X$ axis	$i = Y$ axis	$i = Z$ axis	isotropic
DA <i>endo</i>	0.35	0.04	0.06	0.63
DA <i>exo</i>	0.28	0.17	0.08	0.43
Menshutkin	1.53	8.25	0.31	0.74
C—Cl activ.	0.07	0.34	0.1	0.70
Natural <i>endo</i>	0.05	2.23	0.78	2.55
Natural <i>exo</i>	0.19	0.36	2.61	2.37

## Cartesian coordinates of the studied systems at $F = 0$

### *Diels-Alder reaction*

#### *Endo reactant complex*

C	-2.098476000	-1.184208000	0.014899000
C	0.881550000	-0.676219000	1.321078000
C	0.881550000	0.676219000	1.321078000
C	-2.098476000	1.184208000	0.014898000
C	-1.523409000	-0.732852000	-1.142252000
C	-1.523409000	0.732852000	-1.142252000
H	-1.115782000	-1.359051000	-1.949116000
H	-1.115783000	1.359050000	-1.949116000
C	-2.545933000	0.000000000	0.831408000
H	-2.130421000	0.000000000	1.865803000
H	-3.654433000	0.000000000	0.968910000
H	-2.254058000	-2.233396000	0.303572000
H	-2.254058000	2.233396000	0.303571000
O	1.809744000	0.000000000	-0.713315000
O	1.707525000	-2.258237000	-0.360259000
O	1.707524000	2.258237000	-0.360259000
C	1.482514000	-1.141857000	0.035283000
C	1.482514000	1.141858000	0.035284000
H	0.547823000	-1.378807000	2.095252000
H	0.547823000	1.378807000	2.095252000

#### *Endo TS*

C	1.638994000	-1.162326000	-0.019236000
C	-0.285769000	-0.702352000	-1.123586000
C	-0.285769000	0.702352000	-1.123586000
C	1.638994000	1.162326000	-0.019237000
C	1.286756000	-0.706583000	1.268087000
C	1.286756000	0.706583000	1.268087000
H	0.948473000	-1.344356000	2.097230000
H	0.948472000	1.344356000	2.097229000
C	2.283559000	0.000000000	-0.740022000
H	2.212613000	0.000000000	-1.844563000

H	3.371500000	0.000001000	-0.480300000
H	1.811671000	-2.217768000	-0.277951000
H	1.811670000	2.217768000	-0.277951000
O	-1.761336000	0.000000000	0.543272000
O	-1.684134000	-2.254613000	0.162876000
O	-1.684134000	2.254613000	0.162876000
C	-1.286190000	-1.151044000	-0.118517000
C	-1.286190000	1.151044000	-0.118517000
H	-0.007208000	-1.365084000	-1.953365000
H	-0.007208000	1.365084000	-1.953365000

*Exo reactant complex*

C	-1.934238000	1.184788000	-0.501773000
C	0.871373000	0.676232000	1.278111000
C	0.871319000	-0.676207000	1.278143000
C	-1.934293000	-1.184673000	-0.501857000
C	-2.513042000	-0.732952000	0.653317000
C	-2.513050000	0.733015000	0.653349000
H	-2.920910000	-1.359475000	1.460789000
H	-2.920903000	1.359500000	1.460857000
C	-1.551772000	0.000078000	-1.348440000
H	-0.481696000	0.000084000	-1.660433000
H	-2.117224000	0.000115000	-2.312170000
H	0.469418000	1.375936000	2.021088000
H	-1.791406000	-2.232118000	-0.802707000
H	-1.791296000	2.232249000	-0.802545000
O	1.954755000	-0.000076000	-0.680566000
O	1.804333000	-2.259177000	-0.344874000
O	1.804599000	2.259053000	-0.344930000
C	1.566344000	-1.142985000	0.042642000
C	1.566560000	1.142896000	0.042661000
H	0.469315000	-1.375845000	2.021155000

*Exo TS*

C	1.459637000	1.162851000	0.460608000
C	-0.251011000	0.702634000	-0.986624000
C	-0.251010000	-0.702634000	-0.986623000
C	1.459637000	-1.162851000	0.460607000
C	2.494729000	-0.706767000	-0.382524000
C	2.494729000	0.706767000	-0.382524000
H	3.121605000	-1.344826000	-1.022733000
H	3.121605000	1.344826000	-1.022733000
C	1.057122000	0.000000000	1.332622000
H	0.025414000	0.000000000	1.731478000
H	1.736586000	0.000000000	2.221123000
H	0.135406000	1.364996000	-1.769831000
H	1.274202000	-2.215385000	0.722273000
H	1.274203000	2.215385000	0.722273000
O	-1.986200000	0.000000000	0.420756000
O	-1.812922000	-2.256917000	0.090729000

O	-1.812922000	2.256917000	0.090729000
C	-1.392589000	-1.150139000	-0.143581000
C	-1.392589000	1.150139000	-0.143581000
H	0.135406000	-1.364996000	-1.769831000

**Menshutkin reaction**

*Reactant complex*

C	0.010472000	-0.308706000	-3.179762000
N	0.079278000	-0.048562000	-0.381658000
C	-1.170678000	-0.293589000	-2.435268000
C	-1.082666000	-0.161079000	-1.045935000
C	1.206529000	-0.065549000	-1.111471000
C	1.226603000	-0.191513000	-2.503871000
H	-0.016377000	-0.410025000	-4.266650000
H	-2.145485000	-0.382390000	-2.918183000
H	-1.993165000	-0.142389000	-0.437782000
H	2.142928000	0.025063000	-0.551640000
H	2.176402000	-0.197479000	-3.041536000
C	-0.056580000	0.022305000	3.163356000
H	0.194701000	-0.954018000	2.735819000
H	-1.038915000	0.349173000	2.809157000
H	0.705782000	0.762241000	2.898674000
Cl	-0.107643000	-0.126715000	4.957953000

*Transition state*

C	0.010472000	-0.308706000	-3.179762000
N	0.079278000	-0.048562000	-0.381658000
C	-1.170678000	-0.293589000	-2.435268000
C	-1.082666000	-0.161079000	-1.045935000
C	1.206529000	-0.065549000	-1.111471000
C	1.226603000	-0.191513000	-2.503871000
H	-0.016377000	-0.410025000	-4.266650000
H	-2.145485000	-0.382390000	-2.918183000
H	-1.993165000	-0.142389000	-0.437782000
H	2.142928000	0.025063000	-0.551640000
H	2.176402000	-0.197479000	-3.041536000
C	-0.056580000	0.022305000	3.163356000
H	0.194701000	-0.954018000	2.735819000
H	-1.038915000	0.349173000	2.809157000
H	0.705782000	0.762241000	2.898674000
Cl	-0.107643000	-0.126715000	4.957953000

## **C—Cl activation**

### *Catalysts*

Pd	0.404964000	3.670032000	0.122024000
P	-1.509835000	3.154017000	1.243720000
H	-1.575087000	2.021861000	2.119721000
H	-2.102427000	4.077793000	2.165077000
H	-2.723903000	2.858070000	0.542384000
P	2.319652000	4.186239000	-0.999798000
H	2.975774000	5.445668000	-0.808060000
H	3.502040000	3.389531000	-0.856186000
H	2.352622000	4.228190000	-2.431781000

### *Substrate*

C	0.125103000	-0.244186000	-0.031843000
Cl	1.751501000	0.446104000	0.061011000
C	-0.508280000	-0.659101000	1.142222000
C	-1.794580000	-1.203850000	1.059910000
C	-2.434342000	-1.330235000	-0.177985000
C	-1.782709000	-0.908575000	-1.342138000
C	-0.496327000	-0.361666000	-1.277539000
H	-0.001646000	-0.556443000	2.102464000
H	-2.295815000	-1.530293000	1.973611000
H	-3.437697000	-1.756391000	-0.235329000
H	-2.274654000	-1.003377000	-2.312526000
H	0.019546000	-0.030187000	-2.179359000

### *TS*

C	0.005400000	0.069805000	0.092557000
Cl	2.082013000	0.064106000	0.253211000
Pd	0.666540000	2.128781000	0.068033000
C	-0.669263000	-0.481097000	1.197923000
C	-1.871556000	-1.155596000	0.984331000
C	-2.381467000	-1.329205000	-0.313781000
C	-1.665446000	-0.830981000	-1.406276000
C	-0.448406000	-0.160450000	-1.218401000
H	-0.265680000	-0.355871000	2.203378000
H	-2.414333000	-1.557183000	1.843929000
H	-3.315694000	-1.871883000	-0.468515000
H	-2.033806000	-0.986985000	-2.423295000
H	0.141350000	0.177974000	-2.071660000
P	-1.137834000	3.064401000	1.240940000
H	-1.578797000	2.498717000	2.483771000
H	-1.186147000	4.429608000	1.680105000
H	-2.435942000	3.073850000	0.634335000
P	1.954232000	3.875273000	-0.976089000
H	1.992557000	5.212449000	-0.461403000
H	3.374223000	3.755950000	-1.132445000
H	1.701959000	4.271538000	-2.331049000

### **Natural product**

### *Endo reactant complex*

C	-0.074510967	2.726564753	2.898426000
O	-2.056085669	3.901766441	2.477392000
C	-1.466850551	2.737283899	2.831752000
O	1.951620159	1.548791993	3.330414000
C	-2.195224549	1.583089214	3.132803000
O	1.387031629	-3.563220898	3.648716000
C	-1.508463775	0.427698324	3.458783000
O	3.241028399	-5.219727215	3.164610000
C	-0.107336160	0.367765468	3.519891000
O	7.692675661	-3.962603431	3.891489000
C	0.599088313	1.561865996	3.248905000
O	2.616846353	-2.735594596	0.705040000
C	0.514296606	-0.931598510	3.720838000
O	3.371722760	1.978763157	0.905512000
C	1.819602885	-1.249332159	3.826937000
O	12.507603857	0.202030933	2.838315999
C	2.229938332	-2.660388967	3.837242000
O	7.897800197	-0.061164807	1.613119000
C	3.654320521	-2.992106306	3.967204000
C	4.620609527	-2.059270156	4.380299000
C	4.101603923	-4.274317293	3.558318000
C	5.962571011	-2.368264991	4.392208000
C	5.467324328	-4.588897807	3.508710000
C	6.380624725	-3.628171380	3.935255000
C	5.688427741	-0.858894713	1.063902000
C	5.219145756	0.458161569	1.058034000
C	4.789659035	-1.913497388	0.919481000
C	3.865497719	0.699413097	0.879460000
C	3.435473495	-1.652897943	0.755433000
C	2.935210337	-0.337170710	0.676909000
C	1.522865723	0.000000000	0.493052000
C	0.534673832	-0.733786384	-0.045246000
C	-0.866575053	-0.267688575	-0.090890000
C	-1.190964502	1.001474959	-0.356916000
C	-1.902728373	-1.320861707	0.205700000
C	5.923155740	-5.890013396	2.889095000
C	5.915643300	-5.761339697	1.384880000
C	6.965301015	-5.738706989	0.554791000
C	6.770419637	-5.564297708	-0.929756000
C	8.403178702	-5.879155899	0.985962000
C	9.146618676	-1.946881907	1.701398000
C	9.136776239	-0.554235025	1.863081000
C	10.240782204	0.195257692	2.237033000
C	11.415347185	-0.516294613	2.467274000
C	11.461994021	-1.917644180	2.326557000
C	10.339076841	-2.636642985	1.946583000
C	7.804404037	-2.297744569	1.319055000
C	7.099676785	-1.139352125	1.296266000
H	-3.012616977	3.792586718	2.469923000
H	2.345975708	2.103713192	2.639692000
H	2.338479932	-4.828743459	3.286880000



H	8.234177458	-3.178570421	4.034400000
H	1.735221196	-2.477663517	1.005903000
H	4.105305574	2.602195517	0.932088000
H	13.255203700	-0.389650757	2.967737999
H	0.477395507	3.635421851	2.683414000
H	-3.279648970	1.587272695	3.086498000
H	-2.072084795	-0.479336890	3.657585000
H	-0.182936840	-1.768849222	3.739649000
H	2.576477691	-0.481685669	3.811288000
H	4.312135272	-1.075905948	4.715370000
H	6.696616020	-1.639413683	4.721119000
H	5.908198818	1.282327041	1.207874000
H	5.110289184	-2.946510685	1.000238000
H	1.240271995	0.981507350	0.855754000
H	0.719553081	-1.723623104	-0.458767000
H	6.910834177	-6.156160379	3.266208000
H	5.232321535	-6.686348351	3.182759000
H	4.921333203	-5.641758435	0.954583000
H	10.205089901	1.271343927	2.353019000
H	12.395257860	-2.438582820	2.521097000
H	10.388733045	-3.715528577	1.846245000
H	7.408669460	-3.286366902	1.136768000
H	-0.436029940	1.743423616	-0.598159000
H	-2.224351531	1.333851128	-0.340617000
H	7.259439454	-4.644935790	-1.275654000
H	5.712804261	-5.511583939	-1.199896000
H	7.228224397	-6.391981111	-1.484740000
H	-2.915771921	-0.916032267	0.150251000
H	-1.748835452	-1.735246669	1.208570000
H	-1.824270261	-2.155681779	-0.500215000
H	8.542368576	-5.722883654	2.056957000
H	8.792396918	-6.869640606	0.721567000
H	9.024438461	-5.148236780	0.454520000

Endo TS

C	-0.846702066	5.414670328	0.833686244
O	-2.420096956	7.107016420	1.232382762
C	-2.062477279	5.808329851	1.392000947
O	0.750828044	3.681855238	0.401641613
C	-2.851938714	4.881378904	2.070968203
O	-0.088996114	-0.685282993	3.046281997
C	-2.402445927	3.571141266	2.185796522
O	1.307759828	-2.057892402	4.602530712
C	-1.183192163	3.145888437	1.658309500
O	5.787042356	-0.910252432	5.354131418
C	-0.417243324	4.098582754	0.961791916
O	2.228776606	-2.482443254	1.594500513
C	-0.761801845	1.729449843	1.836960568
O	3.705647831	1.504086074	-0.602733484
C	0.546727900	1.419106597	2.244265720
O	12.594631400	-0.682674596	2.189394369
C	0.801249996	0.218456200	2.975188505
O	7.926543780	-0.693146606	1.168730485
C	2.099471142	0.003888621	3.653634162
C	3.194729881	0.868198809	3.499556761
C	2.295885515	-1.170907750	4.425856345
C	4.421735601	0.598250328	4.067536155
C	3.536658140	-1.468166153	5.007260515
C	4.590233840	-0.581418355	4.805178972
C	5.537782091	-1.075858163	1.230547408
C	5.294880752	0.073471601	0.474228007
C	4.488362092	-1.930657506	1.559020515
C	3.994045905	0.378433126	0.099230684
C	3.190342787	-1.615556402	1.183247310
C	2.902394086	-0.453905096	0.430147716
C	1.556690162	0.000000000	0.115864444
C	0.444215058	-0.793762134	-0.019779657
C	-0.876049656	-0.287606105	-0.056297876
C	-1.124855564	1.081368240	-0.039786911
C	-2.011593582	-1.254374269	0.139202797
C	3.754303736	-2.789441839	5.707915489
C	4.143437991	-3.844563344	4.702952046
C	5.288497076	-4.533390397	4.629265799
C	5.515595485	-5.534476806	3.524929073
C	6.434699199	-4.399146826	5.599834862
C	8.703097848	-1.931047010	2.899684069
C	9.038430606	-1.050615747	1.861606826
C	10.326870978	-0.615048760	1.593931515
C	11.324447445	-1.099908708	2.435153224
C	11.025606271	-1.981152566	3.493717186
C	9.725517545	-2.398797550	3.731389437
C	7.277787616	-2.106290413	2.807830267
C	6.868557388	-1.347557225	1.759591584
H	-3.269588214	7.261054045	1.657835190

H	1.159380505	4.406772155	-0.081930641
H	0.544607008	-1.706050502	4.062509318
H	6.469117266	-0.321215652	5.015677846
H	1.397995885	-2.013652798	1.759121424
H	4.510928819	2.014233859	-0.733989607
H	13.194807947	-1.082128252	2.826545106
H	-0.249178449	6.145600101	0.297634235
H	-3.803086334	5.176854057	2.502810722
H	-3.018389956	2.848707168	2.713576398
H	-1.525462135	1.103257858	2.293746262
H	1.320825625	2.163111887	2.131622848
H	3.096857936	1.764857155	2.899678940
H	5.259525193	1.272147942	3.917862476
H	6.110642469	0.741962378	0.219778537
H	4.648600841	-2.812062893	2.168334678
H	1.478503547	1.058614986	-0.102484635
H	0.548890822	-1.873742049	0.018485844
H	4.509496057	-2.678628033	6.487382753
H	2.820278898	-3.087045195	6.194330831
H	3.388406916	-4.022437430	3.937270620
H	10.558156170	0.063934295	0.782629232
H	11.831064096	-2.335402514	4.130886841
H	9.511677384	-3.076198555	4.551418365
H	6.630976677	-2.671195497	3.463353406
H	-0.398725242	1.757539420	-0.478021427
H	-2.156940350	1.406639116	-0.134011547
H	6.368082028	-5.233091791	2.902421013
H	4.639783587	-5.635030909	2.878582974
H	5.758275428	-6.522866861	3.933511926
H	-2.942703505	-0.884595920	-0.295802217
H	-2.171246602	-1.401505618	1.214198592
H	-1.783714678	-2.231669174	-0.294531122
H	6.381662863	-3.486808911	6.195597531
H	6.470292494	-5.259292767	6.279228806
H	7.388009716	-4.391654649	5.057952676

*Exo reactant complex*

C	-2.236347958	1.089407702	4.186624255
O	-2.899561841	3.386541576	4.455928187
C	-1.959925263	2.455412567	4.172753890
O	-1.453574823	-1.157499690	3.896720863
C	-0.678600578	2.913963601	3.848693555
O	2.860285852	-2.260136408	2.306943110
C	0.310708955	1.993013208	3.555676155
O	5.137253954	-3.156822724	1.784956864
C	0.077686039	0.610223841	3.578557249
O	8.934360615	-0.630193669	2.845050426
C	-1.226116939	0.176536169	3.886287228
O	2.528415019	2.544546857	0.998291100
C	1.107712469	-0.365956336	3.253768233
O	3.645230114	-1.646432639	-1.004898771
C	2.436511711	-0.160801716	3.270508333
O	11.938255330	3.484920473	2.819215653
C	3.344972249	-1.217597717	2.801334388
O	7.546689747	2.259758823	1.207185126
C	4.800081914	-1.048930620	2.883419188
C	5.409924811	0.083341953	3.449637715
C	5.648084440	-2.046637799	2.326001715
C	6.777990762	0.235908616	3.465393623
C	7.042632078	-1.903491849	2.318608194
C	7.586381366	-0.749936160	2.878729290
C	5.756419266	1.063006830	0.120599897
C	5.341631985	-0.148021530	-0.427360448
C	4.812414486	1.980552091	0.585272449
C	3.983980773	-0.442895042	-0.478850092
C	3.458570314	1.672175861	0.526510978
C	3.005702817	0.445433721	0.006029611
C	1.605895979	0.000000000	0.084668943
C	0.508421617	0.743264553	-0.105622291
C	-0.876007669	0.268074030	0.086372322
C	-1.238309927	-1.011338583	-0.065418974
C	-1.868945581	1.339679356	0.457509138
C	7.926258594	-2.951941201	1.678213696
C	8.440523603	-2.535997313	0.319775138
C	7.966698111	-2.902395564	-0.876772404
C	8.608169034	-2.400145859	-2.145924811
C	6.778731149	-3.802138751	-1.094268118
C	9.418585436	1.391784294	0.277775688
C	8.901658885	2.266656967	1.239746480
C	9.680729781	2.999142896	2.127796730
C	11.059476366	2.831815564	2.014390545
C	11.614932342	1.965050346	1.052406706
C	10.808045839	1.247898434	0.185821403
C	8.270230230	0.811830701	-0.363911748
C	7.181904420	1.342231621	0.244716853
H	-3.234547340	0.734440802	4.430579281

H	-0.488516462	3.980232375	3.816073040
H	1.288589694	2.346651189	3.248104335
H	-3.739249651	2.958994881	4.652722085
H	-2.383269815	-1.332724738	4.072299893
H	0.761580234	-1.352796955	2.958939400
H	2.846989194	0.790774787	3.583206291
H	4.803375915	0.863761553	3.892182379
H	7.230942575	1.122333889	3.897301232
H	4.149578486	-3.059810096	1.855377401
H	9.192781983	0.256977400	3.119409177
H	6.059074012	-0.895732891	-0.746338154
H	5.137373855	2.922433365	1.015498625
H	2.977437459	3.320400704	1.348441516
H	2.687526211	-1.710216739	-1.083153913
H	1.476022032	-1.033701613	0.411162013
H	0.621602880	1.794356509	-0.359118864
H	-0.533148852	-1.775696712	-0.377832112
H	-2.261008133	-1.329819485	0.111768831
H	-1.549928214	1.863552671	1.364445368
H	-2.865418510	0.925327112	0.626787154
H	-1.938013225	2.089479695	-0.339418922
H	8.786874482	-3.129718201	2.331818676
H	7.369891216	-3.887858311	1.617014221
H	9.281863695	-1.845287425	0.347054181
H	9.495160380	-1.792072482	-1.946139296
H	7.899546544	-1.799068928	-2.731173968
H	8.908592220	-3.236344274	-2.788553224
H	6.293069875	-4.098454061	-0.164729659
H	7.071288864	-4.700356953	-1.651596815
H	6.025593963	-3.284453070	-1.701136948
H	9.236223054	3.663391704	2.861417467
H	12.694509441	1.873010815	1.012505170
H	11.249708364	0.577140954	-0.543600037
H	8.258203571	0.079172414	-1.154783664
H	11.459191630	4.055321925	3.428396516

Exo TS

C	-3.505213291	0.362540763	3.850230804
O	-3.857676636	2.608042399	4.650510917
C	-3.068906813	1.668677682	4.069099436
O	-3.049440821	-1.835604042	2.996419038
C	-1.784904684	2.051171714	3.681992271
O	1.341084802	-3.146192797	1.258814911
C	-0.950559377	1.116078139	3.086912782
O	3.675060930	-4.074776403	1.014288037
C	-1.348227160	-0.205993202	2.864271783
O	7.223597247	-2.087120044	3.360130070
C	-2.650811528	-0.560989361	3.248450909
O	2.330071948	2.191269457	1.580717008
C	-0.483154563	-1.193727614	2.175549367
O	3.681998214	-1.383030555	-1.280989611
C	0.913638250	-1.059239442	2.232419393
O	11.129000826	1.616137507	5.433337541
C	1.778293759	-2.172250100	1.930735516
O	7.159434208	1.324076951	2.684725109
C	3.190774042	-2.151265868	2.362220531
C	3.688528719	-1.201030688	3.265547057
C	4.101513415	-3.108921156	1.839690869
C	5.017959668	-1.169929382	3.627498572
C	5.465514671	-3.072533821	2.165325567
C	5.902077237	-2.093357378	3.056826426
C	5.613534035	0.706855162	0.939763310
C	5.274378428	-0.259579703	-0.002672934
C	4.640109482	1.578899511	1.435594772
C	3.950046189	-0.396488035	-0.390256704
C	3.315326637	1.419278591	1.051524083
C	2.926642560	0.406327838	0.152482278
C	1.539430290	0.000000000	-0.034544704
C	0.424780851	0.800128021	-0.135161473
C	-0.880833102	0.271359371	-0.075693476
C	-1.083378039	-1.071487392	0.245399654
C	-2.060969964	1.206259964	-0.113195444
C	6.450616706	-4.040224958	1.545475598
C	7.386659421	-3.372894544	0.562637419
C	7.241454306	-3.300429901	-0.765236507
C	8.264570581	-2.590327481	-1.615634199
C	6.075113586	-3.866171147	-1.530683503
C	9.136173023	0.472479410	1.982779087
C	8.466744130	1.150121807	3.007574473
C	9.064395751	1.565269441	4.191222785
C	10.418351358	1.271381364	4.327746464
C	11.126198983	0.591958374	3.315653738
C	10.498655378	0.192548113	2.149163917
C	8.140885462	0.225746354	0.974761596
C	6.979435765	0.741892668	1.447484135
H	-4.508478565	0.063558151	4.144825615

H	-1.461317131	3.072594513	3.845398581
H	0.035022053	1.432486149	2.758555149
H	-4.712504058	2.225183188	4.871168974
H	-3.952407135	-1.964053913	3.302433180
H	-0.849359493	-2.215804820	2.195328702
H	1.348151635	-0.169288236	2.663200010
H	3.017893515	-0.474252836	3.707861036
H	5.386569130	-0.418507026	4.318365984
H	2.690710056	-3.942259363	0.939232019
H	7.428266111	-1.325041352	3.912312948
H	6.003891232	-0.973140987	-0.367201486
H	4.907781359	2.333441901	2.168077399
H	2.706563909	2.775365105	2.246777279
H	2.791226087	-1.285653771	-1.631712184
H	1.412016675	-1.054283440	-0.264933383
H	0.544550569	1.878777511	-0.123307904
H	-0.369754269	-1.835421969	-0.049616122
H	-2.109623022	-1.425448602	0.311958055
H	-1.756449728	2.248616840	0.008776346
H	-2.773035293	0.962773030	0.681608123
H	-2.591679941	1.117819430	-1.067961203
H	7.052479814	-4.489738746	2.343008216
H	5.893809494	-4.848471791	1.070050287
H	8.249059126	-2.882609652	1.010717081
H	9.122485600	-2.251320366	-1.027944706
H	7.820009882	-1.719195261	-2.115318656
H	8.636709965	-3.246950398	-2.411120154
H	5.319826292	-4.316084223	-0.885313980
H	6.415914961	-4.612268463	-2.258972890
H	5.581001007	-3.067072825	-2.095365241
H	8.504119738	2.087654261	4.959249616
H	12.178733501	0.389037737	3.478689668
H	11.055775774	-0.332307034	1.380480239
H	8.271495251	-0.281320355	0.031161152
H	10.558615901	2.076696394	6.056678492