

# Supplementary Material (ESI) for Organic and Biomolecular Chemistry  
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**A Theozyme for the Antibody Aldolases. Characterization of  
the Transition-State Analogue.**

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**Supplementary Material**

MP2/6-31G\*\* energies, imaginary frequencies and cartesian coordinates.

**8**

EUMP2 = -0.15337846718502D+03

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.222756050000
C	1.240926649643	0.000000000000	2.069476181755
H	-0.952507958694	-0.000020150768	1.783857313489
H	1.244699882216	-0.877602759725	2.716820852913
H	1.245291587985	0.878336900302	2.715848376855
H	2.122105163630	-0.000513267386	1.434663990176

**9**

EUMP2 = -0.21188168212238D+03

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.345315000000
N	1.187856294290	0.000000000000	2.098686888682
C	-1.266514717064	-0.098895874261	2.147307302094
C	1.253615411161	0.863204063696	3.272960163788
H	-0.919059634559	-0.116562730643	-0.551933869272
H	0.917747669900	0.083377013867	-0.566269786955
H	1.989436362372	0.146201784132	1.497251735738
H	2.250335597143	0.783369679968	3.701852367461
H	0.544989875904	0.523117579284	4.024631910315
H	1.050713599575	1.919133595781	3.060407073291
H	-1.202857399924	-0.922703652100	2.858744978126
H	-2.114478818408	-0.269420443332	1.488667191029
H	-1.458649600013	0.813890562181	2.712278484096

**12**

EUMP2 = -0.26877389974828D+03

C	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.228219690000
C	1.230441505550	0.000000000000	-0.854048213582
H	1.829490733419	0.007322360946	2.000285914212
O	2.774940946404	0.205848892011	2.079764971636
C	2.869729728278	1.567381339197	2.468727368255
H	-0.962127675532	0.000557811077	-0.539280463822
H	1.205516778538	0.864451631822	-1.518925341029
H	1.227524762822	-0.888419082961	-1.487007106564
H	2.121116113470	0.022033769317	-0.233027254415
H	3.927145186092	1.817596427592	2.503587409938
H	2.380652464758	2.239227521159	1.757144218732
H	2.441099625195	1.745962946934	3.458284983635

**MC-1**

EUMP2 = -0.36530084818064D+03

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.225417280000
C	3.194609497674	0.000000000000	1.318577024668
C	3.081260022334	1.287596238272	0.930700922646
N	2.539044156006	1.652743352425	-0.307066073852
C	3.617019194645	2.416508706692	1.765493807026
C	1.716817374022	2.854714710507	-0.381021952892
C	-0.079698344162	-1.236639182945	2.070360252607
H	0.046170858064	0.950872341420	1.783799250999
H	3.732209249678	-0.257921707132	2.217714219089
H	2.824590161410	-0.807580761143	0.701850846931
H	-0.981278486201	-1.203493978331	2.683679073902
H	0.777763930786	-1.266599520065	2.741723115422
H	-0.093447307232	-2.119134621126	1.437152525531
H	2.049091062809	0.872220084585	-0.727663751342
H	1.353868629278	2.953373479093	-1.401378798757
H	2.315737704253	3.734139943870	-0.155098542660
H	0.849657699406	2.839891283084	0.287953448144
H	4.306093857316	3.027430159944	1.181644602766
H	4.145918267413	2.024818942269	2.630863961326
H	2.819427119423	3.069052760907	2.122868991079

**MC-2**

EUMP2 = -0.36527375474512D+03

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.226060380000
C	3.385282907628	0.000000000000	1.819210310288
C	3.028947084500	0.504300439144	0.618916144052
N	2.934765437807	-0.244835219576	-0.553633431963
C	2.752717109849	1.966208827517	0.407975727490
C	2.968762925705	-1.690262123042	-0.443576243917
C	-0.235471596448	-1.217424262903	2.070058219126
H	0.173673307303	0.935502644451	1.784057791017
H	3.531211310768	0.664207149751	2.656838155307
H	3.600246691196	-1.046174830428	1.971422290699
H	2.158957522311	0.070958314929	-1.122524933103
H	3.454308650705	2.382886974572	-0.314455196411
H	2.838459799438	2.519042863432	1.340652844465
H	1.745076736956	2.103555730464	0.011432045731
H	2.792764575730	-2.119887207009	-1.426668523372
H	2.222290627342	-2.084642357964	0.255124668276
H	3.954168517454	-2.005736733660	-0.103274834365
H	-1.081249783605	-1.047385817694	2.737450963432
H	0.644884999725	-1.391524102711	2.688341380598
H	-0.426124643944	-2.078991952716	1.436315740912

**MC-3**

EUMP2 = -0.48066242459486D+03

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.350152880000
N	1.180185338638	0.000000000000	2.098498663008
C	1.227423931628	0.755109854674	3.344836210246
C	-1.274391278493	-0.087034697713	2.141903311156
C	1.058339014656	2.923773705355	0.312232251684
O	2.139948161883	2.564621534757	0.774899347913
C	0.812303651178	3.196928403302	-1.139374896443
H	3.687500902240	2.897240744386	-0.413906904495
O	4.319422027830	3.158225583539	-1.100326168719
C	4.163981556115	4.548348505516	-1.324947105804
H	1.979155523944	0.221475812399	1.517211406752
H	-0.918258469890	-0.137492691437	-0.549520166850
H	0.923258677551	0.035967460548	-0.562639565402
H	0.201805491736	3.073284543152	0.987086753625
H	-1.235640786784	-0.928440262793	2.834205875583
H	-2.121663204171	-0.223871511017	1.474579283755
H	-1.447643674622	0.815411620070	2.729588558733
H	2.227450829116	0.657070886952	3.760766562433
H	0.527229860367	0.335468705826	4.063499831507
H	1.013910783176	1.821636909875	3.221984402834
H	0.577816278912	4.254394342939	-1.273353320777
H	-0.051407406091	2.622048955661	-1.469779343301
H	1.691394613209	2.934242917379	-1.720669599057
H	4.911932092621	4.838235093081	-2.058933704758
H	3.179749666199	4.807015048053	-1.726578670798
H	4.328928268399	5.139369921099	-0.419232623270

**TS-1**

EUMP2 = -0.36524554356963D+03

1 imaginary frequencies -530.3636

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.287184160000
C	1.850344951593	0.000000000000	1.883158536529
C	2.371361046640	1.042445729191	1.103807168529
N	2.315310171574	0.860268822060	-0.220357160053
C	2.732242725565	2.379076972248	1.679864746529
C	2.482746084086	1.963249248309	-1.155832767657
C	-0.485893856373	-1.255253573554	1.996896658128
H	-0.335470967029	0.921322451913	1.799718692583
H	1.893041737963	0.110762066896	2.958999491642
H	2.030239257200	-1.005027378576	1.527190833488
H	-1.565699288901	-1.328384907758	1.858960693460
H	-0.273370785728	-1.236993426313	3.065767851604
H	-0.028166758965	-2.133057023960	1.544517576445
H	1.467954813377	0.234346079937	-0.425355840760
H	2.522607421527	1.553989533232	-2.161449083470
H	3.415998122979	2.485259814887	-0.958567370682
H	1.656608026610	2.675174507852	-1.100662326035

H	3.735219704648	2.677070187601	1.371852747455
H	2.707743131913	2.339913750440	2.765374388242
H	2.040722385153	3.151789752169	1.337541034710

**TS-2**

EUMP2 = -0.36522050825330D+03

1 imaginary frequencies -432.4589

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.340168580000
C	1.543526896304	0.000000000000	1.834296122453
C	2.118750151762	0.805050939969	0.750900677802
N	2.745984599002	0.273292842340	-0.259885655247
C	1.933417241821	2.282286804422	0.766074472767
C	2.683425289961	-1.154069069921	-0.592841600874
C	-0.719903500053	-1.182329510408	1.995040465327
H	-0.407824671067	0.928345409884	1.820370855829
H	1.705317483998	0.467832113947	2.806238506135
H	1.923883017221	-1.018593044337	1.841978374185
H	2.989922092978	0.900929251765	-1.015117554606
H	2.577202070225	2.788205599419	0.048221608452
H	2.100032403244	2.688963708380	1.759913609951
H	0.890732307794	2.428421352371	0.481536596319
H	3.151904704025	-1.288907299402	-1.562462950989
H	1.620626525645	-1.396080260310	-0.614010686135
H	3.221216489675	-1.736855983323	0.150309019460
H	-1.764704430961	-1.156727630523	1.687084686486
H	-0.670609932638	-1.165006398585	3.087309982543
H	-0.285550999037	-2.114445053348	1.630285064901

**TS-3**

EUMP2 = -0.48064404260747D+03

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.396676550000
N	1.192547331082	0.000000000000	2.005919188282
C	1.373768691289	0.392303753161	3.395670001008
C	-1.245726324301	0.219529502606	2.199906976675
C	0.826690871907	1.763111825176	-0.330157514739
O	1.908502388926	1.804401025093	0.362106440638
C	0.951667288884	1.691916162443	-1.842373416563
H	2.898360429820	3.229399610611	-0.251140550002
O	3.264233772242	4.026358819115	-0.675311552100
C	2.292690058541	5.040114500300	-0.514331940589
H	1.923947449921	0.357685544879	1.363764976569
H	-0.956781960606	-0.057763627671	-0.501374954234
H	0.806232620020	-0.524523201155	-0.493318488114
H	-0.022923125067	2.388760076971	-0.000945791347
H	-1.362526202211	-0.556605940802	2.956920742080
H	-2.117205594893	0.197210681978	1.551977193244
H	-1.212574777206	1.181509143366	2.715055123336
H	2.389357171195	0.143701881118	3.690065924550
H	0.685940949860	-0.157065793002	4.032573970291

H	1.219522656019	1.463814842874	3.534126035216
H	1.375455534820	2.638401342644	-2.180513931247
H	-0.007619909048	1.530706427241	-2.333103751614
H	1.647336607888	0.902716321391	-2.120847675095
H	2.668208207098	5.934380836819	-1.008052436639
H	1.330349368343	4.783132962744	-0.971130223506
H	2.108817470029	5.284488536813	0.537185247142

## 10

EUMP2 = -0.36530084818064D+03

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.421001430000
C	1.422594716162	0.000000000000	1.977770782010
C	2.256364506079	1.195188104019	1.584261285698
N	1.820150410191	1.968115089508	0.649573975501
C	3.584819065202	1.366331214235	2.282957217342
C	2.643709450112	3.110760916924	0.262683815920
C	-0.773041255634	-1.226965586611	1.863386625287
H	-0.503663871108	0.900221857230	1.799986509730
H	1.389034636813	-0.057652380578	3.070814198550
H	1.938089730392	-0.905848601148	1.637700814850
H	-1.778125979442	-1.196063028658	1.447724584279
H	-0.841317020546	-1.279207368319	2.949902532745
H	-0.278336942651	-2.125456725357	1.496060525875
H	0.485569747916	0.810941320202	-0.222697013436
H	2.233513962527	3.543375820440	-0.645803617179
H	3.683735730820	2.833824073286	0.077245838223
H	2.631096871462	3.877917481152	1.040156508718
H	3.678770310547	0.678781108388	3.119668466726
H	3.702920030783	2.384950604776	2.653244154451
H	4.406421729345	1.175015204887	1.589621523855

## 11

EUMP2 = -0.36521891473122D+03

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.324524240000
C	1.448330714152	0.000000000000	1.889320606883
C	2.112885654824	1.157181348921	1.310695550241
N	2.616927508488	1.123926830400	0.109529609843
C	2.056791937833	2.469560209558	2.018487466106
C	2.683371187361	-0.051091526481	-0.776178617253
C	-0.686174856448	-1.234196158587	1.950475575953
H	-0.483415517984	0.893925504959	1.815506442530
H	1.462745665030	0.069781834029	2.977930280323
H	1.906966855591	-0.936118937223	1.575637978800
H	2.972550368331	1.997357244172	-0.259031630071
H	2.510153974628	3.277283993246	1.446225941707
H	2.549726061855	2.391844760009	2.986012767278
H	1.006661214923	2.702925641931	2.198069651824
H	2.766348363801	0.323139957694	-1.791709832824
H	1.730352500893	-0.570363982561	-0.652893136678

H	3.567907024620	-0.637632151351	-0.528508879965
H	-1.719302375736	-1.246011855984	1.607998552876
H	-0.672391989211	-1.239975992449	3.044470589799
H	-0.196253674730	-2.133593854405	1.574846370592

### 13

EUMP2 = -0.48069898935972D+03

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.510139150000
N	1.133381231776	0.000000000000	2.123769160716
C	1.136525901931	0.010770244832	3.584366646959
C	-1.349046783782	-0.003770105892	2.188296260977
C	1.339916746982	0.351372225108	-0.636391763074
O	2.337465258513	-0.600382782352	-0.249516399407
C	1.281191221212	0.341316519761	-2.150807631676
H	3.922019085103	-0.062680430346	-1.068121517356
O	4.651373561782	0.376149727299	-1.540966044487
C	4.712617697226	1.700385002027	-1.047932996753
H	2.339597800436	-0.535465977657	0.727111405064
H	-0.764284210432	0.702824878894	-0.347588367626
H	-0.310831328364	-0.991481661606	-0.347939834279
H	1.628747345808	1.350650236553	-0.286219920479
H	-1.372123810653	-0.701791192795	3.024040443764
H	-2.131375808753	-0.277001176688	1.483976011583
H	-1.579494042263	0.989445406893	2.579635442685
H	2.131486332015	0.283508587524	3.925434221965
H	0.904529811592	-0.982834303643	3.973552874347
H	0.418640009882	0.718676592280	4.002244940110
H	2.269915454546	0.549212962462	-2.554128022762
H	0.577830206578	1.088521149217	-2.517397415863
H	0.966799029560	-0.641512419802	-2.500274215047
H	5.550357247809	2.192414522882	-1.537762142391
H	3.807462719827	2.276361225127	-1.269528829394
H	4.881436182924	1.739927543964	0.033208636672

### TSA-1

EUMP2 = -0.36411794773018D+03

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.254432040000
C	1.199460599642	0.000000000000	2.048173910910
C	2.462731704300	0.000422838987	1.494116487591
N	2.649316931678	0.000093676190	0.157298478086
C	3.689560623420	0.000546679618	2.360511834380
C	3.932373103922	0.002199258794	-0.508900511052
C	-1.321724380967	0.000015570088	1.995831642825
H	-1.399264062448	-0.879614564078	2.635407229178
H	-2.135568748530	0.000026870311	1.276277868260
H	-1.399245635270	0.879647003904	2.635408118739
H	1.114051166228	-0.000128886695	3.124802592396
H	1.779161744470	0.000407190969	-0.374561661152
H	3.408862488851	0.002182283549	3.409839560817

H	4.303558178260	-0.879959026047	2.167716554616
H	4.305108538610	0.879448671667	2.165376668144
H	3.751456906815	-0.000131942200	-1.580175006716
H	4.520623508319	0.889070130285	-0.266886175097
H	4.524790068274	-0.880984604015	-0.263802374868

**TSA-2**

EUMP2 = -0.72369849273318D+03

O	0.000000000000	0.000000000000	0.000000000000
S	0.000000000000	0.000000000000	1.532823300000
C	1.666708972260	0.000000000000	2.107289478634
C	2.701418484291	-0.509544088163	1.383200263214
N	2.506996179186	-1.168271581958	0.191063369821
C	4.106187302204	-0.425890290643	1.910447745527
C	3.592673406159	-1.353624382044	-0.757036261993
C	-0.415562104726	-1.695743225467	2.009559378123
H	1.836987892864	0.520840055917	3.037297488037
H	1.607256576624	-0.924916155706	-0.231593393590
H	4.115832042494	0.065273345890	2.879714559275
H	4.532224896778	-1.423155262112	2.024092379633
H	4.750042757066	0.135347345287	1.232845166791
H	3.210540336148	-1.937089333138	-1.591052651431
H	3.992400120521	-0.414250773743	-1.151196575963
H	4.408398089117	-1.914204172705	-0.305500325566
H	-0.382736956483	-1.778228781161	3.094088224905
H	-1.419127996191	-1.909218150849	1.647067314117
H	0.300925068389	-2.374711939460	1.552564751122