

S1

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

Luis R. Domingo, Mónica Oliva and Juan Andrés

Cartesian coordinates with the computed total energies

4

E(RB+HF-LYP) = -194.101057937 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.348875060000
C	1.387210975527	0.000000000000	1.835142154830
C	2.229319699084	-0.000895517703	0.781420309254
C	1.424163924147	0.000459228780	-0.492262405064
H	3.312945976010	-0.001599276514	0.812348424506
H	1.668678356506	-0.000022619072	2.883347718756
H	-0.874319421324	0.000406465972	1.991951472024
H	-0.865795530927	0.000575766755	-0.652348935986
H	1.644042212971	0.879194211589	-1.118375438621
H	1.643957143463	-0.876946293814	-1.120235325769

11

E(RB+HF-LYP) = -381.637063094 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.479600000000
C	1.119630742631	0.000000000000	2.258827701096
N	-1.220081996498	0.054774132361	2.078839414797
C	-1.378388141880	0.082890271966	3.393040558849
C	-0.267374826789	0.074433250728	4.229808568803
C	0.983129229067	0.036411708014	3.661284507238
N	0.930617659206	-0.468345011947	-0.714337428781
C	0.983820328682	-0.446061269744	-2.201419185375
H	-0.845443322566	0.430745150806	-0.511422147924
H	1.051501009720	-1.467409483537	-2.545272630313
H	1.862575989278	0.109786558535	-2.493346711942
H	0.091908098153	0.027232832626	-2.579573262036
H	2.100842130304	0.003234584398	1.823378507543
H	-2.387151786078	0.113401453826	3.759212564777
H	-0.406532366063	0.104723037367	5.293517151117
H	1.863182175761	0.040144754670	4.277760885844
H	1.716789583525	-0.912493232828	-0.269240862516
H	-2.053487080656	0.057793454378	1.517287040230

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12-en

E(RB+HF-LYP) = -575.794903212 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.521100000000
C	1.284042702428	0.000000000000	1.934664188900
C	2.156279561820	0.009598732934	0.692313704759
C	0.517075457157	-1.397746625853	-0.488687938794
C	1.275448838226	0.852514271783	-0.263539821419
C	-0.345930234861	-2.560444837827	-0.069271327991
C	-0.431249961352	-3.023651500907	1.241686006002
N	-1.143308711302	-3.162574311942	-1.034991692129
C	-1.982561498396	-4.194338326289	-0.731413995232
C	-2.059940128620	-4.678472803527	0.579077132374
C	-1.282462919322	-4.088479039602	1.570477146270
N	1.977912035200	-1.434404999006	0.077611746417
C	3.007522415542	-1.735561169500	-0.971105310594
H	3.222612608266	0.298354816002	0.818311198970
H	1.685157403582	0.055981272537	2.949752117921
H	-0.909856645543	0.051877079940	2.122346116943
H	-0.935149879005	0.333105921558	-0.487164026608
H	0.592580332639	-1.360062148512	-1.612123052161
H	1.172640792646	1.903293515679	0.070236715147
H	1.611334332535	0.902991703084	-1.315252711728
H	2.844006849860	-2.724062361374	-1.430183150881
H	4.022163400720	-1.736947825699	-0.532458632296
H	3.005812851920	-0.980680981542	-1.777650454539
H	0.143903036669	-2.532464802382	2.044383374915
H	-2.599770971030	-4.636523425886	-1.539474787861
H	-2.740050735921	-5.515874166256	0.809855726563
H	-1.337951801490	-4.447517294319	2.611399220973
H	2.045325335703	-2.122407740630	0.808187761923
H	-1.105368026236	-2.824478342459	-1.969274363399

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12-ex

E(RB+HF-LYP) = -575.793019107 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.523100000000
C	1.286164276004	0.000000000000	1.928690205913
C	2.158414335486	-0.031069208828	0.685478422669
C	0.501229616636	1.434649553400	-0.395463804078
C	1.264243081199	-0.864935708327	-0.263484614543
C	0.262817214085	1.757514842793	-1.849177373256
C	0.834619722571	1.033079379054	-2.892844652693
N	-0.625375420116	2.778648280824	-2.162668978068
C	-0.928941132686	3.092232627393	-3.455168245278
C	-0.344940299083	2.381684103847	-4.509997175503
C	0.538876427024	1.344848161802	-4.227449508842
N	2.016304356905	1.386301219973	0.003992816402
C	2.433481228678	2.515895631530	0.896730696767
H	3.218407505948	-0.336442796880	0.825060156052
H	1.690467725243	-0.036846549997	2.943495631936
H	-0.911090915103	-0.022783015749	2.124828085277
H	-0.939067739377	-0.314404509800	-0.490005709231
H	-0.008305020540	2.192251238114	0.263201346691
H	2.580933556681	1.401479314905	-0.827627037975
H	1.597583921536	-0.917363242571	-1.319901311598
H	1.148842118982	-1.914656312164	0.069505718349
H	2.271136599189	3.495045293523	0.418553898192
H	3.507207581026	2.438706774389	1.146087069467
H	1.878732681066	2.502958978712	1.852761999568
H	1.501551247763	0.178466790897	-2.671574173710
H	-1.056836867413	3.284882920724	-1.423615530161
H	-1.646817447918	3.914230173689	-3.651155668118
H	-0.598425646069	2.647670452325	-5.550317958381
H	0.998980387802	0.764199387190	-5.044075559013

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13

E(RB+HF-LYP) = -381.046669526 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.478957970000
C	1.192854568568	0.000000000000	2.216856984838
N	-1.217070649021	0.000077592376	2.052169579936
C	-1.272277557986	0.000141492034	3.387925722191
C	-0.143586106389	0.000149031469	4.209103813881
C	1.115616678074	0.000060591302	3.604854917010
N	1.074912745697	0.000616778655	-0.681773650448
C	0.961710149278	0.000691225063	-2.126749099756
H	-1.004551060276	-0.000552073434	-0.449662769392
H	1.480254130840	-0.879045778109	-2.527725961681
H	1.478160437035	0.881828594022	-2.527467906867
H	-0.077447745278	-0.000367276967	-2.494117258009
H	2.139685379905	-0.000063849249	1.687964980167
H	-2.270179104598	0.000245884599	3.823838474169
H	-0.251488546543	0.000259209333	5.289724376901
H	2.019768936174	0.000096245419	4.207925314535

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MC1

E(RB+HF-LYP) = -575.769679737 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.360027390000
C	1.382480859088	0.000000000000	1.833142349914
C	2.232058015734	0.029640514790	0.761994163209
C	2.970500920997	4.031361259743	1.145760461329
C	1.414931777942	-0.016677556604	-0.503840282502
C	4.357526376060	3.733033909595	1.477147711916
C	4.816646822076	2.603381725221	2.154123384068
N	5.284576367994	4.672664263710	1.098638015025
C	6.603066395034	4.558848539856	1.341671430259
C	7.087636836671	3.437093492258	2.009684877992
C	6.185136286452	2.452389739656	2.414566965103
N	1.976088241694	3.214834190576	1.289211053049
C	0.573377050236	3.550224757000	0.999587838009
H	3.309744001470	-0.096169216024	0.788767343434
H	1.667010664276	-0.090473701311	2.878238286764
H	-0.870667211313	-0.038776795389	2.004871503431
H	-0.870637673505	-0.032587151201	-0.645289926467
H	2.735017472555	5.020700078633	0.754084659331
H	1.638315771319	0.775912237287	-1.232995443915
H	1.617586700169	-0.958464511294	-1.040042462116
H	0.019204201909	3.556566623631	1.943860769392
H	0.156913803918	2.762076290901	0.363436915659
H	0.510103245970	4.526305015224	0.516736135825
H	4.115194462944	1.851414134255	2.497148501063
H	7.234465303273	5.369984173120	0.994344083529
H	8.150916809343	3.351907175318	2.207799997767
H	6.538215695833	1.571959151480	2.943414905585
H	4.970666546003	5.507189403826	0.603188421369
H	2.126281339612	2.210780983183	1.527841981999

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TS1-en

E(RB+HF-LYP) = -575.767090924 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.407100000000
C	1.330028629318	0.000000000000	1.895016729776
C	2.187858538189	0.128871879092	0.821227157176
C	0.086904310066	-2.107674946516	-0.389919223327
C	1.409245311268	0.356753531040	-0.428362954467
C	-1.154488990436	-2.630531450707	0.244655239990
C	-1.229463667831	-3.356969746006	1.429934549213
N	-2.322132297941	-2.410616248549	-0.427464109753
C	-3.534043061310	-2.847575182752	-0.010095170504
C	-3.633485381424	-3.563703685159	1.170278004814
C	-2.464678623678	-3.821963816650	1.893268341907
N	1.301181323404	-2.543847832780	-0.015001943342
C	2.384423172589	-2.885453405682	-0.958840366344
H	3.271900448435	0.155220483716	0.875110158803
H	1.619787001180	-0.066836222423	2.937639693895
H	-0.885977494747	-0.030781548560	2.034043390642
H	-0.871549120243	0.288347005751	-0.581715029270
H	0.002339290716	-1.944121279136	-1.462429454229
H	1.422912232623	1.439983677363	-0.646701396703
H	1.809348984096	-0.122403670393	-1.325688445749
H	2.363765505609	-3.959275406217	-1.173182643932
H	3.348954184565	-2.623309541728	-0.522027864772
H	2.246341793372	-2.336369555686	-1.892013827383
H	-0.331860580589	-3.580056972084	1.995455191926
H	-4.379142790032	-2.610751955649	-0.647337955962
H	-4.602087233431	-3.917758505164	1.505831110480
H	-2.510150923518	-4.393587201085	2.815652310932
H	1.430237703393	-2.886057913883	0.930957015164
H	-2.291100817330	-1.907371168730	-1.312752128902

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TS1-ex

E(RB+HF-LYP) = -575.767770772 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.408400000000
C	1.330521417913	0.000000000000	1.898743508650
C	2.190324488816	-0.117367918040	0.828043414749
C	0.002702629967	2.118320200584	-0.359435924177
C	1.414325597593	-0.340366803509	-0.426008430740
C	-0.403555549007	2.111167054256	-1.790781282403
C	0.444688080132	2.194304707197	-2.891595397632
N	-1.744745535164	2.048184459686	-2.041085604805
C	-2.288494660817	2.058062389194	-3.280412387724
C	-1.463015150092	2.132836715730	-4.389765089737
C	-0.081838139792	2.205389757211	-4.188143135595
N	1.198809588066	2.601357459595	0.015847002178
C	1.402002817957	3.347848046933	1.271316796455
H	3.274370525193	-0.135817721270	0.883099347926
H	1.615566115107	0.068661794416	2.942442645657
H	-0.888473998321	0.020770182944	2.033605657211
H	-0.869117244231	-0.315515359520	-0.570394805101
H	-0.801756571542	2.360905046487	0.329073825678
H	1.944660386960	2.674544037577	-0.666303912643
H	1.813884463113	0.160361766903	-1.312957370509
H	1.442588113730	-1.418391787929	-0.662863181900
H	1.157872124321	4.405850022890	1.125878585194
H	2.443243557884	3.253940735995	1.580404451448
H	0.758576182905	2.932414012660	2.049559906590
H	1.518289553180	2.262959698413	-2.756851161201
H	-2.389276857570	2.016530998480	-1.252713311512
H	-3.370868652205	2.013765165090	-3.333904991920
H	-1.896135974852	2.143040086232	-5.383969541743
H	0.590051077275	2.276567167750	-5.038502980729

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TS2-en

E(RHF) = -572.038033994 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.498635050000
C	1.262597276882	0.000000000000	1.974040841264
C	2.128336869787	0.101700069827	0.848689673898
C	0.183831461638	-1.470008625929	-0.562335926201
C	1.370139796550	0.649552537082	-0.301093071012
C	-1.025751155875	-2.371981848318	-0.325805111086
C	-1.305637478507	-3.051442077337	0.835013439163
N	-1.893765529936	-2.502489636964	-1.347529107082
C	-3.006283122883	-3.247568996897	-1.300906974063
C	-3.319684137041	-3.939356284835	-0.159190165569
C	-2.453600054303	-3.838394444863	0.919793822472
N	1.450110999564	-1.976354120958	-0.076262673743
C	2.258370270454	-2.744701716375	-1.038498259046
H	3.195045736928	-0.025268060994	0.875941881750
H	1.579379380454	-0.104813218476	2.993283341745
H	-0.888412124772	-0.062601624538	2.100244506704
H	-0.858413393397	0.484383081249	-0.444709696466
H	0.282525392194	-1.350496434800	-1.633600091138
H	1.310688281672	1.728908475341	-0.185139446342
H	1.797315969270	0.428615445796	-1.267358499821
H	1.746224523030	-3.633135135639	-1.392516014811
H	3.176176047235	-3.043838408838	-0.553890772174
H	2.505947227073	-2.117777530004	-1.884473271256
H	-0.646374633455	-2.987225603309	1.678689763660
H	-3.606892602665	-3.266031995423	-2.189465710873
H	-4.207475028717	-4.539573885108	-0.119382183148
H	-2.665188988468	-4.370451243090	1.829011525703
H	1.356462323229	-2.495474521551	0.774046543905
H	-1.701515276981	-2.027359928698	-2.209112010055

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TS2-ex

E(RB+HF-LYP) = -575.771898731 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.483330650000
C	1.284697531789	0.000000000000	2.014761890241
C	2.184944847405	-0.036140536630	0.956433848256
C	-0.733019080338	1.312309770874	-0.609957667707
C	1.495935881830	-0.144320860820	-0.350007360810
C	-0.901744845471	1.174108560512	-2.116835641565
C	0.053199533839	1.515629476691	-3.067350256083
N	-2.093962998360	0.699737385280	-2.573326592530
C	-2.399764889998	0.539217151093	-3.883309610413
C	-1.462571451998	0.867813010272	-4.847506330808
C	-0.224871567565	1.366287156978	-4.432000636293
N	-0.014180703992	2.508218434664	-0.270343187565
C	-0.383895883517	3.139753421024	1.000160223641
H	3.267769581776	-0.021931810290	1.062009974425
H	1.538416602404	0.020496028244	3.068727790512
H	-0.909582519412	-0.017587582620	2.080893610167
H	-0.600426344799	-0.854131781080	-0.347064700131
H	-1.742709442273	1.291978281631	-0.162883551947
H	-0.003755303757	3.190883315569	-1.021943467050
H	1.891134933597	0.583204509635	-1.064854293340
H	1.714345106697	-1.136554065295	-0.780639220562
H	-1.452356291716	3.392370877172	1.063070208343
H	0.207275741424	4.048595675243	1.127223974831
H	-0.145249822111	2.472680085551	1.838351226951
H	1.009463036410	1.914885890569	-2.748217055511
H	-2.820173303297	0.475243967256	-1.894721902117
H	-3.391111581040	0.160571509669	-4.106611112369
H	-1.704410470405	0.743630827230	-5.897391612430
H	0.525353500915	1.642647624302	-5.167166621684

S10

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TSc-en

E(RB+HF-LYP) = -575.098537148 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.411739210000
C	1.317299373544	0.000000000000	1.869465059583
C	2.169924304788	-0.004730099388	0.749590492833
C	0.662326050138	-2.004969117734	-0.348750029285
C	1.358105088946	0.524736305472	-0.408251949322
C	-0.320636841414	-2.790160604533	0.441255613019
C	0.026604161561	-3.377716845218	1.667621810145
N	-1.547577063172	-2.915233185612	-0.099899244367
C	-2.459786969279	-3.617389938281	0.578581940779
C	-2.217781289163	-4.220885717273	1.814044739273
C	-0.941027246793	-4.095721302557	2.363816095883
N	1.950656089428	-1.964583570347	0.045337573267
C	2.930282009191	-2.032382923252	-1.033804721264
H	3.249799009586	0.079868997063	0.809084362656
H	1.630057999403	-0.140950006890	2.898061856221
H	-0.878943957382	-0.134922886873	2.033122408034
H	-0.894943772151	0.119406518471	-0.601295632667
H	0.415346471743	-1.964260558852	-1.416539989853
H	1.344228965861	1.625214501855	-0.354004245110
H	1.701341713260	0.245306539460	-1.405098153420
H	3.134230766222	-3.089313684404	-1.253700952079
H	3.877099127005	-1.579038806444	-0.721017130433
H	2.613186452239	-1.562337173736	-1.981122219275
H	1.042341726371	-3.269899865135	2.030508093526
H	-3.439401401101	-3.702993936022	0.108972412658
H	-3.002052164581	-4.777230347294	2.318837489321
H	-0.700927598537	-4.560830933887	3.316944189461

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

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TSc-ex

E(RB+HF-LYP) = -575.103569819 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.406765980000
C	1.323274343809	0.000000000000	1.863787821660
C	2.173770878032	0.028364281361	0.742245527819
C	0.645979764241	2.019462999782	-0.371279090628
C	1.372248036852	-0.489624982716	-0.419358679939
C	0.413737803049	2.060974668022	-1.841614675334
C	1.479443058816	2.090393068509	-2.755817904596
N	-0.873444957119	2.117647475356	-2.235419753140
C	-1.124920425839	2.190574486267	-3.545678467549
C	-0.135092635519	2.204825232168	-4.529950074142
C	1.196957886429	2.155240101124	-4.116994198213
N	1.899785233946	1.995608434496	0.114196947851
C	2.089891374395	2.795288282356	1.321697964508
H	3.255585720889	-0.030075276771	0.788273902641
H	1.633138724037	0.138164797546	2.893842540725
H	-0.880928063286	0.114652650018	2.030509220483
H	-0.889062321057	-0.117510353170	-0.609810964201
H	-0.150276870228	2.516765778648	0.191639725600
H	1.718460500324	-0.170471378690	-1.402144247298
H	1.377517584482	-1.590933602760	-0.391271290711
H	2.225664071321	3.845803689316	1.029395481758
H	2.996643084410	2.475664548624	1.846033026317
H	1.243912500923	2.757092267386	2.026335929933
H	2.495268526598	2.083191191037	-2.376076905832
H	-2.176942510875	2.240354484542	-3.825009366893
H	-0.403041906645	2.262678225547	-5.580680868877
H	2.004201016595	2.180144997584	-4.844931786084

S12

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

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TS3-ex

E(RB+HF-LYP) = -559.479418407 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.429399210000
C	1.316031288102	0.000000000000	1.916667330477
C	2.173994941369	-0.130071210403	0.836125224697
C	0.067083748705	1.799482943177	-0.484776204434
C	1.398083833681	-0.478912336621	-0.384042025049
C	-0.270225486004	1.810147814053	-1.947288074960
C	0.698260363905	1.775988614239	-2.961981963274
C	-1.626312048593	1.865721207623	-2.304810213233
C	-2.006726684858	1.894399787643	-3.645016455663
C	-1.035774667529	1.862075304814	-4.647573895399
C	0.316318324859	1.805205323460	-4.302714011434
N	1.298472869833	2.286356787760	-0.072759712905
C	1.377741117321	3.207880535856	1.060840216119
H	3.257819805885	-0.105507030878	0.885243432249
H	1.609305396505	0.123894927583	2.952576227259
H	-0.891362313803	0.079026341237	2.045178007828
H	-0.873352289982	-0.366571077885	-0.532726873012
H	-0.749958331551	2.196420758212	0.114733226760
H	1.967028244044	2.471683111982	-0.810648540551
H	1.803470622056	-0.106269465387	-1.325278397911
H	1.362593103308	-1.577655340449	-0.468892610527
H	0.928873794837	4.180785548406	0.824166340753
H	2.423842272343	3.352005623112	1.338103614671
H	0.846070505511	2.779024794679	1.915377926779
H	1.760931255289	1.736850506434	-2.731361797331
H	-2.388896660228	1.898247945607	-1.529790708450
H	-3.059546517965	1.947516389259	-3.904554716058
H	-1.329698777149	1.885369881874	-5.692372108592
H	1.076710742555	1.787464737523	-5.077405181255

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

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TS4-ex

E(RB+HF-LYP) = -575.772473278 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.409318470000
C	1.329587408313	0.000000000000	1.902407689998
C	2.189983715051	-0.122013371195	0.834301879672
C	-0.030810059393	2.067522122496	-0.394881523027
C	1.416032395408	-0.351061614105	-0.419705878392
C	-0.437403937225	2.059445341914	-1.834987872980
C	0.454791645134	2.111844322225	-2.924071216845
C	-1.800576695410	2.052996715096	-2.130015584544
N	-2.218751892133	2.088294571377	-3.412916244614
C	-1.381648377655	2.131821876782	-4.472401924099
C	-0.014720006340	2.143484445640	-4.237534106104
N	1.150932082770	2.588846379933	-0.013899145465
C	1.324556481757	3.340061946715	1.240859974289
H	3.273910769630	-0.136904759330	0.890269441645
H	1.612874729601	0.075267874432	2.946035760742
H	-0.889714477698	0.025299629772	2.032523206856
H	-0.867860478796	-0.331889561615	-0.562326796509
H	-0.846837954348	2.308624136384	0.279011857132
H	1.901808362014	2.676509486112	-0.687849936885
H	1.823018207947	0.143958152459	-1.306488441577
H	1.440404652699	-1.430361186496	-0.649297068394
H	1.040244053858	4.388676298610	1.100012398603
H	2.367813231858	3.285439392115	1.553058607097
H	0.696250035079	2.900094627670	2.018386305070
H	1.528936711488	2.138256103216	-2.766503910324
H	-2.578550883148	2.031433388826	-1.374468115625
H	-3.223840443249	2.094291748187	-3.590271198958
H	-1.831662928822	2.161767125474	-5.458467842522
H	0.671219842822	2.186124667087	-5.076577633971

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

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TS5-ex

E(RB+HF-LYP) = -575.776168802 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.412417130000
C	1.327636147213	0.000000000000	1.902970643859
C	2.188546259465	-0.117441124594	0.831703085048
C	-0.004212753022	2.059684826376	-0.371310435179
C	1.414302908770	-0.355937370908	-0.420134420050
C	-0.439889590842	2.044246712138	-1.800762585645
C	0.439573799276	2.199354412606	-2.889026378914
C	-1.816309376260	1.921289251849	-2.078597997687
C	-2.271275788817	1.956498364617	-3.383225405819
N	-1.383245796002	2.105491376655	-4.392587072247
C	-0.054748509263	2.226932271492	-4.181655461880
N	1.192233546056	2.561046236944	-0.004388647560
C	1.380380463928	3.340599973475	1.231483041176
H	3.272624839636	-0.128950499749	0.887800720195
H	1.613151933511	0.074015871591	2.946123059604
H	-0.890231418718	0.027647969320	2.034672978235
H	-0.869435479097	-0.329176912797	-0.561143409153
H	-0.808401543287	2.316537253382	0.311221135197
H	1.941097377436	2.621847467850	-0.683234759272
H	1.817470770539	0.131020824547	-1.312986927141
H	1.437155512921	-1.437692592782	-0.638660758368
H	1.077573161417	4.381966231283	1.076816881485
H	2.430945929329	3.307382400480	1.521422285786
H	0.776297523383	2.906349626151	2.031324271694
H	1.509613216781	2.321335769036	-2.764762525718
H	-2.544053827305	1.814936725232	-1.280550986283
H	-3.318192702507	1.879305277015	-3.654691753850
H	-1.731882090543	2.137562381358	-5.350869478619
H	0.572964986514	2.351676518998	-5.056912755221

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

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IN-en

E(RHF) = -572.044572014 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.498950410000
C	1.255571613073	0.000000000000	2.039324890465
C	2.164885643655	-0.022330440454	0.990313396514
C	-0.806307745257	-1.153277044881	-0.673902733991
C	1.504718360218	-0.055396744893	-0.332338206443
C	-2.327654987069	-0.942176308735	-0.575580329095
C	-3.139783822000	-1.471530079116	0.397815378148
N	-2.911519096800	-0.193925727347	-1.531887233151
C	-4.224614387292	0.067137302947	-1.589436020342
C	-5.064524744560	-0.435146334964	-0.629399417254
C	-4.510591415188	-1.218487425859	0.373252387988
N	-0.320629586630	-2.421963756581	-0.222342417270
C	-0.597806400039	-3.576321729898	-1.077603914923
H	3.234748924009	-0.012312344613	1.111231525251
H	1.499718338581	0.024295016971	3.082996348834
H	-0.900198421026	0.026303121216	2.088562446468
H	-0.417697980646	0.957470124563	-0.310102910179
H	-0.563330975936	-1.087231083597	-1.730073605066
H	1.851949710026	0.772699756545	-0.945363159574
H	1.788676630496	-0.972863674319	-0.841056950189
H	-1.658016644714	-3.776347197580	-1.210520183382
H	-0.136275126474	-4.447631075032	-0.636553538123
H	-0.147526948867	-3.418602909043	-2.049498903439
H	-2.728725548661	-2.101605642015	1.161769137950
H	-4.557992355368	0.667565803215	-2.413372280350
H	-6.116369924290	-0.231246737002	-0.673694605317
H	-5.141551864258	-1.640244077115	1.133913549983
H	-0.538524751282	-2.619331149227	0.733745215366
H	-2.343203703511	0.169868120034	-2.273264307328

S16

A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine

Derivatives: A Shift from a Concerted to Stepwise Molecular Mechanism

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IN-ex

E(RB+HF-LYP) = -575.772314837 au.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.498950410000
C	1.255571613073	0.000000000000	2.039324890465
C	2.164885643655	-0.022330440454	0.990313396514
C	-0.806307745257	-1.153277044881	-0.673902733991
C	1.504718360218	-0.055396744893	-0.332338206443
C	-2.327654987069	-0.942176308735	-0.575580329095
C	-3.139783822000	-1.471530079116	0.397815378148
N	-2.911519096800	-0.193925727347	-1.531887233151
C	-4.224614387292	0.067137302947	-1.589436020342
C	-5.064524744560	-0.435146334964	-0.629399417254
C	-4.510591415188	-1.218487425859	0.373252387988
N	-0.320629586630	-2.421963756581	-0.222342417270
C	-0.597806400039	-3.576321729898	-1.077603914923
H	3.234748924009	-0.012312344613	1.111231525251
H	1.499718338581	0.024295016971	3.082996348834
H	-0.900198421026	0.026303121216	2.088562446468
H	-0.417697980646	0.957470124563	-0.310102910179
H	-0.563330975936	-1.087231083597	-1.730073605066
H	1.851949710026	0.772699756545	-0.945363159574
H	1.788676630496	-0.972863674319	-0.841056950189
H	-1.658016644714	-3.776347197580	-1.210520183382
H	-0.136275126474	-4.447631075032	-0.636553538123
H	-0.147526948867	-3.418602909043	-2.049498903439
H	-2.728725548661	-2.101605642015	1.161769137950
H	-4.557992355368	0.667565803215	-2.413372280350
H	-6.116369924290	-0.231246737002	-0.673694605317
H	-5.141551864258	-1.640244077115	1.133913549983
H	-0.538524751282	-2.619331149227	0.733745215366
H	-2.343203703511	0.169868120034	-2.273264307328