

Supporting Information

Computational Part

The Cinchona Primary Amine-Catalyzed Asymmetric Epoxidation and Hydroperoxidation of α,β -Unsaturated Carbonyl Compounds with Hydrogen Peroxide

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Computational Details

(a) Methodology

Geometry optimizations were carried out using the BP86^{1,2} functional in combination with def2-SVP basis sets.³⁻⁵ The resolution-of-identity (RI) approximation⁶⁻⁸ was applied in conjunction with the approximate auxiliary basis sets to speed up the calculations. All relevant stationary points were characterized as minima or first-order transition states by evaluating the harmonic vibrational frequencies at the same level (RI-BP86/def2-SVP) that had been applied for geometry optimization.

To check the sensitivity of the computed energy profiles, single-point energies at the optimized RI-BP86/def2-SVP geometries were calculated using the standard B3LYP^{1,9,10} hybrid functional and the modern M06 and M06-2X functional,¹¹ in conjunction with different basis sets, i.e., def2-TZVP,¹² 6-31G*,¹³ and TZVP.¹⁴ The influence of the solvent environment (THF, dielectric constant $\epsilon = 7.426$) on the relative energies was investigated through single-point calculations with the conductor-like screening model (COSMO).¹⁵ Empirical Grimme-type dispersion corrections were incorporated at the B3LYP level using the latest parametrization (DFT-D3);¹⁶ the corresponding results are denoted as B3LYP-D. Zero-point energies (ZPE) were computed from the harmonic vibrational frequencies (RI-BP86/def2-SVP). Relative free energies (ΔG) at standard pressure (1 bar) and 323.15K were determined at the RI-BP86/def2-SVP level. The required thermal and entropic contributions were evaluated within the rigid-rotor harmonic-oscillator approximation.

The DFT computations were performed with TURBOMOLE (version-6.4)^{17,18} and Gaussian09.¹⁹

(b) Survey of computational results presented as Supporting Information

Four different geometric orientations were considered for transition state modeling, namely, the anion and hydrogen peroxide approaching from the (β)-*re*-face or (β)-*si*-face, combined with two different orientations of the quinoline group. Out of a total of 30 starting geometry configurations, the lowest-lying pathways for each of the four orientations were computed and analyzed to explain the origin of stereoselectivity: These are denoted as pathway-1 and pathway-3 [(β)-*si*-face approach of hydrogen peroxide and TFA with the quinoline group oriented toward (β)-*si*-face and (β)-*re*-face, respectively] and pathway-2 and pathway-4 [(β)-*re*-face approach of hydrogen peroxide and TFA with the quinoline group oriented toward (β)-*re*-face and (β)-*si*-face, respectively]. In the gas-phase calculations using BP86 and B3LYP, the energy and free energy values always show the same trend, with a consistent preference for pathway-1, in agreement with the experimental selectivity, and the rotation of the quinoline group has little influence on the stereoselectivity, since both pathway-1 and pathway-3 are energetically favored over pathway-2 and pathway-4 (Tables 1-4). The gas-phase calculations with the M06 functionals also reproduce the experimental selectivity, but prefer pathway-3 (Table 4). When including the solvent environment, the position of the quinoline group becomes more relevant. The BP86 and B3LYP calculations again predict the same trend and a clear preference for pathway-1, but pathway-3 with rotated quinoline is now destabilized such that pathway-2 becomes the second lowest one (Table 4).

In the main paper, we consider the free energy difference between the lowest transition states for (β)-*si*-face and (β)-*re*-face attack that give rise to different stereoisomer products. In the case of BP86 and B3LYP, these lowest transition states are always associated with pathway-1 and pathway-2, respectively. The corresponding energy difference is 1.0 kcal/mol at the BP86/def2-SVP level that has been used during geometry optimization (Table 1), and 2.2 kcal/mol at the single-point B3LYP/def2-TZVP(COSMO)//BP86/def2-SVP level, which

is expected to provide the most realistic estimate for the reaction in solution (Table 4). The computed difference is slightly decreased by zero-point vibrational energy corrections (-0.1 kcal/mol, Table 1) and dispersion corrections (-0.7 kcal/mol, Table 4, B3LYP-D/def2-TZVP vs. B3LYP/def2-TZVP), while it is increased by thermal and entropic corrections (+1.0 kcal/mol, Table 2). Applying the resulting overall correction of 0.2 kcal/mol yields a best estimate of 2.4 kcal/mol [based on B3LYP/def2-TZVP(COSMO)//BP86/def2-SVP] for the free energy difference between pathway-1 and pathway-2, which rationalizes the observed stereoselectivity.

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ENERGIES

Table 1. Relative energies (in kcal/mol) with respect to the free reactants, obtained at the BP86/def2-SVP level with and without zero-point energy (ZPE) corrections.

Method and basis set	Pathway	Free Reactants	Reactant Complex (RC)	Transition state (TS)	Product (PRDT)
BP86/def2-SVP	<i>Pathway-1 (TS-1)</i>	0	-114.1	-110.2	-119.1
	<i>Pathway-2 (TS-2)</i>	0	-110.1	-109.2	-115.4
	<i>Pathway-3 (TS-3)</i>	0	-111.8	-109.9	-119.1
	<i>Pathway-4 (TS-4)</i>	0	-108.4	-103.0	-110.8
BP86/def2-SVP + ZPE	<i>Pathway-1 (TS-1)</i>	0	-110.9	-108.0	-115.6
	<i>Pathway-2 (TS-2)</i>	0	-107.3	-107.1	-112.1
	<i>Pathway-3 (TS-3)</i>	0	-108.9	-107.5	-115.5
	<i>Pathway-4 (TS-4)</i>	0	-105.5	-102.2	-108.0

Table 2. Thermal and entropic energy contributions (in kcal/mol), relative to the values for the free reactants, which are needed to convert the computed relative energies to free energies (ΔG in kcal/mol) at standard pressure (1 bar) and 323.15K. These contributions are evaluated at the BP86/def2-SVP level (see methodology section).

Method and basis set	Pathway	Free Reactants	Reactant Complex (RC)	Transition state (TS)	Product (PRDT)
BP86/def2-SVP	<i>Pathway-1 (TS-1)</i>	0	29.6	29.8	29.8
	<i>Pathway-2 (TS-2)</i>	0	29.7	30.8	29.7
	<i>Pathway-3 (TS-3)</i>	0	29.2	30.4	29.5
	<i>Pathway-4 (TS-4)</i>	0	29.8	28.9	28.9

Table 3. Relative free energies (in kcal/mol) with respect to the free reactants, obtained at the BP86/def2-SVP level with and without zero-point energy (ZPE) corrections.

Method and basis set	Pathway	Free Reactants	Reactant Complex (RC)	Transition state (TS)	Product (PRDT)
BP86/def2-SVP	<i>Pathway-1 (TS-1)</i>	0	-84.5	-80.4	-89.3
	<i>Pathway-2 (TS-2)</i>	0	-80.4	-78.4	-85.7
	<i>Pathway-3 (TS-3)</i>	0	-82.6	-79.5	-89.6
	<i>Pathway-4 (TS-4)</i>	0	-78.6	-74.1	-81.9
BP86/def2-SVP + ZPE	<i>Pathway-1 (TS-1)</i>	0	-81.3	-78.2	-85.8
	<i>Pathway-2 (TS-2)</i>	0	-77.6	-76.3	-82.4
	<i>Pathway-3 (TS-3)</i>	0	-79.7	-77.1	-86.0
	<i>Pathway-4 (TS-4)</i>	0	-75.7	-73.3	-79.1

Table 4. Relative energies (in kcal/mol) with respect to the free reactants, obtained from single-point calculations at different levels of theory (see methodology section).

Method and basis set	Pathway	Free Reactants	Reactant Complex (RC)	Transition state (TS)	Product (PRDT)
B3LYP/def2-TZVP	<i>Pathway-1 (TS-1)</i>	0	-95.8	-86.8	-97.9
	<i>Pathway-2 (TS-2)</i>	0	-86.9	-84.4	-94.3
	<i>Pathway-3 (TS-3)</i>	0	-91.2	-85.1	-97.8
	<i>Pathway-4 (TS-4)</i>	0	-91.9	-80.9	-89.9
B3LYP-D/def2-TZVP	<i>Pathway-1 (TS-1)</i>	0	-110.0	-99.0	-108.4
	<i>Pathway-2 (TS-2)</i>	0	-101.1	-97.5	-105.4
	<i>Pathway-3 (TS-3)</i>	0	-104.8	-98.3	-108.4
	<i>Pathway-4 (TS-4)</i>	0	-109.1	-95.2	-103.7
BP86/def2-TZVP (solvent single point)	<i>Pathway-1 (TS-1)</i>	0	-81.6	-75.2	-80.4
	<i>Pathway-2 (TS-2)</i>	0	-77.8	-74.3	-78.1
	<i>Pathway-3 (TS-3)</i>	0	-79.1	-72.9	-80.6
	<i>Pathway-4 (TS-4)</i>	0	-76.3	-68.6	-72.8
B3LYP/def2-TZVP (solvent single point)	<i>Pathway-1 (TS-1)</i>	0	-92.6	-81.3	-89.3
	<i>Pathway-2 (TS-2)</i>	0	-84.5	-79.1	-86.5
	<i>Pathway-3 (TS-3)</i>	0	-88.3	-78.3	-89.4
	<i>Pathway-4 (TS-4)</i>	0	-88.1	-75.1	-81.6
M06-2x/TZVP	<i>Pathway-1 (TS-1)</i>	0	-107.3	-94.4	-111.3
	<i>Pathway-2 (TS-2)</i>	0	-94.3	-93.8	-108.2
	<i>Pathway-3 (TS-3)</i>	0	-99.4	-95.1	-111.5
	<i>Pathway-4 (TS-4)</i>	0	-106.5	-92.0	-105.5
M06/6-31G*	<i>Pathway-1 (TS-1)</i>	0	-119.8	-106.9	-122.2
	<i>Pathway-2 (TS-2)</i>	0	-107.2	-105.0	-118.3
	<i>Pathway-3 (TS-3)</i>	0	-112.2	-107.1	-122.2
	<i>Pathway-4 (TS-4)</i>	0	-116.2	-102.2	-116.1

CARTESIAN COORDINATES OF OPTIMIZED GEOMETRIES (BP86/def2-SVP, Å)

Reactant Complex (RC) [Pathway-1]

75

c	-1.1954886479	-0.8071356089	3.5217763637
o	1.1350360862	0.8775302800	3.3324293269
c	-0.8056715284	-0.3285165724	5.8993345446
c	-1.7134754880	-0.7370395861	4.8833261894
c	-3.0409664314	-1.0787209304	5.2557103473
c	-3.4448194368	-1.0038395995	6.5955706889
c	-2.5425846030	-0.5718670204	7.5842923966
c	-1.2232974519	-0.2328333559	7.2316332376
c	-1.8445157634	-0.5966946266	2.3143049166
c	-3.2799536354	-0.1633873704	2.1349775477
c	-0.9860036577	-0.7204203238	1.1726383512
n	-1.3713181928	-0.4866464354	-0.0636786978
c	-0.5067349719	-0.4815935109	-1.2540805131
c	-1.4168658681	-0.0012970733	-2.4271122115
c	-0.6489036498	0.5215907281	-3.6719453122
c	-1.3807182979	1.7891229431	-4.1741291229
c	-2.9073034486	1.5204055712	-4.3621353589
c	-3.4703220445	1.1169843819	-2.9432469704
n	-2.3937497832	1.0072866761	-1.9413279367
c	-1.7575716343	2.3378044628	-1.7527715297
c	-1.2193479157	2.8916583927	-3.1070369033
c	-3.2221504056	0.4969286608	-5.4220508489
c	-3.8867763530	0.7424306510	-6.5660851189
c	0.0986414094	-1.8564952256	-1.5351772859
c	1.5026428978	-2.0612760415	-1.7632875719
c	1.9310481447	-3.4109571174	-2.0885967363
n	1.0715126208	-4.4712490748	-2.1653986414
c	-0.2092953948	-4.2451919461	-1.9193689876
c	-0.7415473763	-2.9667227359	-1.6052620681
c	2.4962832716	-1.0393169177	-1.6761113218
c	3.8348811605	-1.3245272483	-1.9066947340
c	4.2483039731	-2.6410576031	-2.2470633968
c	3.3147446182	-3.6622859387	-2.3341199872
h	4.5779991286	-0.5194030807	-1.8087762236
o	1.7575018051	-0.2683466559	2.6769285567
o	0.6793559315	1.9774516621	0.9118240567
h	-2.2760329710	-0.0062719282	-0.2952666779

h	-2.0357839353	-0.8763972530	-2.7210409999
h	0.3965312420	0.7889333125	-3.4143369646
h	-0.5925288625	-0.2590709993	-4.4569401596
h	-2.5260380607	3.0067123950	-1.3151257323
h	-0.9557122492	2.2511274828	-0.9906559890
h	-4.2009947635	1.8688692773	-2.5827066172
h	-4.0039819100	0.1446875457	-2.9968234157
h	-0.9469998765	2.1176109350	-5.1397368095
h	-1.7755144331	3.8007514447	-3.4180233089
h	-0.1546113093	3.1800402212	-3.0126230827
h	-3.3694521443	2.4816130757	-4.6734872504
h	-2.8800995149	-0.5379228379	-5.2262368891
h	-4.2557345232	1.7528901554	-6.8112190178
h	-4.0862460504	-0.0530824026	-7.3010309596
h	0.0763356338	-0.9859224379	1.3469895130
h	-3.3708619671	0.6097366641	1.3430148791
h	-3.9399183279	-1.0086591992	1.8426250454
h	-3.6863412636	0.2766052738	3.0637488591
h	-0.1160935751	-1.0137465863	3.4463456474
h	0.2163022548	-0.0486076467	5.6006533280
h	-3.7459263108	-1.4533124815	4.5001973593
h	-0.5145650898	0.1036057774	8.0035425313
h	-4.4704175470	-1.2909810453	6.8736153162
h	-2.8667928636	-0.5079502301	8.6343758816
h	0.2882270175	0.2711501738	-1.0804279969
h	-1.8221480833	-2.8673774520	-1.4163011809
h	-0.8881479142	-5.1165122911	-1.9739177821
h	2.2234963408	-0.0147548671	-1.3960541612
h	5.3138784643	-2.8487253337	-2.4297908598
h	3.5973534722	-4.6957758950	-2.5819100910
h	2.3326636929	0.2169627544	1.9849154994
h	0.7814374845	1.3696668479	2.5216618625
c	1.8779746855	1.9943415055	0.5040380926
o	2.8494147016	1.2775210697	0.8472368898
c	2.1847199844	3.0109705694	-0.6453821866
f	3.4491895741	3.4616511594	-0.6242061050
f	2.0033277739	2.3820130388	-1.8644331966
f	1.3601863813	4.0791461256	-0.6414621400

Transition State (TS-1) [Pathway-1]

75

c	-0.8676263188	-0.3129970602	3.4429142091
o	-0.4817575607	1.5825799461	3.5705142689
c	-0.5709040293	-1.3950121390	5.6594944786

c	-1.3320003796	-0.5392843275	4.8292942971
c	-2.4837836882	0.0790070367	5.3733307444
c	-2.8758179516	-0.1827415576	6.6933890860
c	-2.1285232264	-1.0634538229	7.4956682753
c	-0.9712968407	-1.6661077368	6.9760402931
c	-1.6709957665	-0.4294225773	2.2591973057
c	-3.1760745738	-0.3062354851	2.2386251493
c	-0.9529494862	-0.5775615384	1.0725583717
n	-1.4542013453	-0.5525203406	-0.1768297575
c	-0.6051910233	-0.5545422006	-1.3719306636
c	-1.5205759509	-0.1618445716	-2.5692601654
c	-0.7477791925	0.2316825847	-3.8637496455
c	-1.3377044932	1.5612514451	-4.3857166347
c	-2.8793707140	1.4424163863	-4.6000035329
c	-3.4957519297	1.0361483149	-3.2038900979
n	-2.4623589677	0.9092576374	-2.1633264758
c	-1.7709887940	2.2099106405	-1.9964760626
c	-1.0834504348	2.6528781230	-3.3248982401
c	-3.2714975469	0.4940227841	-5.7016496651
c	-3.9106649599	0.8397765182	-6.8344587823
c	0.0624636211	-1.9100901305	-1.6071867279
c	1.4522884407	-2.0491172135	-1.9501427094
c	1.9443658826	-3.3924567642	-2.1982448745
n	1.1563699049	-4.5063367233	-2.1121864718
c	-0.1124709045	-4.3364242339	-1.7726444990
c	-0.7011402023	-3.0711572971	-1.5105974622
c	2.3786802142	-0.9638106596	-2.0446443668
c	3.7093779529	-1.1859772134	-2.3733417384
c	4.1832288493	-2.5010494106	-2.6317564313
c	3.3174151080	-3.5800245400	-2.5440046377
h	4.4028807650	-0.3330950691	-2.4232359114
o	0.6592758678	1.8404643803	4.3946027227
o	0.3599109694	2.2262637755	1.3073594928
h	-2.3639433857	-0.0938898718	-0.3724985017
h	-2.1618421412	-1.0456162984	-2.7776216855
h	0.3349094969	0.3711170721	-3.6633177983
h	-0.8201574206	-0.5700881213	-4.6257297040
h	-2.5355228451	2.9436540826	-1.6698094020
h	-1.0441064593	2.1321180973	-1.1634549764
h	-4.2366470424	1.7905109837	-2.8697340209
h	-4.0327349442	0.0672393277	-3.2824318162
h	-0.8563984233	1.8365768746	-5.3459298976
h	-1.4832442312	3.6258235801	-3.6783006614
h	0.0069033115	2.7889400628	-3.1745481308
h	-3.2470640706	2.4534458988	-4.8782777473
h	-3.0158613067	-0.5719572410	-5.5462351377
h	-4.1956024454	1.8862173091	-7.0375190489
h	-4.1730070372	0.0939073913	-7.6009070318
h	0.1361320947	-0.7472158364	1.1325373122
h	-3.6038805144	-0.8371754431	1.3633129394

h	-3.6301140734	-0.7527584846	3.1444821295
h	-3.5199962720	0.7500362977	2.1844126508
h	0.1924501481	-0.5843968536	3.2981678649
h	0.3448261457	-1.8577151936	5.2596637414
h	-3.0448682063	0.8095661556	4.7749669036
h	-0.3688728281	-2.3409796986	7.6030495198
h	-3.7662470520	0.3159225947	7.1060487389
h	-2.4398554161	-1.2659057593	8.5319484410
h	0.1722910063	0.2289710511	-1.2514843043
h	-1.7615297888	-3.0138308927	-1.2199730452
h	-0.7327093134	-5.2489532672	-1.6977073086
h	2.0518940211	0.0642133819	-1.8393764902
h	5.2408324914	-2.6592847560	-2.8930845842
h	3.6480844850	-4.6128898506	-2.7269988634
h	1.4173827855	1.8200911513	3.7093924341
h	-0.1645684911	1.8670662967	2.5542317167
c	1.6343960836	2.2160549145	1.3769995712
o	2.3536726171	1.9261995920	2.3539724501
c	2.3607475762	2.6779946325	0.0789032545
f	3.5873703177	2.1402507907	-0.0384987202
f	1.6612768119	2.3254882567	-1.0473716964
f	2.4828865836	4.0217650266	0.0630171375

Product (PRDT) [Pathway-1]

75

c	-0.6451210580	0.0570180525	3.5319433131
o	-0.3866154650	1.5017404378	3.6827278504
c	-1.2274002861	-1.9232088648	4.9792518129
c	-1.2423590817	-0.5242643126	4.8036893867
c	-1.8414358465	0.2818708512	5.7903772156
c	-2.4169743973	-0.3032504591	6.9311593229
c	-2.4027495599	-1.6975271229	7.0980502581
c	-1.8040299635	-2.5074913375	6.1171808726
c	-1.5052725709	-0.0478970233	2.2992679745
c	-2.9686937419	0.3184505215	2.3581949637
c	-0.8767890586	-0.3800604455	1.1271287058
n	-1.4442195218	-0.4282390747	-0.1224749335
c	-0.6163753604	-0.4845907125	-1.3242268990
c	-1.5526093573	-0.1909484810	-2.5333327532
c	-0.8133625979	0.0221506253	-3.8885011190
c	-1.3893241297	1.2908464747	-4.5555407863
c	-2.9409862388	1.1944180361	-4.6989414829
c	-3.5117779602	0.9958943111	-3.2397861205
n	-2.4417888559	0.9568621343	-2.2306504209

c	-1.7040199415	2.2380965494	-2.2509173064
c	-1.0663490924	2.4994638431	-3.6513996122
c	-3.3988405505	0.1203408992	-5.6493723371
c	-4.0596450469	0.3313687750	-6.8027420544
c	0.0778561179	-1.8370467944	-1.4890109436
c	1.4563374916	-1.9714504622	-1.8788377316
c	1.9687522070	-3.3174571048	-2.0601953616
n	1.2120437553	-4.4391199214	-1.8649452716
c	-0.0443344458	-4.2716197440	-1.4792820296
c	-0.6512292051	-3.0044106423	-1.2762067763
c	2.3555049330	-0.8771625119	-2.0805789993
c	3.6743741982	-1.0927781164	-2.4580293324
c	4.1652714570	-2.4121775094	-2.6553874068
c	3.3292231757	-3.4995823053	-2.4559331288
h	4.3472834511	-0.2329877599	-2.5978486256
o	0.6742003640	1.7289104995	4.6745589121
o	0.4451176510	2.6541268363	1.5304996083
h	-2.2931593541	0.1319435465	-0.3003306286
h	-2.2318905110	-1.0670984443	-2.6165229565
h	0.2778429240	0.1589385017	-3.7384538978
h	-0.9244965463	-0.8652926334	-4.5427493950
h	-2.4237611635	3.0360795866	-1.9775454280
h	-0.9397228075	2.2260835340	-1.4477517314
h	-4.2089360807	1.8177933444	-2.9784761741
h	-4.0880467212	0.0494506548	-3.1727856998
h	-0.9382229046	1.4286797127	-5.5591308168
h	-1.4629841507	3.4315198002	-4.1051676407
h	0.0331845315	2.6261743385	-3.5690801102
h	-3.2920866275	2.1705052521	-5.0982690291
h	-3.1761869811	-0.9231807139	-5.3542491505
h	-4.3146996232	1.3500064086	-7.1414981116
h	-4.3716516482	-0.5022916891	-7.4511743651
h	0.1885200112	-0.6720175070	1.1549988906
h	-3.5531526537	-0.2334211426	1.5922982544
h	-3.4020650730	0.0675465118	3.3471393057
h	-3.1502080949	1.4039928899	2.1932976978
h	0.3401076891	-0.4228411381	3.3379582734
h	-0.7605109209	-2.5617151819	4.2117076697
h	-1.8342580527	1.3741280767	5.6678996173
h	-1.7822154221	-3.6013384236	6.2412497628
h	-2.8764975002	0.3390468026	7.6985350897
h	-2.8517468572	-2.1533521113	7.9940098034
h	0.1591978835	0.3149327449	-1.2883257875
h	-1.6966213670	-2.9413039723	-0.9374555375
h	-0.6382318150	-5.1899072528	-1.3143765914
h	2.0126761681	0.1542154120	-1.9185982948
h	5.2127887821	-2.5660771403	-2.9569010567
h	3.6749528470	-4.5354665412	-2.5864791302
h	1.4566016645	1.8122820553	4.0549949388
h	0.0282675543	2.2007812237	2.3759628505

c	1.7522773008	2.5820724030	1.6182981195
o	2.4136702757	2.1390174419	2.5503846134
c	2.4438212970	3.1612002040	0.3523324575
f	3.7523826252	2.8872184877	0.3536951142
f	1.9016840097	2.6312688913	-0.7789151197
f	2.2783801115	4.4980466576	0.3006955759

Reactant Complex (RC) [Pathway-2]

75

c	-1.2029894088	-1.7785645356	-2.6214680177
o	1.0153612021	-1.5419230843	-2.9543766817
c	-3.3338298775	0.7451269240	4.7776827008
c	-1.8949759435	1.0015583478	5.2718401819
c	-0.9736476619	-0.0651461591	4.6374144779
c	-0.9365082747	0.1898558070	3.1048343831
n	-1.9827235306	1.1626295042	2.7039317061
c	-3.3143898998	0.7723992522	3.2177613021
c	-1.6180611254	2.4814755743	3.2535513385
c	-1.4814930879	2.4402205030	4.8258420983
c	-1.0396642773	-1.0986076431	2.2322959402
c	0.1419613586	-2.0373236962	2.4451113309
c	1.4964188056	-1.7238464333	2.0650586386
c	2.5302312537	-2.6548963280	2.4807877486
n	2.2690064215	-3.8064966533	3.1735393145
c	1.0088678915	-4.0788197951	3.4663948890
c	-0.0814051575	-3.2300258227	3.1288899726
c	3.8921855372	-2.3742973603	2.1591145486
c	4.2331347402	-1.2381491548	1.4397851375
c	3.2210195731	-0.3435372535	1.0012574596
c	1.8861447535	-0.5777778748	1.3071438090
h	3.4739661546	0.5348916513	0.3907083534
c	-0.1120571571	2.8507966727	5.3022054314
c	0.1372281582	3.8270982026	6.1938462129
n	-1.2587163730	-0.6499738417	0.8569875887
c	-1.1506344174	-1.3726314556	-0.2650612581
c	-1.5054903497	-0.9117607491	-1.5450498498
c	-2.1413122088	0.4512013856	-1.6883083558
c	-1.5652980673	-1.6251623111	-4.0277330839
c	-1.4731000579	-0.3916692860	-4.7249007004
c	-1.8382957093	-0.3101634084	-6.0763639080
c	-2.2888888251	-1.4500042489	-6.7621241649
c	-2.3486969688	-2.6877375098	-6.0960413088
c	-1.9736207247	-2.7761489176	-4.7507921343
o	1.4097513447	-1.0901692731	-4.2423753787

o	1.3265595756	0.6064179071	-1.5981350782
c	1.3586576812	1.5563736094	-2.4388287905
c	1.4134892722	2.9775707208	-1.8042636671
f	2.1958331376	3.0044019946	-0.6981688795
o	1.3045774849	1.4932846982	-3.6898595024
f	1.8714542339	3.9094890255	-2.6558588760
f	0.1583202045	3.3545385631	-1.4151958579
h	0.0256390300	0.6736829274	2.8367397544
h	-1.3736199747	-1.0761745771	4.8689542366
h	0.0469040350	-0.0311732596	5.0674617344
h	-4.0520414881	1.4946444195	2.8130492615
h	-3.5834764939	-0.2154898458	2.7907897076
h	-2.3933744373	3.2118622062	2.9459698678
h	-0.6667020680	2.8050721765	2.7831836678
h	-1.8480543353	0.9353485423	6.3774881731
h	-4.0197330518	1.5176495490	5.1832949724
h	-3.6953491468	-0.2338140761	5.1560222054
h	-2.2183063377	3.1411852620	5.2736188047
h	0.7463150444	2.3038693232	4.8669461194
h	-0.6797141792	4.4110068671	6.6510982075
h	1.1639693410	4.0825831123	6.4987546051
h	-0.7223102301	-2.3827901317	-0.1462431179
h	-2.8651139639	0.6364863866	-0.8663538531
h	-1.3914908859	1.2695228563	-1.6523889384
h	-2.6999973137	0.5422584751	-2.6375286510
h	-0.9170440344	-2.8034939847	-2.3362698480
h	-2.0100598952	-3.7484972650	-4.2344619531
h	-1.0695218898	0.4988285552	-4.2241950182
h	-2.6802305425	-3.5895240839	-6.6331034083
h	-1.7509363837	0.6522832382	-6.6032772973
h	-2.5745260547	-1.3796548862	-7.8229920694
h	-1.9457137716	-1.6578036253	2.5696112730
h	-1.1029053700	-3.5178419115	3.4251024809
h	1.1356042286	0.1105596203	0.8987287941
h	0.8151285198	-5.0206010873	4.0127319934
h	4.6442999511	-3.1019791232	2.4969742395
h	5.2862962556	-1.0370145595	1.1901891684
h	-1.6404742657	0.3148310092	0.8451071902
h	1.3723876775	-0.0686267212	-4.1442518764
h	1.1560509913	-0.6982375837	-2.3344060126

Transition State (TS-2) [Pathway-2]

75

c	-1.0851720853	-1.7070301177	-2.6152361007
o	0.8084602071	-1.5867344642	-2.8084152614

c	-3.4579846659	0.5598077759	4.7351116921
c	-2.0656002551	0.8461343017	5.3348589698
c	-1.0563844594	-0.1338626060	4.6950737792
c	-0.9593318181	0.1981027231	3.1779258055
n	-2.0063866476	1.1713174535	2.7814873161
c	-3.3531470518	0.7146843872	3.1856958711
c	-1.7133105451	2.4582629710	3.4353372789
c	-1.6948356981	2.3273995416	5.0088657493
c	-1.0003725222	-1.0515483991	2.2449927914
c	0.2151166920	-1.9507475626	2.4545436738
c	1.5576654093	-1.5938877206	2.0686250172
c	2.6217493573	-2.4986918633	2.4637894339
n	2.4020395078	-3.6623772353	3.1508589853
c	1.1529418674	-3.9727252463	3.4532597946
c	0.0348834876	-3.1558536792	3.1288187302
c	3.9713615537	-2.1794241272	2.1255120891
c	4.2726896330	-1.0307455793	1.4088492919
c	3.2320074221	-0.1576863323	0.9936927428
c	1.9089898159	-0.4291922381	1.3189107955
h	3.4578290241	0.7288845237	0.3841709914
c	-0.3889255376	2.7725625617	5.6137395236
c	-0.2565038675	3.7135562815	6.5665218655
n	-1.1840818787	-0.5576959054	0.8847940795
c	-1.0995400167	-1.2830434933	-0.2505974240
c	-1.3941337536	-0.8123420903	-1.5272722946
c	-1.9099539176	0.5954486345	-1.7161858794
c	-1.5904843795	-1.5611410989	-3.9961631705
c	-1.4226322726	-0.3796371991	-4.7585102569
c	-1.9359384741	-0.2944130224	-6.0611045101
c	-2.6219868998	-1.3817615408	-6.6278166039
c	-2.7748106934	-2.5689837388	-5.8915715861
c	-2.2498233451	-2.6608166267	-4.5951486344
o	1.3361494352	-1.5456380703	-4.1316815907
o	1.5046468586	0.5850975714	-1.8906555609
c	1.7160479595	1.3718986670	-2.8787921713
c	2.0454560435	2.8320913860	-2.4583373668
f	2.8529161101	2.8720386840	-1.3717070281
o	1.6388551564	1.1129037803	-4.0948313136
f	2.6434136957	3.5187253495	-3.4441163926
f	0.8933543201	3.4812113355	-2.1339344118
h	0.0037449116	0.7113319255	2.9745087856
h	-1.4092794408	-1.1751421267	4.8577562509
h	-0.0618382896	-0.0670525134	5.1786617715
h	-4.0841206135	1.4543808422	2.8005013342
h	-3.5750468669	-0.2390113877	2.6646626047
h	-2.4769770305	3.1948204687	3.1128953368
h	-0.7345458599	2.8237169996	3.0613074690
h	-2.0833036072	0.7087354924	6.4347605295
h	-4.2069121209	1.2611671285	5.1581563112
h	-3.7851071274	-0.4636773954	5.0140628981

h	-2.4990079163	2.9641922717	5.4367370940
h	0.5257023405	2.2848681028	5.2249662179
h	-1.1334101178	4.2380791880	6.9828742991
h	0.7299604956	3.9973657609	6.9651525475
h	-0.7283905200	-2.3146075136	-0.1222795456
h	-2.5800942515	0.8902342049	-0.8811709192
h	-1.0878142734	1.3426085403	-1.7576425599
h	-2.4986784108	0.6919455203	-2.6477565825
h	-0.9891286443	-2.7603196396	-2.3061920203
h	-2.3594965149	-3.5974338184	-4.0257275424
h	-0.8510494100	0.4667321031	-4.3526903804
h	-3.2960602953	-3.4317973842	-6.3337819121
h	-1.7862939612	0.6277117194	-6.6431415628
h	-3.0242340193	-1.3096053238	-7.6500255712
h	-1.8898371162	-1.6592264657	2.5423072721
h	-0.9757145175	-3.4801657027	3.4246319467
h	1.1257131633	0.2411936921	0.9443293407
h	0.9919895461	-4.9234739982	3.9948823430
h	4.7468359736	-2.8895151780	2.4477968345
h	5.3163751477	-0.8015302419	1.1441065302
h	-1.5535149221	0.4080110969	0.8793536122
h	1.4350214763	-0.5437026311	-4.2872607256
h	1.1185492314	-0.5825268119	-2.3306812929

Product (PRDT) [Pathway-2]

75

c	-0.8036209244	-1.6561365327	-2.6641058455
o	0.6107850038	-1.2575375550	-2.7554062870
c	-3.5742397978	0.3539198522	4.7591052987
c	-2.2028350333	0.6860365944	5.3836798099
c	-1.1431232737	-0.2288735522	4.7289031069
c	-1.0404804992	0.1515306124	3.2231267813
n	-2.1306160764	1.0825223206	2.8408018596
c	-3.4562347645	0.5484876332	3.2147616500
c	-1.9094685793	2.3627742462	3.5317495764
c	-1.8963608001	2.1909723468	5.1021946719
c	-0.9979819118	-1.0691466678	2.2524738066
c	0.2624750952	-1.9063621709	2.4676164884
c	1.5902972691	-1.4784374355	2.1005157869
c	2.6931777990	-2.3454505962	2.4700300124
n	2.5271214409	-3.5352429659	3.1267164459
c	1.2926195409	-3.9067719984	3.4207103559
c	0.1391180378	-3.1349981225	3.1114236521
c	4.0274035652	-1.9597833206	2.1381734516

c	4.2786020421	-0.7793946288	1.4553113925
c	3.2006704860	0.0634276277	1.0724428801
c	1.8909081186	-0.2747540679	1.3891796227
h	3.3967477468	0.9793674993	0.4957821546
c	-0.6156162493	2.6771120435	5.7279404771
c	-0.5282102823	3.6102610121	6.6937634829
n	-1.1633783956	-0.5514005491	0.9050349248
c	-1.0007237319	-1.2623728936	-0.2502798075
c	-1.3057151664	-0.8183917138	-1.5141142395
c	-1.9134641162	0.5450363552	-1.7461167262
c	-1.5525322373	-1.5068462167	-3.9748775900
c	-1.2601278509	-0.4827323726	-4.8992729077
c	-2.0076276937	-0.3545849734	-6.0814594122
c	-3.0625988829	-1.2419788195	-6.3537245278
c	-3.3613733958	-2.2651042481	-5.4380300607
c	-2.6065831660	-2.3974100881	-4.2613984468
o	1.3078354588	-1.8543644579	-3.9112596772
o	1.7167026396	0.9660226320	-2.1528657528
c	2.2221000082	1.3752328034	-3.2950550296
c	2.9108394746	2.7591147357	-3.1372364263
f	3.7219755608	2.7763234728	-2.0559492279
o	2.1679908551	0.8079278569	-4.3795982638
f	3.6384618573	3.0600857052	-4.2197203956
f	1.9701612930	3.7164961537	-2.9713528843
h	-0.1033725598	0.7210490554	3.0527735625
h	-1.4531633752	-1.2888002776	4.8552886614
h	-0.1588954738	-0.1347148203	5.2292302610
h	-4.2204009644	1.2570321307	2.8348699845
h	-3.6187538994	-0.4036635370	2.6700034681
h	-2.7076205268	3.0685789939	3.2233833762
h	-0.9476581001	2.7891679813	3.1779282330
h	-2.2265098439	0.5178302470	6.4792347814
h	-4.3576530753	1.0128821879	5.1882602205
h	-3.8601578148	-0.6888150956	5.0104621659
h	-2.7308951829	2.7802784805	5.5401305369
h	0.3208340005	2.2300884149	5.3421441770
h	-1.4284960406	4.0950684069	7.1084953012
h	0.4429213010	3.9266767164	7.1054664621
h	-0.5346912496	-2.2545769011	-0.1200987092
h	-2.6211214192	0.8143036729	-0.9332187763
h	-1.1525530932	1.3577883841	-1.7939100248
h	-2.4845906917	0.5806104055	-2.6941888481
h	-0.7945378013	-2.7317073794	-2.3798253714
h	-2.8371028041	-3.2072860875	-3.5506143072
h	-0.4289986302	0.2101834191	-4.7041795520
h	-4.1809595997	-2.9705813994	-5.6445571772
h	-1.7601399638	0.4444237581	-6.7973092581
h	-3.6462799469	-1.1409398011	-7.2815924676
h	-1.8555731503	-1.7352003200	2.5241174636
h	-0.8567296511	-3.5154107328	3.3897777064

h	1.0692014334	0.3711677102	1.0546801047
h	1.1741696431	-4.8764890454	3.9393007375
h	4.8327929484	-2.6453731392	2.4396074345
h	5.3110317769	-0.4985989549	1.1962162987
h	-1.6259606633	0.3695175214	0.9009589795
h	1.5958132859	-1.0099920811	-4.3552719652
h	1.2288393158	0.0631319114	-2.3143871604

Reactant Complex (RC) [Pathway-3]

75

c	3.3613708563	0.5148236472	0.9367811235
o	3.7016199076	0.6804325823	-1.4459922275
c	5.8313475868	0.4117389007	0.7586787138
c	4.6779951593	1.0191508411	1.3252170333
c	4.8602169080	2.0353901516	2.3002353619
c	6.1478273565	2.4348826416	2.6842614880
c	7.2778230395	1.8410614428	2.0962428694
c	7.1130898406	0.8308804385	1.1304820225
c	2.1106316503	1.1452942216	1.0278485659
c	1.9004925714	2.6336552772	1.1956372586
c	0.9998741431	0.3085127010	0.7741478368
n	-0.2645370853	0.7086468044	0.6696667175
c	-1.3456302047	-0.1429442705	0.1536437391
c	-1.6768013069	-1.3408259283	1.0360819092
c	-2.0020078380	-1.2398779110	2.4371581608
c	-2.3790172745	-2.4615802745	3.1204821912
n	-2.4258453905	-3.6827840543	2.5041615925
c	-2.0992633887	-3.7371529258	1.2240098916
c	-1.7189463621	-2.6037701437	0.4518433464
c	-2.7229031223	-2.4123608795	4.5055722387
c	-2.6958906923	-1.2157094798	5.2051552782
c	-2.3154642325	-0.0171378002	4.5436758282
c	-1.9754064373	-0.0286873634	3.1964270062
h	-2.2830556723	0.9293140118	5.1050315402
c	-2.5733640933	0.7830350741	-0.0973416820
c	-3.6503449346	0.1588554241	-1.0300431198
c	-4.0794789472	1.2425626250	-2.0454998356
c	-2.8699068859	1.5622344209	-2.9489948079
c	-1.6837798521	1.9949199967	-2.0339856066
n	-2.1153526498	2.0955675443	-0.6158242745
c	-3.2341936368	3.0480606346	-0.5098983518
c	-4.4994753032	2.5588290412	-1.3172900540
c	-5.7194657966	2.4096548426	-0.4467221327
c	-6.9043740327	3.0112508231	-0.6591100374

o	4.5250454908	-0.3378724383	-2.0403133402
o	1.2842446299	-0.2290989008	-2.0782848024
c	1.5033964963	-1.3264905580	-2.6777214885
c	0.2646797727	-2.0544714443	-3.2883476092
f	0.4734070178	-2.4076598995	-4.5675141396
o	2.5885056882	-1.9282770212	-2.8391213507
f	-0.0151657409	-3.1871964625	-2.5828228410
f	-0.8662651196	-1.2925859890	-3.2551522674
h	-3.0319164036	1.0044815324	0.8897324996
h	-3.2423722507	-0.7127415914	-1.5839372433
h	-4.5130032793	-0.2144071322	-0.4433453072
h	-1.2848153016	2.9877718449	-2.3253699662
h	-0.8364900017	1.2825501150	-2.1035853594
h	-2.8874066686	4.0323153991	-0.8843820434
h	-3.4841283898	3.1791256662	0.5640989321
h	-4.9311656432	0.8759127194	-2.6533302057
h	-3.1375990432	2.3639938865	-3.6681008101
h	-2.5948367179	0.6700319840	-3.5461811697
h	-4.7363854618	3.3038822384	-2.1065997443
h	-5.6144929108	1.7558448783	0.4407685695
h	-7.0642194106	3.6792536327	-1.5226966803
h	-7.7589156343	2.8603281107	0.0188791092
h	1.1669562212	-0.7738511947	0.6512556288
h	1.1320693105	3.0068740585	0.4847631781
h	1.5568051575	2.9049677869	2.2173279350
h	2.8272401770	3.1973647767	0.9856056528
h	3.3431956030	-0.5545845225	0.6739659012
h	5.6976899583	-0.3517406001	-0.0233212337
h	3.9895998436	2.4864075392	2.7957162287
h	7.9945605406	0.3646031108	0.6644823936
h	6.2704932451	3.2121524588	3.4540309683
h	8.2878379243	2.1603511301	2.3963144194
h	-1.0049698815	-0.5374145075	-0.8285875636
h	-1.4510010606	-2.7390514411	-0.6068296860
h	-1.6599056147	0.9069185711	2.7154243440
h	-2.1303400025	-4.7321020786	0.7430720604
h	-3.0033159599	-3.3632299354	4.9815063371
h	-2.9619959494	-1.1911951667	6.2728914180
h	-0.5075064578	1.7149175975	0.5439513182
h	3.8388860509	-1.0396621195	-2.3378095448
h	2.7430960135	0.3948565889	-1.6894407675

Transition State (TS-3) [Pathway-3]

75

c	3.4172248314	0.4152707893	0.5436725109
o	3.8081715884	0.6124944586	-1.3131250229
c	5.9409788276	0.5070245209	0.7561041200

c	4.6598325042	0.9101437891	1.2043612624
c	4.5742047468	1.7086787663	2.3695328589
c	5.7321981279	2.1053393167	3.0567181082
c	6.9976805750	1.7171730600	2.5891152815
c	7.0950712057	0.9176309247	1.4366481500
c	2.1489891001	1.0818687081	0.6544311913
c	2.0107842761	2.5902836330	0.6719164550
c	1.0133922565	0.2855745542	0.5367100185
n	-0.2553538863	0.7348667369	0.4879457325
c	-1.3876269240	-0.0992765655	0.0731789074
c	-1.6649193097	-1.2887258121	0.9863735845
c	-1.8829220347	-1.1794387204	2.4071164436
c	-2.2342869812	-2.3917183768	3.1203139386
n	-2.3463258938	-3.6139646914	2.5143203986
c	-2.1090139253	-3.6788041445	1.2150790336
c	-1.7671194492	-2.5538460705	0.4137642486
c	-2.4803087418	-2.3308519884	4.5255964234
c	-2.3792843162	-1.1324692557	5.2153284702
c	-2.0184824015	0.0554023480	4.5239105824
c	-1.7736901750	0.0333370129	3.1564244173
h	-1.9233749758	1.0015910538	5.0786474557
c	-2.6217109932	0.8375014872	-0.0818927226
c	-3.8101909377	0.1867569770	-0.8485483427
c	-4.3030758097	1.1970129742	-1.9083600736
c	-3.1671790820	1.4151260711	-2.9305252345
c	-1.9151017223	1.9359118548	-2.1589613144
n	-2.2121539178	2.1139027214	-0.7172174038
c	-3.3123694603	3.0794587789	-0.5632636060
c	-4.6395357318	2.5749662693	-1.2550598000
c	-5.8046305967	2.5284494348	-0.3022372231
c	-6.9771385797	3.1658983641	-0.4753133363
o	4.6913609901	-0.3681797111	-1.8880479864
o	1.6681841153	-0.0699183547	-2.4019648578
c	1.7884631710	-1.3061265527	-2.6915759407
c	0.5401520776	-1.9896640436	-3.3226055987
f	0.7835337011	-2.3452705700	-4.5978199366
o	2.7834675224	-2.0447320488	-2.5339858923
f	0.2089103526	-3.1074112731	-2.6287052604
f	-0.5579366282	-1.1868504664	-3.3221675645
h	-2.9558731072	1.1168027580	0.9395398190
h	-3.4943181429	-0.7476123093	-1.3591052546
h	-4.6221072175	-0.0976269180	-0.1504707971
h	-1.5799471950	2.9195202332	-2.5456367092
h	-1.0519719977	1.2499713107	-2.2696349482
h	-2.9897992855	4.0478658597	-0.9964378005
h	-3.4791147043	3.2493521125	0.5212295766
h	-5.2078133381	0.8032412364	-2.4139441162
h	-3.4898502094	2.1381223951	-3.7083281310
h	-2.9384348953	0.4628523645	-3.4516937464
h	-4.9061511602	3.2693337371	-2.0808784711

h	-5.6652316084	1.9256312959	0.6160378679
h	-7.1686397376	3.7870529492	-1.3669128006
h	-7.7892738798	3.0930874256	0.2648913312
h	1.1234913730	-0.8117988198	0.4959474125
h	1.4087022147	2.9412369430	-0.1958132580
h	1.5014509087	2.9615855917	1.5882635540
h	2.9927256502	3.0924713474	0.6050638531
h	3.3572815443	-0.6864013998	0.4748742560
h	6.0159536855	-0.1126238359	-0.1487738294
h	3.5880815204	1.9950402171	2.7621528951
h	8.0829588567	0.6043065935	1.0651953822
h	5.6418139286	2.7184989810	3.9666207164
h	7.9065135373	2.0305604771	3.1257312188
h	-1.1627301038	-0.5181984003	-0.9335956038
h	-1.5755615875	-2.6947111408	-0.6611828870
h	-1.4640954379	0.9555335617	2.6468982513
h	-2.1891336520	-4.6751125110	0.7423899880
h	-2.7461620887	-3.2739622835	5.0248408236
h	-2.5692930588	-1.0988934172	6.2990245908
h	-0.4521957809	1.7362455597	0.3015353221
h	4.0411355013	-1.1303578149	-2.1187410736
h	2.8296329473	0.3787002440	-1.7885430594

Product (PRDT) [Pathway-3]

75

c	3.4698996954	0.2479071327	0.2736918716
o	3.7868316640	0.4011189971	-1.1588337010
c	5.6694164848	1.5149844930	0.6455430989
c	4.6340199763	0.6994121638	1.1410524333
c	4.6541032393	0.3162829307	2.4979903376
c	5.6867035478	0.7437682189	3.3463225480
c	6.7161612729	1.5607619581	2.8466586660
c	6.7042951314	1.9420908308	1.4952439538
c	2.1840722693	1.0108014726	0.4566213293
c	2.1852106925	2.5202090991	0.4970627035
c	1.0220039005	0.2848286938	0.4629909862
n	-0.2536111129	0.7912901788	0.5082107790
c	-1.4022120006	-0.0403858263	0.1555824289
c	-1.6862864876	-1.1735062203	1.1393541682
c	-1.8606727412	-0.9859083119	2.5577809823
c	-2.2327304356	-2.1466712473	3.3425573917
n	-2.3946893578	-3.3958572645	2.8061809824
c	-2.1920994304	-3.5356651464	1.5068310229
c	-1.8410158722	-2.4643002130	0.6396138733

c	-2.4465781450	-2.0014034547	4.7470111440
c	-2.2930486956	-0.7707274862	5.3667099735
c	-1.9063900126	0.3648355083	4.6047136245
c	-1.6911905036	0.2610464209	3.2363231896
h	-1.7646689484	1.3349160161	5.1058488329
c	-2.6301699168	0.8981845177	-0.0291174012
c	-3.8671814109	0.1992589230	-0.6696707221
c	-4.3788478605	1.0894803715	-1.8240318220
c	-3.2718885862	1.1693182178	-2.8966676682
c	-1.9968212321	1.7736694800	-2.2292056007
n	-2.2399073804	2.0990188048	-0.8067788580
c	-3.3259015291	3.0861951506	-0.7143123278
c	-4.6761305231	2.5385463569	-1.3251149757
c	-5.8256455372	2.6256781837	-0.3565794552
c	-6.9806761788	3.2800632501	-0.5779731998
o	4.8573723057	-0.5281563427	-1.5498440554
o	1.8208805318	-0.1302435702	-2.7416317393
c	1.9752414213	-1.4029973216	-3.0225176598
c	0.8079612334	-1.9378096529	-3.8984607119
f	0.7396812031	-1.2620815930	-5.0621024069
o	2.8906332756	-2.1375665559	-2.6691434225
f	0.9630916311	-3.2392327101	-4.1615229607
f	-0.3786468288	-1.7741129626	-3.2504563939
h	-2.9046738377	1.2811614833	0.9763745659
h	-3.5987681413	-0.7990781321	-1.0753441310
h	-4.6574923066	0.0226217904	0.0867094531
h	-1.6814464968	2.7115197271	-2.7300405086
h	-1.1328794320	1.0830786802	-2.2989796592
h	-3.0066367288	4.0094128265	-1.2397063447
h	-3.4629585016	3.3536326452	0.3542484566
h	-5.3033383094	0.6555046097	-2.2554093341
h	-3.6123031142	1.7915852951	-3.7505578920
h	-3.0637626226	0.1566465976	-3.3003720321
h	-4.9431218282	3.1426040852	-2.2196997475
h	-5.6886690293	2.1151156502	0.6162012758
h	-7.1675983911	3.8122566041	-1.5262611770
h	-7.7820458363	3.3104917804	0.1768162125
h	1.0734577598	-0.8187304153	0.4564712438
h	1.9242997813	2.9757823035	-0.4848692575
h	1.4524198156	2.9056113631	1.2383949040
h	3.1803854987	2.9132196627	0.7822605156
h	3.2850794946	-0.8362298317	0.4453940066
h	5.6700452254	1.7948616559	-0.4173656735
h	3.8475063848	-0.3221348385	2.8935482492
h	7.5113790599	2.5746540583	1.0939629619
h	5.6902693272	0.4338841094	4.4028737525
h	7.5292958714	1.8940247717	3.5098241570
h	-1.2190996338	-0.5340772735	-0.8302497540
h	-1.6944725057	-2.6612506222	-0.4344197852
h	-1.3501698797	1.1347079888	2.6654851930

h	-2.3132691205	-4.5529980701	1.0903715489
h	-2.7312632756	-2.9061972864	5.3036985760
h	-2.4593308667	-0.6718093091	6.4505216256
h	-0.4100449985	1.7643800200	0.1990925234
h	4.2958857332	-1.2733735769	-1.9139427080
h	2.5866602399	0.1632108059	-2.0925901787

Reactant Complex (RC) [Pathway-4]

75

c	-1.0712708284	2.6705954322	-1.4884361100
o	2.4525922942	1.6707421339	-0.0963925354
c	-1.0025700065	4.9858449658	-2.3438432109
c	-1.5632117546	4.0428633836	-1.4399537873
c	-2.5270212305	4.5026559256	-0.5024867491
c	-2.9397219631	5.8412803668	-0.5039622582
c	-2.4094908088	6.7480908375	-1.4388720640
c	-1.4343501752	6.3169010053	-2.3561524104
c	-1.7078061374	1.4945627011	-1.1424458013
c	-3.1354192592	1.3460477659	-0.6826515696
c	-0.8668664842	0.3258485604	-1.2115294455
n	-1.2727043587	-0.8835881964	-0.9024546896
c	-0.4787319122	-2.1322196043	-0.8321119541
c	-0.8533745005	-2.7527189123	0.5371143757
c	-0.2348397352	-4.1364003259	0.8551419242
c	-1.3134056912	-4.9533694719	1.6049111957
c	-1.9572173974	-4.1132372477	2.7574200188
c	-2.6818554787	-2.8902145805	2.0789685794
n	-2.3407549309	-2.7968575871	0.6419685362
c	-2.9003481098	-3.9733185013	-0.0618364950
c	-2.4272553361	-5.3046944314	0.5972076775
c	-0.9718678204	-3.6794180088	3.8184074073
c	-0.8417023078	-4.2671204873	5.0219448606
c	0.9986093100	-1.9075949024	-1.0941366526
c	1.5337534981	-2.0341845626	-2.4275750457
c	2.9278057368	-1.6928525246	-2.6116401781
n	3.7334916715	-1.2713053327	-1.5854699436
c	3.2076005813	-1.2048067383	-0.3704360937
c	1.8490617761	-1.5085990434	-0.0692523366
c	0.7843688349	-2.4376077760	-3.5742484832
c	1.3760996210	-2.5152420267	-4.8294149053
c	2.7468875864	-2.1867618796	-5.0027146482
c	3.5048653489	-1.7812210828	-3.9137852000
h	0.7766457281	-2.8335501417	-5.6959679152
o	2.0711079799	1.5340140056	-1.5022610200

o	0.1682318324	1.3152608228	1.2076032944
h	-2.1966910659	-1.0715158489	-0.4480547737
h	-0.5238942598	-2.0246291484	1.3091784425
h	0.0673768343	-4.6798573086	-0.0676676453
h	0.6801036467	-4.0161734917	1.4674959174
h	-4.0056886874	-3.8805667033	-0.0501509786
h	-2.5980653562	-3.9252117163	-1.1289241629
h	-3.7840024527	-2.9819771223	2.1647833746
h	-2.3905286078	-1.9397115824	2.5661190320
h	-0.8679159742	-5.8737379344	2.0326112542
h	-3.2655141589	-5.8146560824	1.1166454180
h	-2.0464017523	-6.0129471380	-0.1683560241
h	-2.7144855683	-4.7692997529	3.2395677915
h	-0.3453949444	-2.7986796029	3.5804537029
h	-1.4677681173	-5.1272427058	5.3173321283
h	-0.1092273007	-3.9069207385	5.7611754065
h	0.1858067645	0.4507741244	-1.5331575880
h	-3.6029789173	0.4388785387	-1.1203251819
h	-3.1871558492	1.2448100394	0.4226533122
h	-3.7551581019	2.2108934258	-0.9807299843
h	-0.0338671824	2.5639674996	-1.8530995392
h	-0.2244877387	4.6533951233	-3.0484534855
h	-2.8999746002	3.8221713383	0.2742550922
h	-0.9982852108	7.0279457384	-3.0741567087
h	-3.6719645168	6.1847141983	0.2425522458
h	-2.7405766870	7.7978745811	-1.4380224729
h	-0.8884268725	-2.7994687707	-1.6220828079
h	1.4711915598	-1.3353738920	0.9547229404
h	3.8727119202	-0.8609801200	0.4397712008
h	-0.2813534753	-2.6926870582	-3.4739316489
h	3.2040080739	-2.2542539472	-6.0017859885
h	4.5685240382	-1.5168454849	-4.0071310274
h	2.7918305192	0.9391116187	-1.8084859847
h	1.5776005540	1.4561777764	0.3741040938
c	-0.1408026806	0.5964892042	2.2009715795
o	0.2640870902	-0.5404932233	2.5358656280
c	-1.2743275872	1.1928723393	3.1062150176
f	-1.0788853782	0.9507197292	4.4155849350
f	-1.4466081289	2.5232257510	2.9510192471
f	-2.4786168726	0.6042752204	2.7651790174

Transition State (TS-4) [Pathway-4]

75

c	-0.7252077013	2.7108175498	-1.1677298379
o	-0.0946763634	3.1834328505	0.6668389671
c	-0.7318520088	4.7359617761	-2.6172837379

c	-1.2738589532	4.0446321258	-1.5086382792
c	-2.3053680094	4.6681819180	-0.7645873624
c	-2.7960192916	5.9269988303	-1.1419430421
c	-2.2697205904	6.5876629367	-2.2666575371
c	-1.2324807837	5.9894947800	-3.0012524477
c	-1.4848902583	1.5180549680	-1.0182320146
c	-2.9634407680	1.4814919267	-0.7112608815
c	-0.7520689877	0.3211007293	-1.1004131668
n	-1.2454741626	-0.8998171510	-0.8769430649
c	-0.5218041748	-2.1852194636	-0.8607476710
c	-0.8265810820	-2.8280667626	0.5168987309
c	-0.2687830250	-4.2598145460	0.7316587560
c	-1.3411127822	-5.0670462162	1.4991067045
c	-1.8519946144	-4.2790471420	2.7492150883
c	-2.5160178165	-2.9542722492	2.2089100479
n	-2.2970040633	-2.7936150813	0.7569308669
c	-2.9940535549	-3.8838932669	0.0401670695
c	-2.5399163848	-5.2852399508	0.5537888702
c	-0.7790609657	-4.0083514206	3.7768627428
c	-0.6547641313	-4.6670169763	4.9439911643
c	0.9573065990	-2.0654395264	-1.1983462752
c	1.4205335678	-2.2430808104	-2.5517119332
c	2.8476332037	-2.1527710545	-2.7858462142
n	3.7502669916	-1.8915359646	-1.7919696542
c	3.2787876109	-1.7039922467	-0.5689546714
c	1.9012159617	-1.7774160604	-0.2163336367
c	0.5690276577	-2.4873104923	-3.6733799349
c	1.0922947213	-2.6494809941	-4.9498763596
c	2.4946024258	-2.5776859888	-5.1714883442
c	3.3521267575	-2.3329979162	-4.1097752668
h	0.4143624298	-2.8330385365	-5.7975891534
o	1.0251470141	4.0829694056	0.5752137656
o	0.7985208320	1.0601952407	1.4275338008
h	-2.1575512608	-1.0221852602	-0.3986190733
h	-0.3924458553	-2.1523405571	1.2828201756
h	-0.0501319982	-4.7644832507	-0.2356450048
h	0.6859009364	-4.2227628387	1.2917885493
h	-4.0848150803	-3.7330583771	0.1764343634
h	-2.8008504149	-3.7731853213	-1.0472412422
h	-3.6093539086	-2.9547214010	2.3960407652
h	-2.0913617117	-2.0702964953	2.7254259588
h	-0.9241729972	-6.0392089782	1.8308226426
h	-3.3625290654	-5.8017897720	1.0916531878
h	-2.2460543081	-5.9433802011	-0.2906774100
h	-2.6305009186	-4.9135131411	3.2259388718
h	-0.0744948221	-3.1871416028	3.5482639721
h	-1.3524802757	-5.4732286513	5.2301914081
h	0.1455282540	-4.4230688374	5.6600933493
h	0.3137445051	0.3596559513	-1.3774974169
h	-3.4431630654	0.5908066720	-1.1686297133

h	-3.1587631195	1.4409610966	0.3818771546
h	-3.4853223962	2.3711445677	-1.1118544392
h	0.3068900090	2.5608579638	-1.5269548709
h	0.0880636060	4.2748397014	-3.1899752322
h	-2.6887643189	4.1799181447	0.1422685441
h	-0.8023962318	6.5055969878	-3.8732415389
h	-3.5919573638	6.4018547751	-0.5476897842
h	-2.6589969662	7.5743067000	-2.5612896099
h	-0.9944562345	-2.8307498307	-1.6348155492
h	1.6031848602	-1.5773362454	0.8264907863
h	4.0202538323	-1.4777723140	0.2189621585
h	-0.5212318040	-2.5349552459	-3.5331935279
h	2.8947731902	-2.7123177215	-6.1880501535
h	4.4418358325	-2.2622531067	-4.2409242926
h	0.5755230941	4.9320424747	0.7725004747
h	0.3614389799	2.1932257742	1.0952214258
c	0.3254850942	0.3873968178	2.4165256807
o	0.5581963287	-0.7979585897	2.6818803272
c	-0.6811449763	1.1567742972	3.3359339213
f	-0.9847055272	0.4614949271	4.4445567841
f	-0.2057978779	2.3647544954	3.7140591983
f	-1.8505214325	1.3731248536	2.6597888794

Product (PRDT) [Pathway-4]

75

c	-0.5218632172	2.7930634580	-0.8124848200
o	-0.2320193357	3.0883314684	0.6177943397
c	-0.8908471475	4.3032016908	-2.8138805612
c	-1.1383084566	4.0247534146	-1.4542811608
c	-1.9819043052	4.8933452445	-0.7267632411
c	-2.5608903355	6.0146626047	-1.3471460622
c	-2.3134243162	6.2770718945	-2.7041470053
c	-1.4768682270	5.4159895340	-3.4363433713
c	-1.3609609759	1.5506112368	-0.7939508737
c	-2.8339676137	1.5971792371	-0.4612618737
c	-0.7026348014	0.3574578041	-0.9954830190
n	-1.2618642999	-0.8847032154	-0.9342262599
c	-0.5340559347	-2.1617851242	-0.8627437958
c	-0.8433918390	-2.8059696402	0.5140445424
c	-0.2584898724	-4.2293314752	0.7366171251
c	-1.3370773989	-5.0826990114	1.4423090395
c	-1.9038283061	-4.3438472451	2.6979289846
c	-2.5626867801	-3.0095462704	2.1728021478
n	-2.3158607035	-2.8086198427	0.7339628591

c	-2.9805735688	-3.8910151083	-0.0224633910
c	-2.4997911670	-5.2980598508	0.4520874702
c	-0.8749439813	-4.0980093059	3.7732902276
c	-0.8141756101	-4.7587146021	4.9444147759
c	0.9496644520	-2.0405340982	-1.1869571715
c	1.4014114495	-2.1038193625	-2.5536968608
c	2.8274342950	-2.0336786885	-2.7949878628
n	3.7456747886	-1.8855336088	-1.7914706224
c	3.2878327475	-1.7929417124	-0.5528152538
c	1.9109244879	-1.8633423903	-0.1963269165
c	0.5292099278	-2.2164382979	-3.6798883011
c	1.0349879639	-2.2806950865	-4.9719205352
c	2.4372413049	-2.2362253419	-5.2032385303
c	3.3135091651	-2.1118999804	-4.1357260315
h	0.3439403001	-2.3633438580	-5.8248509187
o	0.7574547253	4.1826256585	0.7201236699
o	0.9508678048	1.0183676073	1.6462728699
h	-2.1684444486	-0.9879638617	-0.4531178979
h	-0.4387537733	-2.1215249924	1.2885389904
h	0.0148056877	-4.7081163922	-0.2295782920
h	0.6714568031	-4.1819265346	1.3361356269
h	-4.0752446372	-3.7687650704	0.1107361948
h	-2.7831053573	-3.7417128350	-1.1038462786
h	-3.6595495173	-3.0223737499	2.3381628348
h	-2.1619919384	-2.1325978757	2.7202768553
h	-0.9094354676	-6.0557858772	1.7578331060
h	-3.3219643040	-5.8595164825	0.9437474490
h	-2.1590039210	-5.9146325063	-0.4062686221
h	-2.6928159830	-5.0000089037	3.1253194733
h	-0.1376283600	-3.2972837867	3.5772934940
h	-1.5399468543	-5.5504472224	5.1991395774
h	-0.0402019075	-4.5318552158	5.6942753980
h	0.3693813602	0.3710738712	-1.2506075407
h	-3.3913154636	0.8062873209	-1.0076813334
h	-3.0352145976	1.4520468319	0.6230049889
h	-3.2879122504	2.5651428982	-0.7516150720
h	0.4583087685	2.5831620071	-1.2919800800
h	-0.2295025518	3.6366853901	-3.3905391291
h	-2.1877975137	4.6825944605	0.3350650569
h	-1.2725620382	5.6180927938	-4.4991432392
h	-3.2127625339	6.6844819871	-0.7650594513
h	-2.7690323702	7.1528358180	-3.1909421349
h	-0.9706100821	-2.8411362009	-1.6313426851
h	1.6350492880	-1.7551910128	0.8636664222
h	4.0405533882	-1.6557725635	0.2452415851
h	-0.5596243885	-2.2294480172	-3.5250462164
h	2.8230049850	-2.2941334609	-6.2326484524
h	4.4034625806	-2.0619125092	-4.2749550128
h	0.1604805281	4.9613490857	0.6333474800
h	0.4635151515	1.8830496394	1.3769575253

c	0.4554086432	0.3583481214	2.6738364008
o	0.7773355025	-0.7782523962	2.9737739914
c	-0.6367729724	1.0964183135	3.5111096834
f	-0.6607048732	0.6421308497	4.7699585150
f	-0.4403501944	2.4323255571	3.5396853952
f	-1.8587110696	0.8673161339	2.9570689193

CARTESIAN COORDINATES OF OPTIMIZED GEOMETRIES (B3LYP/SVP, Å)

Monoprotonated iminium cation 41 (Figure 2)

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C	0.222830	0.219656	-0.215985
C	1.694439	0.691136	-0.328093
C	2.105162	1.506954	-1.565633
H	1.934932	1.247332	0.588019
C	2.633761	-1.298462	-1.545828
C	3.970376	-0.117134	0.154251
C	3.483037	1.005338	-2.048974
H	1.365913	1.390074	-2.374580
H	2.128024	2.576467	-1.315674
H	3.182712	-2.229712	-1.347402
H	1.601019	-1.571040	-1.797579
C	3.306824	-0.414436	-2.619488
C	4.504415	0.933256	-0.873914
H	4.593437	-1.021738	0.191549
H	3.907071	0.293880	1.171387
H	3.879019	1.676813	-2.823818
H	4.282837	-0.832552	-2.908715
H	2.686518	-0.389659	-3.527645
H	5.448182	0.548906	-1.291213
N	2.588572	-0.535489	-0.249356
C	4.796522	2.269320	-0.234958
H	3.968222	2.756902	0.295791
C	5.981609	2.883731	-0.279322
H	6.842284	2.439531	-0.791057
H	6.137667	3.857306	0.193047
N	0.206269	-0.869802	0.766362
C	-0.914609	-1.270847	1.257871
C	-1.061573	-2.381738	2.188678
H	-1.853242	-0.755680	0.986805
C	0.159345	-3.183734	2.558618
H	0.950051	-3.042757	1.808989
H	0.574488	-2.876771	3.534301
H	-0.065747	-4.258180	2.618695
C	-2.337018	-2.597151	2.638147
H	-3.097050	-1.934465	2.207610
C	-2.895569	-3.558164	3.583140
C	-4.305499	-3.682638	3.619369
C	-2.140949	-4.349108	4.481893
C	-4.933069	-4.571564	4.488673
H	-4.911483	-3.069592	2.946337
C	-2.772501	-5.231284	5.357604
H	-1.057086	-4.260046	4.521778
C	-4.166799	-5.351921	5.361415
H	-6.022678	-4.652823	4.492632

H	-2.172095	-5.826883	6.049665
H	-4.655067	-6.045589	6.050423
H	-0.056739	-0.210733	-1.196065
C	-0.710070	1.405934	0.003868
C	-0.708576	2.205540	1.196919
C	-1.566674	1.769112	-1.023747
C	0.071616	1.928285	2.360750
C	-1.566216	3.361235	1.196573
C	-2.389344	2.914553	-0.899656
H	-1.610356	1.179563	-1.944055
C	0.028451	2.779310	3.457618
H	0.666494	1.018318	2.401776
C	-1.573493	4.215466	2.340857
H	-3.066398	3.190264	-1.717403
C	-0.797220	3.942251	3.435719
H	-2.227776	5.088593	2.306168
H	-0.796689	4.585191	4.318342
N	-2.379754	3.688847	0.161551
O	0.718015	2.599610	4.602960
C	1.536096	1.462334	4.765573
H	1.977712	1.534953	5.768126
H	0.952689	0.526620	4.695127
H	2.350854	1.435812	4.018121
H	2.082504	-1.110872	0.466292