

Mechanism and Selectivity of Cinchona Alkaloid Catalyzed [1,3]-Shifts of Allylic Trichloroacetimidates

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ENERGETICS

M05-2X/6-31+G(d,p)//B3LYP/6-31G(d)

Structure	Lowest Frequency cm ⁻¹	E_{gas} a.u.	$E_{\text{zpe+thermal}}$ a.u. 298.15K, 1atm	G_{gas} a.u.	ΔG_{sol} kcal/mol	G_{toluene} a.u.
trimethylamine	266.1	-174.449072	0.093888	-174.3551843	-1.79	-174.358043
1-Conformer 1	17.7	-2163.465358	0.179053	-2163.286305	4.86	-2163.278559
1-Conformer 2	14.9	-2163.465664	0.178438	-2163.287226	4.49	-2163.280076
1-Conformer 3	19.6	-2163.465366	0.179082	-2163.286284	4.87	-2163.278517
1-Conformer 4	17.3	-2163.464835	0.178916	-2163.285919	4.50	-2163.278748
1-Conformer 5	13.3	-2163.464882	0.178389	-2163.286493	4.22	-2163.279776
1-Conformer 6	13.0	-2163.463733	0.178220	-2163.285513	4.73	-2163.277983
2-Conformer 1	11.5	-2163.499868	0.180939	-2163.318929	2.91	-2163.314286
2-Conformer 2	15.7	-2163.499726	0.181225	-2163.318501	2.73	-2163.314159
2-Conformer 3	6.7	-2163.496475	0.178828	-2163.317647	2.30	-2163.313984
2-Conformer 4	8.2	-2163.497609	0.180427	-2163.317182	3.04	-2163.312333
3-Conformer 1	8.6	-2163.493558	0.178616	-2163.314942	4.32	-2163.308055
3-Conformer 2	9.2	-2163.491898	0.178471	-2163.313427	4.12	-2163.306867
3-Conformer 3	9.9	-2163.491847	0.178178	-2163.313669	4.12	-2163.307108
3-Conformer 4	6.5	-2163.491830	0.177937	-2163.313893	4.14	-2163.307300
TS-[3,3]-1	i438.5	-2163.423087	0.179415	-2163.243672	2.56	-2163.239588
TS-[3,3]-2	i441.9	-2163.422459	0.179382	-2163.243077	2.55	-2163.239019
TS-[3,3]-3	i471.2	-2163.415390	0.178795	-2163.236595	2.88	-2163.231998
TS-[3,3]-4	i422.8	-2163.406855	0.177367	-2163.229488	2.73	-2163.225144
TS-[3,3]-5	i459.1	-2163.413958	0.178763	-2163.235195	2.81	-2163.230713
TS-[3,3]-6	i398.6	-2163.405914	0.177450	-2163.228464	2.15	-2163.225033
TS-[1,3]-1	i252.1	-2163.382780	0.173512	-2163.209268	-3.63	-2163.215055
TS-[1,3]-2	i263.1	-2163.382584	0.173220	-2163.209364	-3.54	-2163.215006
Radical 1	57.3	-1587.192253	-0.003716	-1587.195969	-0.50	-576.164885
Radical 2	38.6	-576.160369	0.152710	-576.007659	0.13	-1587.039335
Ion 1	40.2	-1587.327070	-0.002381	-1587.329451	-21.20	-575.939351
Ion 2	43.9	-575.903185	0.155280	-575.747905	-28.49	-1587.217196
TS-SN2'-1a	i164.1	-2337.907698	0.298683	-2337.609015	3.67	-2337.603166
TS-SN2'-1b	i164.9	-2337.901740	0.298834	-2337.602906	2.54	-2337.598851
TS-SN2'-1c	i167.4	-2337.905351	0.297566	-2337.607785	5.33	-2337.599285
TS-SN2'-1d	i160.1	-2337.903177	0.299012	-2337.604165	4.52	-2337.596961
TS-SN2'-1e	i150.4	-2337.896524	0.297107	-2337.599417	2.51	-2337.595424
TS-SN2'-1f	i166.3	-2337.890480	0.297090	-2337.593390	1.01	-2337.591782
INT	12.9	-2337.919066	0.298351	-2337.620715	2.00	-2337.617533
TS-SN2'-2	i157.7	-2337.912598	0.300094	-2337.612504	2.59	-2337.608369

Reactions of Hindered Allylic Trichloroacetimidates:

Structure	Lowest Frequency cm ⁻¹	E_{gas} a.u.	$E_{\text{zpe+thermal}}$ a.u. 298.15K, 1atm	G_{gas} a.u.	ΔG_{sol} kcal/mol	G_{toluene} a.u.
4	16.5	-2201.579006	0.188118	-2201.390888	1.75	-2201.388094
[3,3]-Shift	i410.3	-2201.532390	0.187902	-2201.344488	0.40	-2201.343851
Amine Catalyzed [1,3]-Shift	i178.0	-2375.995524	0.307748	-2375.687776	-1.51	-2375.690184

Quinidine (QD) Catalyzed [1,3]-shift

Structure	Lowest Frequency cm ⁻¹	E_{gas} a.u.	$E_{\text{zpe+thermal}}$ a.u. 298.15K, 1atm	G_{gas} a.u.
QD	24.9	-1036.442844	0.361489	-1036.081355
(S)-TS-QD	i152.1	-3199.903211	0.566951	-3199.336260
(R)-TS-QD-I	i162.0	-3199.900084	0.565897	-3199.334187
(R)-TS-QD-II	i131.7	-3199.907217	0.569590	-3199.337627
(S)-INT-QD	12.3	-3199.917095	0.565165	-3199.351930
(R)-INT-QD	9.2	-3199.914910	0.566731	-3199.348179
(S)-TS2-QD	i166.6	-3199.908884	0.567694	-3199.341190
(R)-TS2-QD	i55.0	-3199.908762	0.568117	-3199.340645

Quinine (QN) Catalyzed [1,3]-shift

Structure	Lowest Frequency cm ⁻¹	E_{gas} a.u.	$E_{\text{zpe+thermal}}$ a.u. 298.15K, 1atm	G_{gas} a.u.
QN	21.3	-1036.442068	0.361292	-1036.080776
(S)-TS-QN	i136.6	-3199.905738	0.569051	-3199.336687
(R)-TS-QN	i155.7	-3199.901854	0.565541	-3199.336313
(S)-INT-QN	10.6	-3199.913628	0.565905	-3199.347723
(R)-INT-QN	13.0	-3199.916287	0.565718	-3199.350569
(S)-TS2-QN	i57.9	-3199.907742	0.567474	-3199.340268
(R)-TS2-QN	i159.8	-3199.907409	0.566460	-3199.340949

Quinidine Methyl Ether (QD-OCH3) Catalyzed [1,3]-shift

Structure	Lowest Frequency cm ⁻¹	E_{gas} a.u.	$E_{\text{zpe+thermal}}$ a.u. 298.15K, 1atm	G_{gas} a.u.
QD-OCH3	17.8	-1075.738786	0.387059	-1075.351727
(S)-TS-QD-OCH3	i155.2	-3239.200462	0.592821	-3238.607641
(R)-TS-QD-OCH3	i153.2	-3239.198660	0.594297	-3238.604363

CARTESIAN COORDINATES (Å)

Reactants and Catalysts

NMe₃

N, -0.1384117921, -0.036764
1737, -0.3428892592\C, -1.199277426, 0.4971927304, 0.4973800721\H, -1.53365
25221, 1.4629666955, 0.1022359751\H, -2.0550471252, -0.1870349227, 0.492044
1574\H, -0.889417583, 0.6481814692, 1.5517178413\C, 0.2789024844, -1.358430
7371, 0.0989491165\H, -0.5800311007, -2.0387650537, 0.0935712685\H, 1.03265
5706, -1.7571647581, -0.5891294109\H, 0.7120713532, -1.3633223085, 1.120145
5998\C, 0.9885107519, 0.8793588068, -0.4273471188\H, 1.7435279042, 0.475368
638, -1.11102617\H, 0.6522911149, 1.8437727496, -0.8241536237\H, 1.47766993
55, 1.0646219059, 0.5509267583\

1 – Conformer 1 $\Delta G_{\text{gas}}=0.6$ kcal/mol

C, 1.0826130268, 0.388736663
, 0.4678378065\C, 2.162737688, -0.6444670748, 0.2295181371\C, 4.2103374158,
-2.5146559781, -0.1909705587\C, 3.087144066, -0.9238542178, 1.2416135004\C
, 2.2682959572, -1.3153486989, -0.9960066156\C, 3.2854351071, -2.2476268418
, -1.2026848556\C, 4.1091118252, -1.8503718894, 1.0325096287\O, -0.18737289
47, -0.069468292, -0.1000940569\C, -0.9652073875, -0.8342854702, 0.67797070
59\N, -0.6628628358, -1.186364271, 1.8534139631\C, -2.2516943992, -1.187513
7403, -0.1175625285\Cl, -3.3659391726, -2.1958529522, 0.8736521972\Cl, -1.8
020723605, -2.1118868843, -1.5964766661\Cl, -3.1081112584, 0.3247292914, -0.
.5863178884\C, 1.3248964731, 1.749427499, -0.1599198605\C, 2.3468242538, 2.
0424045785, -0.970814192\C, 0.372665862, 2.8609620507, 0.1745660942\O, 0.35
34745943, 3.9448456189, -0.3713567241\O, -0.4565820072, 2.5261753386, 1.187
7305954\C, -1.3913215228, 3.5445011865, 1.5789190896\H, -1.3860381004, -1.7
579762153, 2.2861281155\H, 0.9256115235, 0.506948048, 1.5418558663\H, 3.091
1165014, 1.3046263242, -1.2479102776\H, 2.4469418637, 3.0479123527, -1.3663
552695\H, -1.9759908068, 3.1074855845, 2.3884949694\H, -2.0357506899, 3.813
6453048, 0.7383519927\H, -0.8621970754, 4.4375449601, 1.921867904\H, 1.5442
312964, -1.1146264856, -1.7799317008\H, 3.354568667, -2.7668553131, -2.1548
814624\H, 5.0017004444, -3.241473712, -0.3533903649\H, 4.8186174238, -2.060
1735858, 1.8283793107\H, 3.0007513015, -0.4192306783, 2.2008339649\

1 – Conformer 2 $\Delta G_{\text{gas}}=0.0$ kcal/mol

C, 0.845138198, -0
.2813525002, 0.2464535273\C, 1.4829436585, 0.5809829434, -0.8326263761\C, 2
.6490119611, 2.1685148444, -2.8238230888\C, 2.241481268, -0.0070617501, -1.
8487235806\C, 1.311989148, 1.9708787178, -0.819152836\C, 1.8877213487, 2.76
07635728, -1.81320747\C, 2.8259621809, 0.7842311483, -2.8384106022\O, -0.59
86009192, -0.0953062744, 0.2412526541\C, -1.3085604893, -0.8036107739, -0.6
467156837\N, -0.8081876263, -1.6606074797, -1.4290467457\C, -2.7990528459,
-0.3843460789, -0.5237379292\Cl, -3.3747873817, -0.7070816827, 1.153800159
8\Cl, -3.8271540884, -1.3112241687, -1.6717994974\Cl, -2.9575158662, 1.3703
268364, -0.8915643529\C, 1.3253735426, 0.0661129372, 1.6423902165\C, 0.5820
078065, 0.6777133647, 2.5706694187\C, 2.7259975281, -0.377230773, 1.9098994
274\O, 3.354107097, -1.1031434865, 1.1625694216\O, 3.22103176, 0.0965150784
, 3.0725351851\C, 4.5562207898, -0.3303482861, 3.3869831057\H, -1.509290791
, -2.1009265457, -2.0220739414\H, 1.0566383481, -1.3315057655, 0.0380354419
\H, -0.4479953195, 0.952711363, 2.3738437582\H, 0.9901524198, 0.8994470013,

3.5501257403\H, 4.6010071353, -1.4189989093, 3.4775636312\H, 4.7965932356, 0.1444403597, 4.3385878868\H, 5.2536052861, -0.009625099, 2.6087917928\H, 0.7254159079, 2.4328507597, -0.0297168671\H, 1.7465461545, 3.8382446515, -1.7965894209\H, 3.102120168, 2.7844237964, -3.5962519569\H, 3.4159016771, 0.317713148, -3.6227869247\H, 2.3728763081, -1.0844775892, -1.860343854\

1 – Conformer 3 $\Delta G_{\text{gas}}=0.6$ kcal/mol

C, 0.5496191778, 0.5086114405, -0.2176870859\C, 1.2516400059, -0.7423395288, -0.7254753859\C, 2.5126661913, -3.0747199925, -1.6324880299\C, 0.9051623765, -1.2986682133, -1.963032506\C, 2.2321658013, -1.3645095634, 0.0542250088\C, 2.8629929849, -2.5237926198, -0.3988073347\C, 1.5300554078, -2.4610993313, -2.4128440493\O, -0.8415686191, 0.1906493947, 0.0912396808\C, -1.1099528493, -0.3141992133, 1.301254526\N, -0.2456430382, -0.4782537585, 2.2094928834\C, -2.6275304352, -0.6406678205, 1.3661015179\Cl, -3.5757539259, 0.865115481, 1.0813021455\Cl, -3.0764491076, -1.3058298583, 2.9761009029\Cl, -3.0277830877, -1.8584349643, 0.1038175975\C, 0.5230398999, 1.641032455, -1.2251239463\C, -0.575296637, 2.0680750151, -1.8572834805\C, 1.815725915, 2.3340477826, -1.5308215689\O, 1.9762876383, 3.155047772, -2.4098538227\O, 2.7990043876, 1.9497899703, -0.6851260023\C, 4.0787263869, 2.5632795182, -0.9087660466\H, -0.6487888014, -0.8656154776, 3.0606695914\H, 1.0282231424, 0.8390363385, 0.7054994112\H, -1.5481044169, 1.630065164, -1.6693388561\H, -0.4993104464, 2.8816783335, -2.571087386\H, 4.4380050729, 2.3387377709, -1.9162514672\H, 4.7429334995, 2.1341499957, -0.1583625972\H, 4.008910666, 3.6475625607, -0.7888412144\H, 2.4907977805, -0.9423966794, 1.0205591448\H, 3.624593526, -2.9984915146, 0.214166303\H, 3.0027756025, -3.9783687204, -1.9852014862\H, 1.2535017621, -2.8851252906, -3.3744532541\H, 0.1474702995, -0.817622126, -2.5752343931\

1 – Conformer 4 $\Delta G_{\text{gas}}=0.8$ kcal/mol

C, 1.118871532, 0.4205129256, 0.4533746377\C, 2.1844829184, -0.6291586499, 0.2270579716\C, 4.2112953118, -2.5254268788, -0.1772903038\C, 3.1370563982, -0.8723531202, 1.2225411267\C, 2.2517680106, -1.3489647819, -0.9727945236\C, 3.2584448511, -2.2946767339, -1.1714794891\C, 4.1484520199, -1.8118080708, 1.0209484684\O, -0.1600444005, -0.018158947, -0.1030166558\C, -0.9471404464, -0.7612533901, 0.6890711113\N, -0.623657858, -1.1406874609, 1.8494759763\C, -2.2698863, -1.0482906407, -0.0718098487\Cl, -3.3855324409, -2.0450986886, 0.9291969315\Cl, -1.9006496652, -1.9514947048, -1.5888883496\Cl, -3.0847850999, 0.5026212161, -0.4740920448\C, 1.3765539249, 1.7698537801, -0.1926840874\C, 2.3822241891, 2.0325166298, -1.0337990704\C, 0.4213043599, 2.8357367286, 0.2463435217\O, -0.3394150155, 2.713913801, 1.1861893794\O, 0.5025264629, 3.9570444196, -0.5015890785\C, -0.3721097187, 5.0235809188, -0.0996989016\H, -1.3583734416, -1.6825616126, 2.300512694\H, 0.9648753403, 0.566945987, 1.5248456442\H, 3.0960812003, 1.2673736024, -1.319556069\H, 2.5159897913, 3.0258413797, -1.4470435146\H, -0.1885422825, 5.8326927755, -0.8071279635\H, -0.1442966044, 5.3445808582, 0.920353575\H, -1.4152173242, 4.7003646586, -0.1453091263\H, 1.5048617628, -1.1767582749, -1.7419520398\H, 3.2970628851, -2.852459607, -2.1034206468\H, 4.9944900923, -3.2626103226, -0.3327366757\H, 4.8796637838, -1.9941048796, 1.8038940205\H, 3.080170763, -0.3298719168, 2.1631063308\

1 – Conformer 5 $\Delta G_{\text{gas}}=0.5$ kcal/mol

C, 0.0658401998, -0.5585486979, 0.5556056721\C, 1.3994117058, -0.7396709057, 1.2630514361\C, 3.8335466943, -1.0961971789, 2.6057670815\C, 2.2821514791, 0.3355567131, 1.

4237512401\C, 1.7419320703, -1.9918705554, 1.7833729106\C, 2.9533329365, -2.1678154395, 2.4550777888\C, 3.4954181469, 0.1558311805, 2.0860750787\O, 0.3119314984, 0.2743628727, -0.6090114215\C, -0.4950308821, 0.1102602809, -1.6676023178\N, -1.4804573983, -0.6801706386, -1.6865175506\C, 0.0116722929, 1.0278777887, -2.8133781121\Cl, -1.036306943, 0.8797095823, -4.2677662616\Cl, 1.6897006743, 0.5586312429, -3.2556501246\Cl, -0.0128439306, 2.7459512656, -2.262586237\C, -0.9914139661, 0.0817633392, 1.44510333\C, -1.2859138165, 1.3854890633, 1.436868283\C, -1.6798583938, -0.882998676, 2.3519489619\O, -1.4808166569, -2.0838492628, 2.3348324267\O, -2.5528637687, -0.2920398473, 3.1939676698\C, -3.2530497355, -1.1842374949, 4.0754349405\H, -1.9610025912, -0.6808075468, -2.5844073077\H, -0.311005231, -1.5236117396, 0.2147391241\H, -0.7885238812, 2.0710420369, 0.7585281995\H, -2.0409187725, 1.7913659299, 2.1000568844\H, -2.5482573231, -1.7266491773, 4.7110893731\H, -3.8430764083, -1.9049865672, 3.5031282435\H, -3.9023449975, -0.5478119131, 4.677224706\H, 1.0510623221, -2.8222447029, 1.6743781977\H, 3.2091542564, -3.1453725979, 2.8550231754\H, 4.778914259, -1.2343987722, 3.1237729357\H, 4.1777866022, 0.9944301495, 2.1970898587\H, 2.026178358, 1.3084985884, 1.0153572551\\

1 – Conformer 6 $\Delta G_{\text{gas}} = 1.1$ kcal/mol

C, 0.7416775206, -0.3628211565, -0.0878686531\C, 1.8062451341, 0.6886107465, -0.3470581371\C, 3.7329909896, 2.6559293482, -0.8726208912\C, 2.2411382838, 1.5434992926, 0.6727065992\C, 2.3468935332, 0.826473665, -1.6295269266\C, 3.3080172444, 1.8033072289, -1.8924184049\C, 3.1956331294, 2.5252375145, 0.4101361899\O, -0.51069059, 0.359086828, 0.1242267435\C, -1.6366505788, -0.2066363423, -0.3348937165\N, -1.6854402048, -1.3466903903, -0.8785047285\C, -2.810481738, 0.7831626974, -0.0998242432\Cl, -2.9454371485, 1.1556463621, 1.6586447562\Cl, -4.3696790687, 0.0764621873, -0.6551539027\Cl, -2.5003240592, 2.2981393125, -1.018190845\C, 1.0350661784, -1.2505127359, 1.1084221642\C, 0.4203945642, -1.147317776, 2.2910560461\C, 2.0877716521, -2.3057103775, 0.958378531\O, 2.4823165067, -3.0303743962, 1.8481963315\O, 2.5529084715, -2.3677402484, -0.3104642595\C, 3.5678037621, -3.3568467076, -0.5459487991\H, -2.6269853677, -1.5946607433, -1.1766312301\H, 0.6145685161, -0.9873799781, -0.972752687\H, -0.3598071239, -0.4153282461, 2.4662746091\H, 0.6952463386, -1.8159085712, 3.1001031124\H, 3.8352718277, -3.255830301, -1.5979901951\H, 3.1798591284, -4.3579492288, -0.3404561901\H, 4.4354359994, -3.1730091425, 0.0927977738\H, 2.0162392669, 0.1621460161, -2.4239432031\H, 3.7228916768, 1.8980941788, -2.892332059\H, 4.481106229, 3.4177633961, -1.0749817594\H, 3.5238040891, 3.1857057036, 1.2082385356\H, 1.8327041579, 1.4371961843, 1.6735887188\\

Quinine (QN)

N, 7.3833615677, 5.94721845, -2.7675875489\C, 7.4480391884, 4.6577392601, -2.3203506703\C, 6.2107248934, 6.5410432055, -2.7218574151\C, 6.3135775739, 3.9366507545, -1.8177870835\C, 8.7065565185, 4.0089718743, -2.3567607601\C, 5.0265045032, 5.9276438864, -2.241900661\H, 6.1721417379, 7.5690831304, -3.0817872291\C, 5.0555479396, 4.6271163691, -1.788899036\C, 6.4927972023, 2.6042040572, -1.3760585373\C, 8.860043856, 2.7109398983, -1.92292042\H, 9.5492574799, 4.5751599956, -2.7408854492\H, 4.0953587136, 6.4842573707, -2.2310429172\C, 3.7907090485, 3.9483119522, -1.2787576111\C, 7.7386199435, 1.9992920535, -1.4250779677\H, 5.6644547473, 2.0197722993, -0.9906218406\H, 9.8371269373, 2.2433205873, -1.9631576504\C, 3.1914192447, 2.988415568, -2.3361365223\O, 2.7993049146, 4.9062581411, -0.9001146091\H, 4.0438000368, 3.3253631943, -0.4098844048\O, 7.7975224364, 0.7131766482, -0.972306431\C, 2.396911027, 3.6984380634, -3.4753364329\N, 2.386094016, 1.9135725672, -1.709934078\H, 4.0513875155, 2.4698792057, -2.7734625551\H, 3.17495363, 5.4441804504, -0.1851452703\C, 9.045541107, 0

.0375508458, -0.9912377318\C, 1.0818497491, 2.9225322867, -3.6989803347\H, 2.9927621959, 3.7431811011, -4.3934887426\H, 2.1559347621, 4.7287464989, -3.1963901344\C, 2.1545271269, 0.8752561012, -2.7265736215\C, 1.0756325613, 2.4115870225, -1.2400711565\H, 9.7899767332, 0.5420718781, -0.3613747173\H, 9.4401163481, -0.0585202727, -2.0112867868\H, 8.8498163668, -0.9574807376, -0.5876233753\C, 1.3589818981, 1.4164999679, -3.9733523444\C, 0.2436207354, 3.0234511739, -2.4093136194\H, 0.5334850259, 3.3520036566, -4.5450432312\H, 1.6076107857, 0.0520600299, -2.2532403862\H, 3.1282910175, 0.4764793839, -3.0353687913\H, 1.2504842379, 3.1512474495, -0.4582265806\H, 0.5546477414, 1.5617989819, -0.7842771389\C, 2.0793614657, 1.1582289457, -5.2675943792\H, 0.3858159954, 0.910209478, -4.0274569326\H, 0.0067638559, 4.0741556264, -2.2044964831\H, -0.7096258379, 2.4947485073, -2.5375037554\C, 1.582824279, 0.4746394278, -6.3005421185\H, 3.0924037893, 1.558100965, -5.3441256173\H, 2.15465518, 0.3143199948, -7.2108329798\H, 0.5819114582, 0.0473645047, -6.2748533101\\

Quinidine (QD)

C, -3.6756799474, 1.244283716
7, -0.1009819771\C, -2.435331501, 0.6829843176, -0.3595533392\C, -4.519926011, -0.8973886608, 0.6367045544\C, -2.1972395525, -0.6926705416, -0.1282176343\C, -4.731652529, 0.4434612831, 0.404479508\C, -3.2652200653, -1.5036038955, 0.3832418163\C, -0.94249606, -1.3417481434, -0.3813432268\C, -0.8516158294, -2.6902376753, -0.1158305902\C, -1.9721002841, -3.392208305, 0.3946873145\N, -3.1401015815, -2.8396897571, 0.640265609\H, -1.8847426791, -4.4580518505, 0.6050138844\H, 0.0791854761, -3.2167567229, -0.2983375041\H, -1.6574203898, 1.3355166158, -0.7408058172\H, -5.7042632297, 0.8763541812, 0.6085199296\H, -5.3119107162, -1.5315126165, 1.0226150781\C, 0.2536500243, -0.5687704626, -0.9208410352\O, 1.201874784, -1.4417018322, -1.5421958032\H, 0.7567380142, -1.8691042654, -2.2910246808\C, 0.9620219758, 0.2407294945, 0.1941310909\H, 0.1548455913, 0.6574114713, 0.8059709252\C, 1.9002968178, -0.6055604587, 1.1089099832\N, 1.6706349906, 1.4239964687, -0.3482901206\C, 3.1842939805, 0.2130936441, 1.3597878013\C, 2.7883515381, 1.6053805258, 1.89236739\C, 1.9666148779, 2.328830916, 0.7786179236\C, 2.9438832933, 1.046586872, -0.9907929727\C, 3.962932389, 0.418211296, 0.02798094\C, 4.6000390951, -0.8344336232, -0.5077169874\C, 5.915013096, -1.0350150789, -0.6167779202\H, -0.0956186707, 0.1669012591, -1.6578741516\H, 3.3677387479, 1.9477923603, -1.448319719\H, 3.9144164848, -1.6128201607, -0.8434829712\H, 6.3229746501, -1.9591976115, -1.0182295322\H, 6.6372833748, -0.280638164, -0.3089178988\H, 4.7664957331, 1.1397537588, 0.2318097728\H, 3.824514911, -0.3052458016, 2.0823167248\H, 3.6840568104, 2.1806547642, 2.1575899537\H, 2.1959036694, 1.4965662338, 2.8097414206\H, 1.0182359951, 2.7132864583, 1.1713362044\H, 1.4049852557, -0.8281006369, 2.0614699244\H, 2.5177164206, 3.1854181288, 0.3743294203\H, 2.7244755116, 0.342914022, -1.7955242595\H, 2.1448003393, -1.5637921097, 0.6430799134\O, -3.7946360354, 2.5785249726, -0.3623683824\C, -5.0401374493, 3.2150598386, -0.1216039834\H, -4.8973998771, 4.2604009868, -0.4012706322\H, -5.32620352, 3.1611714153, 0.9370506557\H, -5.8421633593, 2.7842213123, -0.7352676892\\

Quinidine methyl ether

H, 7.4543023483, 2.7852867447, -
0.4024324312\C, 6.7718815569, 1.9469144748, -0.3218662762\C, 5.3949702048, 2.15841939, -0.0545635972\C, 7.2465433439, 0.6639319863, -0.4802005383\C, 4.5297207491, 1.0811332606, 0.0474924426\O, 4.83678215, 3.3926058898, 0.1158335545\C, 6.3898831242, -0.4600422188, -0.383181607\H, 8.2955888134, 0.4755576053, -0.6859409767\C, 4.9972472482, -0.2455080988, -0.1098192574\H, 3.4849781252, 1.2930004148, 0.2473841172\C, 5.6692152264, 4.5382977041, 0.0244758694\N, 6.9414299415, -1.6977444603, -0.5559187326\C, 4.160171913, -1.4062

78063, -0.0107466544\H, 5.0138218601, 5.3948797563, 0.1922465354\H, 6.13130
 43211, 4.627138777, -0.9675498053\H, 6.4559182673, 4.5313833239, 0.79033224
 81\C, 6.1355336936, -2.7332103233, -0.459589949\C, 4.7478710514, -2.6390336
 848, -0.188761119\C, 2.6625717518, -1.2854649654, 0.2539365757\H, 6.5873865
 294, -3.7150862784, -0.5999601771\H, 4.1480799606, -3.5399847978, -0.114066
 6006\O, 2.1335696908, -2.4857859028, 0.8140648955\C, 1.8917387886, -0.92922
 83253, -1.04225008\H, 2.4824902301, -0.4612336429, 0.9583895544\H, 2.512980
 5432, -0.1815597093, -1.5472420444\C, 1.6631154692, -2.1285586424, -2.01161
 03676\N, 0.6175393048, -0.2277434964, -0.7560701174\C, 0.2421180402, -1.998
 7047291, -2.6007700174\H, 2.4076534913, -2.1172332282, -2.8162715251\H, 1.7
 714224984, -3.0826453919, -1.4887054762\C, 0.1812552744, 0.437066875, -1.99
 92417793\C, -0.4358606233, -1.1718421416, -0.337617001\C, 0.0736493153, -0.
 5788516581, -3.1805351864\C, -0.8216627758, -2.179321414, -1.4798287378\H,
 0.0871707806, -2.7521844416, -3.3809951711\H, 0.8897892281, 1.2409015368, -
 2.2298233146\H, -0.7861747106, 0.9101797702, -1.7955761552\H, -1.311170082
 7, -0.5884154144, -0.030113744\H, -0.0762322582, -1.7134096212, 0.538337131
 7\H, -0.8928684759, -0.4873415545, -3.6913556857\H, 0.8507148584, -0.390515
 8108, -3.9323105459\C, -0.9417993511, -3.5889563382, -0.9702823671\H, -1.79
 3850826, -1.8936198285, -1.905028032\C, -2.0289536297, -4.3543546532, -1.08
 61549856\H, -0.0674919161, -3.9857819539, -0.4527430606\H, -2.0628336876, -
 5.3664782099, -0.6910644126\H, -2.9304096105, -3.9977420204, -1.5817105015
 \C, 2.3945794297, -2.6320884864, 2.2014431294\H, 1.9340121804, -3.573563901
 8, 2.5112274216\H, 3.4715517586, -2.6720315665, 2.4133532969\H, 1.950683885
 4, -1.8073805358, 2.778769258\

Thermal [3,3]-rearrangement

TS-[3,3]-1

C, -1.3068685244, 0.4291246408, -0.623698624\C, -2.5961276774, -0.26730663
 45, -0.2777488855\C, -5.0825336437, -1.4790651509, 0.2208344823\C, -3.64499
 18822, 0.4648033901, 0.2958659797\C, -2.8132549112, -1.6127231566, -0.61179
 79953\C, -4.0444289173, -2.2136764167, -0.3579600207\C, -4.879819045, -0.13
 78227665, 0.543465489\O, -0.1277500667, -0.7953153607, -0.4739582803\C, 0.7
 647031061, -0.7155755449, 0.4541683701\N, 0.5860933203, -0.1555994594, 1.60
 62205614\C, 2.1419787754, -1.2976122433, -0.0099949369\Cl, 2.8092624318, -0
 .1979547891, -1.2721592748\Cl, 1.8958843905, -2.9362623151, -0.6958233405\
 Cl, 3.3159186887, -1.4111636334, 1.3541999823\C, -0.8418377267, 1.550191862
 9, 0.1633433488\C, -0.7200446107, 1.3149048968, 1.5342833736\C, -0.01386442
 01, 2.6108732579, -0.4206036352\O, 0.630827191, 3.4306338673, 0.2144005589\
 O, -0.0758224103, 2.631563077, -1.7831849817\C, 0.675721615, 3.677379357, -2
 .4103957452\H, 1.4253323352, -0.071572952, 2.1757356488\H, -1.1765688957, 0
 .5628827642, -1.6949817357\H, -1.4664978694, 0.7256322536, 2.0515537964\H,
 -0.1909440451, 2.049023539, 2.1346021643\H, 1.7384115489, 3.593009674, -2.1
 66575277\H, 0.3185960638, 4.6588196353, -2.0859237389\H, 0.5187254929, 3.54
 9175076, -3.4824397013\H, -2.0090481865, -2.1889106142, -1.0563245148\H, -4
 .1943897434, -3.2589385714, -0.6147548696\H, -6.0427167322, -1.9494604074,
 0.4149214403\H, -5.6815830899, 0.4449094649, 0.9890540563\H, -3.4918416318
 , 1.5126631493, 0.5343338852\

TS-[3,3]-2

C, 1.7434590537, 0.3794839021, -0.5036161921\C, 1.8209332521, 1.
 8030523316, -0.0298607207\C, 2.1278712917, 4.4790886378, 0.7724071157\C, 2.
 6794957941, 2.1378928027, 1.0266232473\C, 1.1277715405, 2.8293836347, -0.68
 99601028\C, 1.2761417948, 4.1545495077, -0.2868396675\C, 2.8313894096, 3.46
 75574809, 1.4247521512\O, 0.1238159212, 0.229996976, -1.0624743257\C, -0.68
 44292857, -0.5764144501, -0.4665558042\N, -0.6567426605, -0.8485115877, 0.7
 993679679\C, -1.6491614506, -1.2934802918, -1.4696961396\Cl, -0.6665096368
 , -2.4676908174, -2.4187440748\Cl, -2.389018702, -0.084583106, -2.565841752

2\Cl, -2.9683143222, -2.1802652424, -0.6121551637\C, 1.9640773586, -0.72417
03151, 0.4022888794\C, 1.1622969835, -0.7391732041, 1.5451591155\C, 2.54102
81197, -1.9457329489, -0.1686185785\O, 3.06753269, -2.0290732927, -1.267008
0496\O, 2.4755087639, -3.0050438484, 0.6890446174\C, 3.0647142848, -4.21642
12371, 0.2010566629\H, -1.2847739708, -1.5958882185, 1.0873639977\H, 2.2030
04542, 0.2199198973, -1.4777389504\H, 0.9376503141, 0.1925690563, 2.0497511
043\H, 1.1433132108, -1.6239908907, 2.1724567412\H, 4.1257325589, -4.070577
99, -0.0198847846\H, 2.5604924477, -4.5550263789, -0.7085231139\H, 2.938697
141, -4.9473767186, 1.0013756803\H, 0.4613810385, 2.5819484806, -1.50913893
35\H, 0.7266590363, 4.9372458258, -0.8030008009\H, 2.2442317006, 5.51407255
98, 1.0825338254\H, 3.5019585262, 3.7089136854, 2.2451426215\H, 3.240845184
4, 1.3527237995, 1.5234181371\

TS-[3,3]-3

C, 1.2258803613, 0.047566365, 1.2531442308\C, 2.3162606929, -0.6609480528,
0.5140505026\C, 4.4550882405, -1.9815069415, -0.7319132166\C, 2.1944399458
, -1.1154830111, -0.8049944899\C, 3.5116295721, -0.8940508846, 1.2066214418
\C, 4.5824243825, -1.5358716144, 0.583211876\C, 3.2557666713, -1.7757121176
, -1.4191882576\O, -0.1764092511, -0.9292337075, 0.8588550175\C, -1.3438292
403, -0.3892995075, 0.9117185829\N, -1.6780483817, 0.5689838563, 1.71645985
9\C, -2.3085489601, -0.945274089, -0.1933218704\Cl, -2.1913593072, -2.72899
36382, -0.2685081438\Cl, -1.7984055888, -0.2290818234, -1.7729881215\Cl, -4
.0233594042, -0.4871478736, 0.1280169833\C, 0.7994706464, 1.4169362798, 1.0
757494347\C, -0.1250895273, 1.8197556561, 2.0380132468\C, 0.8660844149, 2.2
367172426, -0.148035102\O, 0.2555759047, 3.2830803816, -0.3014078894\O, 1.7
235606809, 1.7558586282, -1.079526853\C, 1.8661096843, 2.5623030469, -2.256
0803818\H, -2.6028339161, 0.9581422694, 1.54448204\H, 1.255750581, -0.21614
89675, 2.3099321734\H, -0.0410482779, 1.4605342569, 3.0566377012\H, -0.6348
804763, 2.7684412882, 1.9045056691\H, 0.905999259, 2.6783306863, -2.7662525
388\H, 2.5756522413, 2.0277511478, -2.889003821\H, 2.2506845869, 3.55356693
82, -2.0006605107\H, 3.6091352207, -0.5639764005, 2.2384735852\H, 5.5061741
567, -1.6998384406, 1.1313112843\H, 5.2808449487, -2.4953218577, -1.2168166
326\H, 3.1457604464, -2.1332204388, -2.4395368874\H, 1.2645292826, -0.96227
61972, -1.3387699619\

TS-[3,3]-4

C, 0.8774692016, -0.180759611, 0.7139666334\C, 1.6798872892, -1.3631425292
, 0.3149688426\C, 3.1529581901, -3.6635104575, -0.3151170342\C, 2.115805690
6, -1.58587975, -0.9989878086\C, 1.9643647891, -2.3192583842, 1.2997729343\
C, 2.714705756, -3.4545907554, 0.9920198843\C, 2.8414251015, -2.7317054384,
-1.310208564\O, -0.4683907473, -0.2586329419, -0.6055951191\C, -1.41347118
68, 0.5922118633, -0.4378524255\N, -1.2313914579, 1.8778163027, -0.36263816
26\C, -2.8160339614, -0.0823988298, -0.1965277096\Cl, -2.8150428581, -0.700
2664527, 1.5169598442\Cl, -3.0588491515, -1.4481533593, -1.3215223574\Cl, -
4.1821203759, 1.081168705, -0.3846100719\C, 1.2569845672, 1.2007113865, 0.7
226010169\C, 0.2931080014, 2.0794204492, 1.1799048972\C, 2.4144876016, 1.83
46665193, 0.0311241125\O, 2.5552831497, 3.0390748066, -0.0731581536\O, 3.33
06580412, 0.9511914314, -0.413817113\C, 4.4907464059, 1.5274688536, -1.0340
098719\H, -2.0887460239, 2.3788072831, -0.1256832501\H, 0.1857004944, -0.42
36947428, 1.5176372028\H, -0.4597841402, 1.7588921662, 1.891005983\H, 0.459
4266514, 3.1450663584, 1.0798093942\H, 4.2053381198, 2.1265180999, -1.90256
9276\H, 5.1077585661, 0.6802668897, -1.334674711\H, 5.0276480559, 2.1638620
995, -0.3255460832\H, 1.6051351381, -2.1696919283, 2.3153498096\H, 2.939638
4438, -4.1800674972, 1.7688079062\H, 3.7234626054, -4.554630025, -0.5629057
527\H, 3.1631485116, -2.9021536326, -2.3340188156\H, 1.8598870814, -0.87053
69591, -1.7711977713\

TS-[3,3]-5

C, 0.1815109254, -0.6560297457, 1.6436411653\C, 0.9966655192, -1.8442181765, 1.2714221389\C, 2.4806491409, -4.1634061708, 0.7327870803\C, 1.6271483731, -2.0077514764, 0.0293837557\C, 1.0969445671, -2.8686424084, 2.2250070129\C, 1.8496346645, -4.0140251326, 1.9673336195\C, 2.3578058894, -3.1627452218, -0.2352700867\O, -1.0524560546, -0.6466822024, 0.3487906851\C, -1.6286658218, 0.462797303, 0.0547976148\N, -1.8849605623, 1.4106902631, 0.9022883527\C, -1.8923280733, 0.6138653299, -1.4855582825\Cl, -2.5329804515, -0.9136278022, -2.1585154575\Cl, -0.3110570213, 1.0148735824, -2.2640502237\Cl, -3.0689224601, 1.9407640044, -1.8334033805\C, 0.6032182633, 0.7219398436, 1.750512385\C, -0.3816306234, 1.5409810152, 2.295131569\C, 1.738010057, 1.3033176279, 1.0145781724\O, 2.5605597619, 0.7047647732, 0.3452614601\O, 1.8166917681, 2.6535306512, 1.2074689233\C, 2.9162420162, 3.2956936899, 0.5505188025\H, -2.2390619843, 2.2639376668, 0.4742119099\H, -0.512324565, -0.9101338552, 2.4428192695\H, -1.0608990998, 1.1442786633, 3.039973815\H, -0.253478609, 2.6169672464, 2.3033062181\H, 3.8686064851, 2.8913336544, 0.9042543072\H, 2.8319466101, 4.3530673616, 0.8058968435\H, 2.8570325879, 3.1580627129, -0.5327943039\H, 0.5885296766, -2.7642350862, 3.1809786775\H, 1.9282906354, -4.7910156039, 2.7227034654\H, 3.0585927095, -5.0590445978, 0.5205042666\H, 2.8374649704, -3.281305748, -1.2028899696\H, 1.5407501882, -1.2344752341, -0.721387148\

TS-[3,3]-6

C, 1.4589613953, 0.3099040036, 1.4947786917\C, 1.9956614267, -0.8135784022, 0.7013913686\C, 3.0635485878, -3.0327271717, -0.640305415\C, 1.6883137463, -1.0390806367, -0.6496614503\C, 2.8145156012, -1.7343812036, 1.3763396232\C, 3.3645305646, -2.8253530245, 0.705966851\C, 2.2156261814, -2.1449821006, -1.3090794887\O, -0.4232294015, -0.0331712618, 1.3138945726\C, -1.1554697331, 0.7109704316, 2.053685413\N, -1.1661566596, 2.0122686616, 2.0019184794\C, -1.9632769237, -0.097626125, 3.1411309437\Cl, -0.7827857732, -0.5375435356, 4.4582619794\Cl, -2.6506362347, -1.5872943888, 2.4372903272\Cl, -3.2983650174, 0.8722877084, 3.8747280673\C, 1.5338765877, 1.7219847865, 1.2612406188\C, 0.9776316481, 2.5116844609, 2.2474981009\C, 1.8858335238, 2.3301988032, -0.0489640658\O, 2.2281522688, 1.735492402, -1.0516593181\O, 1.8266954635, 3.685405138, 0.0032588339\C, 2.1560415547, 4.3571069139, -1.221194122\H, -1.7410303113, 2.4211783656, 2.7401428417\H, 1.4539703248, 0.0746579795, 2.5562725626\H, 0.8887414372, 2.1410372534, 3.2627558836\H, 0.8781620166, 3.5797942339, 2.1108900073\H, 3.1799204782, 4.1235462241, -1.5250947682\H, 2.0526083135, 5.4211897976, -1.0061355568\H, 1.4723104237, 4.0583123341, -2.0201419215\H, 3.0300068227, -1.587323637, 2.4321481851\H, 4.010431945, -3.5181583763, 1.2379650782\H, 3.4778064374, -3.8895008591, -1.1651678967\H, 1.9651539145, -2.3150133408, -2.352402238\H, 1.0301808108, -0.3564521142, -1.1686062779\

Thermal [1,3]-rearrangement

TS-[1,3]-1

C, 1.4950365479, 0.5276895965, -0.6821039611\C, 1.3485528472, 1.8714498314, -0.1965758277\C, 1.1256101332, 4.5599913338, 0.5698565711\C, 0.794357606, 2.8303838603, -1.0777840912\C, 1.8081920751, 2.2968280252, 1.0706450702\C, 1.6990819377, 3.6297973131, 1.4436850866\C, 0.6732108894, 4.1569622873, -0.6920004749\O, -0.7652097506, 0.1423047845, 0.3942126261\C, -1.2360411966, -0.3083386574, -0.6765216801\N, -0.6215752368, -0.3469798258, -1.8217576933\C, -2.7186531489, -0.8488170244, -0.5133906492\Cl, -2.7095862649, -2.1888848452, 0.6977485374\Cl, -3.4482354894, -1.4917864333, -2.0470464003\Cl, -3.7655649422, 0.4901941909, 0.0821015847\C, 2.029422157, -0.6229706515, 0.0306967686\C, 1.7061964514, -0.963677127, 1.2964024585\C, 2.94093

36954, -1.4773683706, -0.8057883828\0, 3.2412288515, -1.2180952324, -1.9536587457\0, 3.3973207398, -2.5539411121, -0.1386357005\C, 4.2804764767, -3.4104747557, -0.884788454\H, -1.1361413473, -0.7905941317, -2.5792073087\H, 1.5162799499, 0.4198317842, -1.7552979171\H, 0.9514444687, -0.4103783515, 1.8405651707\H, 2.1380025726, -1.8460663754, 1.7553953713\H, 3.7675777429, -3.8138080459, -1.7612982246\H, 4.5565942512, -4.210412973, -0.1978521969\H, 5.1648191809, -2.8569317907, -1.2103970832\H, 2.2835588998, 1.585729645, 1.7366644837\H, 2.0672437255, 3.9508856788, 2.4136389385\H, 1.039749349, 5.6009983081, 0.8689427049\H, 0.2293058496, 4.8810693838, -1.3685904975\H, 0.4227456983, 2.4940832005, -2.0408920836\

TS-[1,3]-2

C, -1.5787660595, 0.248612144, 0.5406984106\C, -1.670054785, 1.6523171925, 0.2532328716\C, -1.9024826592, 4.4204762451, -0.1277374949\C, -1.178799237, 2.5586200804, 1.2237200842\C, -2.3001456162, 2.1671310266, -0.903139997\C, -2.4152285895, 3.5386758906, -1.0854238068\C, -1.2838626128, 3.9270876444, 1.0274033423\0, 0.6615196212, 0.4060928808, -0.7249482341\C, 1.2729944075, -0.070587226, 0.2577426227\N, 0.757283534, -0.357884824, 1.4182929554\C, 2.8198634071, -0.2880218998, -0.0311130133\Cl, 2.995888423, -1.3963546631, -1.4436248189\Cl, 3.7442504898, -1.0084531051, 1.3581339945\Cl, 3.5611681847, 1.3075121934, -0.4234272088\C, -1.9969454578, -0.8466093732, -0.3166785785\C, -1.6911990516, -0.9576370019, -1.6271409207\C, -2.7719006147, -1.9809182739, 0.3036394877\0, -3.2117772679, -2.9242834144, -0.3172127183\0, -2.9379747724, -1.8137411792, 1.6310459063\C, -3.645335208, -2.8720033826, 2.3031113426\H, 1.3995874676, -0.7842013343, 2.0824646087\H, -1.4630038501, -0.007213788, 1.5809889264\H, -1.0337253908, -0.2445581445, -2.1070247668\H, -2.0390409885, -1.8240737631, -2.18126653\H, -4.6514428638, -2.978306261, 1.8901273489\H, -3.6856567733, -2.5738581021, 3.3505906022\H, -3.1090249586, -3.8173060787, 2.1905757205\H, -2.7278157055, 1.4859468946, -1.6300984024\H, -2.9114624214, 3.9261247209, -1.9702894913\H, -1.9923437241, 5.4928384938, -0.2776348019\H, -0.8858197433, 4.6144025322, 1.7678815494\H, -0.6717768539, 2.1574427355, 2.0958823896\

Radical 1

0, 1.4721261519, 1.7456071392, -0.1021441646\C, 1.2656321519, 0.5516041392, -0.0972431646\N, 2.2945301519, -0.3646608608, -0.1914011646\C, -0.1924908481, -0.0215378608, -0.0111891646\Cl, -0.4291178481, -0.5878488608, 1.6922508354\Cl, -0.3305978481, -1.4259158608, -1.1336521646\Cl, -1.3843208481, 1.2219991392, -0.4218591646\H, 2.1710531519, -1.1326138608, 0.4829838354\

Radical 2

C, -0.045121957, -0.5257950323, -0.048111\C, -1.457081957, -0.2401630323, 0.003761\C, -4.262073957, 0.1433759677, 0.091117\C, -2.358529957, -1.3097580323, -0.229426\C, -2.015936957, 1.0234219677, 0.317799\C, -3.394111957, 1.2062049677, 0.359087\C, -3.733775957, -1.1194900323, -0.197477\C, 1.057862043, 0.3522649677, -0.18744\C, 1.030207043, 1.6810229677, -0.550783\C, 2.393419043, -0.3166130323, 0.029083\0, 2.545790043, -1.5058150323, 0.227569\0, 3.427543043, 0.5520519677, -0.018943\C, 4.724612043, -0.0298310323, 0.180154\H, 0.225108043, -1.5754880323, 0.023794\H, 0.107377043, 2.1756279677, -0.82589\H, 1.946079043, 2.2517039677, -0.628851\H, 5.429172043, 0.8000299677, 0.116343\H, 4.935183043, -0.7740110323, -0.592571\H, 4.783661043, -0.5108290323, 1.16012\H, -1.364367957, 1.8486529677, 0.580321\H, -3.796136957, 2.1834939677, 0.613538\H, -5.337656957, 0.2937199677, 0.12123\H, -4.398698957, -1.9566260323, -0.392863\H, -1.953188957, -2.2940140323, -0.450763\

Ion 1

0, -2.1378679114, -0.7680371266, -0.00
 09870506\C, -1.5228009114, 0.3083428734, -0.0007860506\N, -1.9111239114, 1.
 5478648734, -0.0010940506\C, 0.1083360886, -0.0069731266, -0.0000030506\Cl
 , 0.5501030886, -0.9893711266, 1.4761479494\Cl, 1.2551490886, 1.4695838734,
 0.0000519494\Cl, 0.5521930886, -0.9905211266, -1.4749380506\H, -1.10896991
 14, 2.1762668734, -0.0011620506\\

Ion 2

C, 0.0751319355, -0.5519209677, 0.20392796
 77\C, 1.4342409355, -0.2546779677, 0.0280599677\C, 4.1857619355, 0.19504403
 23, -0.2019450323\C, 2.3698219355, -1.3169929677, 0.2471439677\C, 1.9279939
 355, 1.0296920323, -0.3678840323\C, 3.2873519355, 1.2438240323, -0.47458703
 23\C, 3.7285719355, -1.0835449677, 0.1549599677\C, -1.0512610645, 0.3303070
 323, 0.3050859677\C, -0.9912770645, 1.5863790323, 0.8195799677\C, -2.381903
 0645, -0.3278719677, -0.0193570323\O, -2.4747440645, -1.5222889677, -0.2012
 660323\O, -3.3727760645, 0.5553450323, -0.0663830323\C, -4.6902350645, 0.02
 04530323, -0.3699050323\H, -0.1964880645, -1.6065699677, 0.2546229677\H, -0
 .0683070645, 2.0109200323, 1.2009229677\H, -1.8958110645, 2.1754020323, 0.9
 298309677\H, -5.3524570645, 0.8840920323, -0.3721720323\H, -4.9820110645, -
 0.6981689677, 0.3979879677\H, -4.6741750645, -0.4656639677, -1.3469690323\
 H, 1.2312609355, 1.8122440323, -0.6463090323\H, 3.6657979355, 2.2094580323,
 -0.7932740323\H, 5.2534679355, 0.3724350323, -0.2961010323\H, 4.4375809355
 , -1.8826789677, 0.3435719677\H, 1.9961129355, -2.3000599677, 0.5186029677\
 \

Catalyzed [1,3]-rearrangement

Model Catalyst (N(CH₃)₃)

TS-S_N2'-1

a

C, 0.9027429947, 0.4692787261, -0.9754738008\C, 1.630790833,
 1.746368005, -0.6450708389\C, 3.0951827128, 4.1225053354, -0.2240403065\C,
 1.0305322399, 2.8627061584, -0.0471842169\C, 2.9768787555, 1.8490253358, -1
 .0402950553\C, 3.701329717, 3.0232937119, -0.8334625937\C, 1.7581470291, 4.
 034966948, 0.1651298465\O, -0.6592100495, 0.5923984132, -0.0051850874\C, -1
 .7263436588, 0.9415451633, -0.6701455716\N, -1.7361406552, 1.566166556, -1.
 7837248554\C, -3.0149254954, 0.4533242933, 0.0878037148\Cl, -3.0497236993,
 -1.3578084362, 0.0961554462\Cl, -4.5420234495, 1.0404139393, -0.6724705669
 \Cl, -2.9838168596, 1.0464066587, 1.7991849872\C, 1.4750846653, -0.78591865
 32, -0.6571548863\C, 2.3756442921, -1.0013883624, 0.4783344732\C, 1.1293235
 189, -1.9856648446, -1.3970451975\O, 1.5163311725, -3.1245465598, -1.122139
 1786\O, 0.3316768677, -1.7541319237, -2.4779618173\C, -0.0189619257, -2.909
 0652866, -3.2429949667\H, -2.6798869262, 1.7121605415, -2.1368759834\H, 0.3
 839540607, 0.512768827, -1.9293434225\H, 3.0021204571, -0.1425656714, 0.726
 7751521\H, 2.9807014224, -1.8960494357, 0.3273413913\H, 0.8697839617, -3.37
 81193068, -3.6760943397\H, -0.6793350343, -2.5467354551, -4.0326064816\H, -
 0.5362217624, -3.6475351706, -2.6234388468\H, 3.4487983666, 1.0018481291, -
 1.5302188428\H, 4.7388033443, 3.0775711077, -1.1538177967\H, 3.6564445703,
 5.0388423939, -0.0607154639\H, 1.2710549369, 4.8866230163, 0.6334359968\H,
 -0.0071702513, 2.8075812807, 0.2534015104\N, 1.6723233856, -1.3155420827, 1
 .915104582\C, 2.7140640159, -1.9036236747, 2.8038799829\H, 3.0387717314, -2
 .8590391878, 2.387779439\H, 3.5630502847, -1.2182511644, 2.8576667287\H, 2.
 3012463261, -2.0568098044, 3.8041688062\C, 1.1482473342, -0.0476685597, 2.5
 14922116\H, 1.9769460794, 0.6506393455, 2.647959316\H, 0.4013290946, 0.3733
 25019, 1.8407992776\H, 0.6962797682, -0.2776122624, 3.4836936002\C, 0.54159

8715, -2.283202323, 1.7390891008\H, -0.2344230147, -1.7909161441, 1.1540437
751\H, 0.9079801511, -3.1553718025, 1.1981846248\H, 0.1587183872, -2.553097
493, 2.7269980089\\

b

C, -0.9487128851, -0.3735441953, -1.0307078596\C, -1.681129
6098, -1.6583106188, -0.7635102814\C, -3.1510289181, -4.0498847696, -0.4622
257284\C, -1.0703970083, -2.818869349, -0.2668277136\C, -3.0391994127, -1.7
271111793, -1.1248797623\C, -3.7667608861, -2.9085142462, -0.9760230218\C,
-1.8005276898, -3.9980140286, -0.1135185981\O, 0.597330573, -0.5194194572,
0.0286305161\C, 1.6879452044, -0.8801211266, -0.5879173376\N, 1.7383138369
, -1.536100615, -1.6825579149\C, 2.9507798192, -0.3714097219, 0.2009121423\
Cl, 2.9928524415, 1.4377294501, 0.1585405147\Cl, 4.5032357865, -0.986125375
8, -0.4814021022\Cl, 2.8538516733, -0.9133247972, 1.9296474143\C, -1.519511
4452, 0.8776930434, -0.7047012783\C, -2.4297706518, 1.0735995126, 0.4239025
602\C, -1.0836751948, 2.0174990367, -1.4977196497\O, -0.3423794808, 1.99313
05803, -2.466539806\O, -1.6386703334, 3.215383686, -1.0648652507\C, -1.3166
910205, 4.3452552112, -1.8820653896\H, 2.6934123993, -1.6843707992, -2.0027
701012\H, -0.3732153349, -0.3769748598, -1.9539823939\H, -3.0707265625, 0.2
153756586, 0.6348172146\H, -3.0275331415, 1.9777521032, 0.3161252551\H, -0.
2358936144, 4.5085916079, -1.9179618891\H, -1.8166607736, 5.1987184031, -1.
4186997617\H, -1.6786693436, 4.2040518664, -2.9046018267\H, -3.5171046609,
-0.8492776399, -1.5505990378\H, -4.8133274111, -2.935150001, -1.2691982951
\H, -3.7141860333, -4.9720265192, -0.3442760738\H, -1.3052236872, -4.883821
1319, 0.2760809624\H, -0.0213729724, -2.7940147089, -0.0057045582\N, -1.733
5281443, 1.3053071272, 1.8935971866\C, -2.7596095454, 1.918829788, 2.782086
599\H, -3.0236947882, 2.9052107848, 2.3960529161\H, -3.6459159008, 1.280198
0617, 2.7946065802\H, -2.3612783103, 2.0135747132, 3.7955063963\C, -1.29563
46737, -0.0113297674, 2.4596892122\H, -2.1644727897, -0.6675354212, 2.54073
93583\H, -0.5483926457, -0.4454835725, 1.7942040638\H, -0.8642378444, 0.158
9026687, 3.4500280041\C, -0.5456948782, 2.2075652243, 1.7726023466\H, 0.199
8025594, 1.7057254956, 1.1562143708\H, -0.858144052, 3.1358904004, 1.295066
8393\H, -0.1481765596, 2.3967142414, 2.7733369046\\

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TS-S_N2'-2

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Quinidine (QD)

TS-S_N2'-1

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Quinine (QN)

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(S)-TS2-QN

C, 1.0868760714, -0.3642215354, 1.2518539993\C, 1.7222793057, -1.6548974005, 0.853542045\C, 3.0650619223, -4.0595691742, 0.2820060515\C, 1.5527732845, -2.2838443654, -0.3868382983\C, 2.5596878659, -2.2560860063, 1.809464881\C, 3.2292798936, -3.4458322143, 1.5249607449\C, 2.2234331958, -3.4765756758, -0.6661484721\O, -0.6872624307, -0.4185290203, -1.91889625\C, -1.3964986302, -0.6309961587, -0.9064906553\N, -1.0095801038, -0.7184889098, 0.335185789\C, -2.94148479, -0.7981561308, -1.2749031136\C1, -3.5207625197, 0.7452570795, -2.0294639108\C1, -4.0291931744, -1.1601631705, 0.1377569291\C1, -3.1164578413, -2.1379496503, -2.4673322085\C, 1.5811167037, 0.8839808158, 0.9349651399\C, 2.6227941514, 1.1204160519, -0.1104692532\C, 1.2135678783, 2.0453207359, 1.7392483602\O, 1.6906612329, 3.1786627033, 1.5979967176\O, 0.3090118445, 1.7951509632, 2.7068237812\C, -0.0617189135, 2.9113585856, 3.5291195299\H, -1.7590694166, -0.9008115027, 0.9967079897\H, 0.5037299167, -0.4120615578, 2.1627606933\H, 3.091224953, 0.1787591495, -0.3926492138\H, 3.3879509367, 1.7809522201, 0.2850883129\H, 0.806741146, 3.3036454972, 4.0649290211\H, -0.7995915819, 2.5199328009, 4.2299038202\H, -0.496836506, 3.7095352642, 2.9222154146\H, 2.6898298695, -1.7844491544, 2.780870148\H, 3.8730837089, -3.8942048615, 2.2772029238\H, 3.5802871568, -4.9903111474, 0.059536195\H, 2.0727861535, -3.9578291507, -1.629045811\H, 0.8649876881, -1.8568372773, -1.1087870774\N, 6.6461391157, 6.4453117829, -2.8480998359\C, 6.9636060614, 5.1692208042, -2.4819196612\C, 5.4315564007, 6.8674072854, -2.5697745701\C, 6.0420498588, 4.2789455937, -1.833911424\C, 8.278084897, 4.7140720001, -2.7517333235\C, 4.4379695643, 6.0742535841, -1.9441921208\H, 5.1964831259, 7.8928206318, -2.8531869734\C, 4.7182164123, 4.7738260994, -1.5904850644\C, 6.4965263031, 2.9913276103, -1.4602276348\C, 8.6927209831, 3.450608049, -2.3947093794\H, 8.9515751776, 5.4054164803, -3.2482440357\H, 3.4597752153, 6.4902110792, -1.7337765582\C, 3.6391633578, 3.9060009235, -0.9492540195\C, 7.7915766776, 2.5791724219, -1.7313312821\H, 5.8575513338, 2.2943700582, -0.9289994401\H, 9.7061575073, 3.1350285684, -2.6140446247\C, 3.179594218, 2.8279990116, -1.983644147\O, 2.56605799, 4.714178862, -0.5190959358\H, 4.1000431766, 3.4168761337, -0.0838439298\O, 8.1147607357, 1.3195210547, -1.3215854678\C, 2.5959071333, 3.477446381, -3.2616913955\N, 2.1676069649, 1.7724490229, -1.4722483952\H, 4.0566145143, 2.2259951805, -2.2364143893\H, 2.2301417475, 4.3170518985, 0.3126735399\C, 9.4332229854, 0.8410739728, -1.5495641464\C, 1.4126495896, 2.6630207141, -3.8021784943\H, 3.3926472943, 3.573609309, -4.0046356575\H, 2.2516126086, 4.4888558342, -3.0250633415\C, 2.1401292268, 0.6519250701, -2.5144323618\C, 0.7532090791, 2.3480911138, -1.3943866343\H, 10.1822249764, 1.4604135893, -1.0398146708\H, 9.667778241, 0.7949060265, -2.6208300896\H, 9.4575662875, -0.1674560286, -1.1334497013\C, 1.786896925, 1.1691728736, -3.9340029618\C, 0.2610517667, 2.7719850477, -2.7939525395\H, 1.1052795001, 3.052056051, -4.7782126316\H, 1.3768016891, -0.0446614741, -2.1666297109\H, 3.1259439996, 0.1814665274, -2.4872530006\H, 0.7973566384, 3.1821940872, -0.7047864964\H, 0.1358846176, 1.5494767525, -0.9912880207\C, 2.8853276792, 0.9004573343, -4.9313752003\H, 0.890456265, 0.6293589097, -4.2582087027\H, -0.1038257933, 3.8037307672, -2.7529365746\H, -0.5716589712, 2.1273745368, -3.0897887536\C, 2.7266756638, 0.1929594838, -6.0504385905\H, 3.8688880822, 1.316980233, -4.7058392422\H, 3.5460431247, 0.0304156, -6.7453215143\H, 1.7691650514, -0.2517650116, -6.3138086477\\

Quinidine methyl ether

TS-S_N2'-1

(R)-TS-QD-OCH₃

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-2.0322135167, 3.242397148, -1.0357334802\C, -0.4638285745, 3.685405872, 0.
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02843308, -1.6997918824\O, -2.9568883832, 0.7290119589, -0.1427319941\C, -4
.249118304, 0.8601300323, -0.0093277587\N, -4.8427118678, 1.8313891567, 0.5
682037082\C, -4.9796894087, -0.3760614525, -0.6500477616\Cl, -4.542596762,
-1.8735989723, 0.2668387361\Cl, -6.7769268478, -0.2130879187, -0.636719907
5\Cl, -4.4563328719, -0.5714035164, -2.3756682678\C, -0.9730248977, 0.78895
21159, 1.5614829911\C, 0.3369920068, 0.4887779901, 0.9581846895\C, -1.25368
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6995, 4.5497764301\H, -5.8539751889, 1.714266475, 0.5799735416\H, -2.753916
9306, 1.9284554075, 1.6666215691\H, 0.7928768555, 1.3305583404, 0.432510367
3\H, 0.9923610345, 0.1207244161, 1.7394684065\H, -2.0351766029, -0.09872465
25, 5.3311582453\H, -3.7576850863, -0.0153475927, 4.8382120041\H, -2.749825
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, 4.5414265674, 0.8175493669, 0.3017579653\C, 6.7405726336, 1.6176264609, -0
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55421718\C, -0.4633159368, -4.2681964709, -0.4122768973\H, -1.6534087486, -
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, 3.3098016862\\

(S)-TS-QD-OCH₃

Cl, -6.6802070606, 0.5780102337, -1.3814238914\C, -4.9566566805
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, -3.9999184191, 0.6989847477, -2.5474483499\C1, -4.8744027649, -1.70145274
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98, 2.7120323083\C, -0.8691451614, 1.5537526789, 0.7826624581\H, -2.7716213
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\C, -1.1321931625, 0.7673030019, 3.7372164508\C, 0.3230901959, 0.6841257632
, 0.7629152266\C, -0.7454991563, 2.7832213203, 0.0306639843\C, -2.734055218
4, -1.467643441, 4.1312525171\H, -3.4992801949, -1.0747527273, 2.1571655449
\C, -1.0564398573, 0.0597008752, 4.9372207984\H, -0.5166560194, 1.650483862
6, 3.5889425448\H, 0.4261503046, 0.0836371639, 1.667111017\H, 1.2152016272,
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92\H, 0.1497116602, -4.3102161418, -0.3107667677\H, -1.6891410758, -5.82712
53872, -0.8173916613\H, -2.5938354682, -4.4727144409, -1.6945497655\C, 2.37
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078264\H, 3.4537812368, -2.3465355411, 2.9700560661\H, 1.9862252974, -1.372
2259194, 3.2981411961\

INT

(R)-QD-OCH₃

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TS-S_N2'-2

(R)-TS2-QD-OCH₃

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 3662897\C, -0.5288933384, -2.2791316026, -1.8375393703\H, 0.7417271196, -2.
 4074103377, -3.6098314316\H, 0.5086379334, 1.4410441201, -1.7470343463\H, -
 1.0506920904, 0.5971809225, -1.696492843\H, -1.4087511009, -1.1953993265, -
 0.1634511926\H, 0.0094540805, -2.1832849606, 0.302356108\H, -0.4668948176,
 -0.251774277, -3.7874284349\H, 1.2487108653, 0.1113369669, -3.5929060504\C
 , -0.5712286756, -3.7734070618, -1.6525851951\H, -1.4640162144, -1.96530375
 58, -2.314375163\C, -1.5904789354, -4.5481604665, -2.0256834077\H, 0.294455
 7891, -4.2302617695, -1.1698599906\H, -1.5755225603, -5.6240983861, -1.8734
 274452\H, -2.4814637954, -4.1340676926, -2.4926747874\C, 2.4962360443, -2.4
 65691865, 2.3967152096\H, 2.0007944614, -3.3893794113, 2.7013333343\H, 3.57
 73055345, -2.5586440355, 2.560000722\H, 2.1054936924, -1.6376343994, 3.0036
 04476\

Reactions of Hindered Allylic Trichloroacetimidates

4

C, 2.5131844002, -0.43221049
 34, 1.2176128457\C, 0.966088582, -0.5534856158, 1.1822534698\H, 0.771794730
 1, -1.9457215361, 2.4647315609\N, 0.2344253941, -1.3474964312, 1.8394879717
 \O, 0.4903713236, 0.3469849355, 0.3120156287\C, -0.9528245494, 0.4310148107
 , 0.1709198715\H, -1.3968962387, 0.3769631757, 1.1666342215\C, -1.270553743
 5, 1.7720322947, -0.4726488761\C, -1.9585798385, 4.2046574362, -1.685909180
 7\C, -2.564495062, 2.2911463422, -0.3331254969\C, -0.3238598811, 2.47894141
 11, -1.221914342\C, -0.668565898, 3.6912339168, -1.8228932351\C, -2.9049397
 405, 3.5003272754, -0.9387871891\H, -3.3004155765, 1.7383373636, 0.24344859
 13\H, 0.6854872243, 2.0941287291, -1.3194607639\H, 0.0771698491, 4.23608703
 66, -2.3960367779\H, -3.9109304097, 3.8943044173, -0.8210618834\H, -2.22365
 17921, 5.149188245, -2.153508211\C, -1.4641886739, -0.7559104012, -0.633711
 8797\C, -0.8592992126, -1.2243410704, -1.7350317705\H, 0.0417833931, -0.743
 9836589, -2.1103345258\C, -1.4101933529, -2.4173153423, -2.4636203677\H, -0.
 6018681465, -3.0174393125, -2.8987811017\H, -2.0452107005, -2.0920093303,
 -3.3012628756\C, -2.2050548893, -3.2696926818, -1.483454096\H, -1.52940991
 25, -3.7402691494, -0.7580563301\H, -2.7830355286, -4.0497440504, -1.983210
 3815\O, -3.1758055651, -2.4870863241, -0.7619421144\C, -2.7703262814, -1.32
 26918379, -0.193471803\O, -3.5032139243, -0.7593859525, 0.5925693087\Cl, 3.
 1707085277, -0.7674814114, -0.4301641486\Cl, 2.9757564452, 1.2275744817, 1.

7275201704\Cl, 3.2255961755, -1.6150168613, 2.3692341188\\

[3,3]-Rerrangement

C, 2.163
0567559, -1.1302074407, 0.78431274\C, 1.1298274529, -0.3300648832, -0.09185
69031\H, 1.149419225, -1.6484998798, -1.5259717689\N, 0.7361918761, -0.7567
905165, -1.2578884565\O, 0.6681828867, 0.6984822019, 0.5013411347\C, -1.183
2463861, 1.0531290447, 0.3364059441\H, -1.3094878401, 1.1159266049, 1.41437
98924\C, -1.1477977837, 2.3611159274, -0.36872208\C, -1.2030062571, 4.89460
31292, -1.5817904582\C, -2.0967214158, 2.6594728708, -1.3589059075\C, -0.23
87307437, 3.3597369469, 0.0209855918\C, -0.2620432677, 4.6109857604, -0.587
0524152\C, -2.1231247166, 3.9184201398, -1.9611646087\H, -2.8373985908, 1.9
140960999, -1.6308907508\H, 0.4979482964, 3.1364880993, 0.7849352971\H, 0.4
533991937, 5.3698922318, -0.282588429\H, -2.8683262827, 4.134837203, -2.721
6702605\H, -1.222544115, 5.8748463666, -2.0502450202\C, -1.7050009368, -0.1
400890166, -0.2366051312\C, -1.3087355028, -0.4965908718, -1.5277050553\H,
-1.0760011588, 0.2821936311, -2.2423851165\C, -1.7538768795, -1.8255105425
, -2.0666540408\H, -1.0870000019, -2.1787808118, -2.8605674583\H, -2.746589
5256, -1.6887669756, -2.520529944\C, -1.831399508, -2.8444951174, -0.935597
5805\H, -0.8237454905, -3.0963934393, -0.5806016568\H, -2.321450898, -3.766
4154121, -1.2564405577\O, -2.6058623552, -2.3657363564, 0.1720813808\C, -2.
3396811735, -1.1171792661, 0.6730685184\O, -2.7217714904, -0.8457313852, 1.
7916023487\Cl, 3.1129691652, -2.3157547407, -0.1987815485\Cl, 3.3025820511
, -0.0027713418, 1.5779953506\Cl, 1.2148560721, -2.0278248509, 2.0305088081
\\

Amine Catalyzed [1,3]-Shift

C, 0.7780605746, 0.6963241452, -0.995230749\C, 1.252402137
4, 2.0290813444, -0.5018251107\C, 2.2373041486, 4.5731592191, 0.2270815915\
C, 0.4076954048, 2.9867671285, 0.0807069146\C, 2.5944119969, 2.3845128336, -
0.7343744118\C, 3.0828217051, 3.641067099, -0.3738073612\C, 0.8993330928, 4
.239703205, 0.4460771152\O, -0.8576515579, 0.3906186192, 0.0601997411\C, -1
.9733587819, 0.6632621753, -0.5466665424\N, -2.1098251676, 1.4909219251, -1
.5124945533\C, -3.1553584666, -0.1865029313, 0.0575266834\Cl, -2.891781436
4, -1.9337239091, -0.3275198147\Cl, -4.7733241589, 0.2942435048, -0.5824985
422\Cl, -3.196896751, 0.0161521027, 1.8616772892\C, 1.5414224795, -0.474061
5007, -0.8436948566\C, 2.4894266927, -0.6832362227, 0.2479291626\C, 1.29830
46982, -1.5364308632, -1.8244809588\O, 0.4637364071, -1.4986412533, -2.7034
590363\O, 2.1028889538, -2.6722540489, -1.8001635289\C, 3.1464601482, -2.87
37217897, -0.8542743457\H, -3.0671973968, 1.5312725717, -1.8567736287\H, 0.
1738305323, 0.7359939036, -1.8981629989\H, 2.872447752, 0.2458323304, 0.669
8243202\H, 3.9700893217, -3.3506056303, -1.3968463021\H, 2.8026425511, -3.6
023380598, -0.1049021329\H, 3.2500940515, 1.6788887997, -1.2370407786\H, 4.
121903594, 3.8910120352, -0.5729147161\H, 2.6130384763, 5.5529137948, 0.510
1770916\H, 0.2264596065, 4.9631231433, 0.899281951\H, -0.6338602166, 2.7441
581457, 0.2383459161\N, 1.7215143577, -1.2756318655, 1.6814162519\C, 2.6976
462834, -1.9375071598, 2.5888550297\H, 3.0501671034, -2.868259955, 2.144236
701\H, 3.540764098, -1.2659708993, 2.7665445011\H, 2.209167866, -2.16009710
34, 3.541950734\C, 1.1449427268, -0.0843192261, 2.3879369987\H, 1.948516061
9, 0.6165570005, 2.6230125137\H, 0.3971155112, 0.3800994498, 1.7449721574\H
, 0.6712304016, -0.4234234798, 3.3137846912\C, 0.5973775838, -2.2093328745,
1.3547130076\H, -0.1386767678, -1.6666382133, 0.7621793295\H, 0.9769234308
, -3.065987655, 0.7994384591\H, 0.145540048, -2.5470591179, 2.2918129883\C,
3.6334679229, -1.5967153793, -0.179533167\H, 4.3287637398, -1.8468604858, 0
.6275660696\H, 4.2073032862, -1.0031416159, -0.9013920134\\

Products

2 – Conformer 1 $\Delta G_{\text{gas}}=0.0$ kcal/mol

C, -2.526893
0458, 0.4592131331, -0.3212873216\C, -2.6618357305, 0.0814546749, -1.734665
3622\C, -3.1185513309, -0.6203613644, -4.4239090977\C, -1.6029918537, -0.36
76727292, -2.5478976391\C, -3.9561438044, 0.1347658277, -2.2904215472\C, -4
.1816476533, -0.1970627859, -3.6230280033\C, -1.8365919935, -0.712995244, -
3.8780947052\O, 1.5577064193, -0.4222583835, -1.3866979121\C, 1.7142634126
, -0.0431503068, -0.2381179\N, 0.9797487277, 0.8897165339, 0.3936420739\C, 2
.8317325564, -0.7149016069, 0.6491673346\Cl, 2.0257276172, -2.0215670508, 1
.6072159091\Cl, 3.5990376256, 0.4608478927, 1.7919262393\Cl, 4.0905270075,
-1.4191563894, -0.3912934198\C, -1.5025200038, 1.0266953211, 0.356325403\C
, -0.1895461162, 1.5235395862, -0.2180351164\C, -1.6305531657, 1.3078767137
, 1.8111673782\O, -0.727296582, 1.8024222063, 2.4720896991\O, -2.8199238576
, 0.9701764497, 2.3491274836\C, -2.9537616876, 1.2179756714, 3.7583155259\H
, 1.131199114, 1.1061085734, 1.3712769543\H, -3.4271167531, 0.2852294639, 0.
2644466663\H, -0.1087759127, 2.5989137618, -0.0234293144\H, -0.1337842461,
1.3677845516, -1.2922477771\H, -2.8382904057, 2.2834483854, 3.9731884296\H
, -2.2010504943, 0.6579250422, 4.3190070672\H, -3.9572295724, 0.8799416844,
4.0178470034\H, -4.7874608671, 0.4541582931, -1.6661912819\H, -5.185862597
6, -0.1352337113, -4.0333798999\H, -3.2912629725, -0.8906728499, -5.4621470
941\H, -1.0090086557, -1.0659511558, -4.4871113065\H, -0.6032113262, -0.486
7669933, -2.1434502083\

2 - Conformer 2 ΔG_{gas} kcal/mol

C, -1.118143
3729, -2.3650185922, -0.3622876758\C, 0.0985882391, -3.1849360286, -0.43613
01629\C, 2.3127914178, -4.9196589346, -0.5828474457\C, 1.4094347508, -2.687
001548, -0.3013235603\C, -0.0751953182, -4.5730335881, -0.6092620541\C, 1.0
177362971, -5.4301095834, -0.6969927443\C, 2.5004088082, -3.5515886053, -0.
3752521889\O, 1.9875171463, 0.6218990748, -0.0081704827\C, 1.0054872286, 1.
3447143568, -0.0163289774\N, -0.1543643126, 1.095425811, -0.6506368259\C, 1
.0695510879, 2.7507260112, 0.6977659206\Cl, -0.4725548193, 3.1184538574, 1.
5744186863\Cl, 1.3300559468, 4.0017141266, -0.5814816165\Cl, 2.4186718643,
2.7844702373, 1.8551579135\C, -1.3536215388, -1.082059322, -0.7217986898\C
, -0.3926688217, -0.1324494953, -1.4113772351\C, -2.7027192664, -0.48601076
37, -0.5302201393\O, -2.9588052065, 0.6766272133, -0.8129556756\O, -3.62335
3237, -1.3252420172, -0.0140422934\C, -4.9274909826, -0.7591761612, 0.19530
47664\H, -0.9601715448, 1.6976577639, -0.5326301158\H, -1.9852829875, -2.90
50166615, 0.0121296738\H, -0.8279167808, 0.1657519055, -2.3720007539\H, 0.5
688332019, -0.6005173121, -1.6053494464\H, -5.5267086189, -1.5627607269, 0.
6239799012\H, -5.356025991, -0.4222071317, -0.7521071744\H, -4.8714590628,
0.0889530481, 0.8824205729\H, -1.0828597823, -4.9744808057, -0.6880012415\
H, 0.8596365276, -6.495014826, -0.8440522702\H, 3.1691482167, -5.5861396588
, -0.6401951312\H, 3.5033785821, -3.1502131148, -0.2598559729\H, 1.58721677
17, -1.6355035614, -0.1016462432\

2 - Conformer 3 $\Delta G_{\text{gas}}=0.8$ kcal/mol

C, -0.592890
7458, 2.575173737, -0.1704462835\C, 0.3427126386, 3.0735273605, -1.18677805
5\C, 2.1839140583, 4.1278791581, -3.039075768\C, 1.3374269128, 3.9844188005
, -0.7815361752\C, 0.2683199291, 2.7329675384, -2.5502810747\C, 1.180810573
7, 3.2554150129, -3.4647757541\C, 2.2573862561, 4.4941525714, -1.6930331073
\O, 1.4378499999, -1.3619714104, -1.1127403173\C, 0.5296623484, -1.67805498
76, -0.3682692753\N, -0.6546987511, -1.0437640399, -0.245434143\C, 0.691294

0479, -2.9168988708, 0.5980721588\Cl, 0.8453323676, -2.2918222096, 2.291729
 5783\Cl, 2.1450538378, -3.8429040078, 0.1702207092\Cl, -0.7576990388, -3.99
 8926873, 0.5024515584\C, -1.1908963646, 1.3665196017, -0.066345753\C, -0.95
 48764887, 0.1798023082, -0.9844225545\C, -2.1796223912, 1.1174578779, 1.018
 4005435\O, -2.774464072, 0.0573085928, 1.1546388677\O, -2.3807879738, 2.167
 5351478, 1.8397919344\C, -3.327733948, 1.9515680253, 2.8993373793\H, -1.362
 6743377, -1.3558582309, 0.408092412\H, -0.8180051017, 3.2868428735, 0.62062
 41189\H, -0.1026548221, 0.3608866261, -1.637162241\H, -1.8388953854, 0.0006
 363375, -1.6105833223\H, -3.0025027193, 1.1300390588, 3.5427209703\H, -4.31
 31086914, 1.7151540493, 2.4899222531\H, -3.3571227833, 2.8882898202, 4.4562
 813018\H, -0.5308473446, 2.0909055795, -2.9056737521\H, 1.1027823048, 2.985
 3003797, -4.5141386597\H, 2.8959874909, 4.5305987232, -3.7539797808\H, 3.02
 72527821, 5.1825481921, -1.355727459\H, 1.3931734395, 4.2765599646, 0.26423
 02158\

2 – Conformer 4 $\Delta G_{\text{gas}} = 1.1$ kcal/mol

C, 1.8599981
 569, -1.3585430391, 1.3778827443\C, 1.2067517305, -1.3799524942, 2.69137452
 76\C, 0.1101418747, -1.5418257961, 5.281549475\C, -0.0384302715, -0.7883203
 927, 2.9817699999\C, 1.867979892, -2.0831850432, 3.7191929079\C, 1.33534650
 44, -2.1517300241, 5.0029976424\C, -0.5748599401, -0.8720722474, 4.26555959
 87\O, -1.6998104725, 1.0180114592, 0.6781146281\C, -1.1769833916, 1.0582432
 645, -0.4216496617\N, 0.1455533075, 1.0428833463, -0.6722014096\C, -2.07936
 74611, 1.0864556915, -1.7168080416\Cl, -1.4415791426, 2.2651179601, -2.9389
 784609\Cl, -3.745182653, 1.5294014942, -1.2938259375\Cl, -2.0479571472, -0.
 5739635534, -2.4352151225\C, 1.8441434174, -0.4522334909, 0.3728227089\C, 1
 .159114728, 0.8996605399, 0.376675744\C, 2.6742903091, -0.7996659043, -0.81
 76405618\O, 3.3397120024, -1.8049787273, -0.9631309018\O, 2.6063975736, 0.1
 71307403, -1.7757134629\C, 3.3897076022, -0.0790395375, -2.9560125211\H, 0.
 4863430648, 1.0395953089, -1.6241497332\H, 2.5137389816, -2.210145278, 1.19
 2122372\H, 1.9082827633, 1.6819804375, 0.211954937\H, 0.6752419854, 1.09604
 24761, 1.3306207875\H, 3.2311036592, 0.7852611709, -3.6015753416\H, 3.05622
 62377, -0.9960046766, -3.4482517439\H, 4.4466191142, -0.1785529587, -2.6972
 410445\H, 2.8167761683, -2.5678894741, 3.5020037162\H, 1.869637163, -2.6885
 782455, 5.7820632272\H, -0.3149741112, -1.6015169512, 6.2798332236\H, -1.54
 06887119, -0.4171874074, 4.4672041475\H, -0.6143491713, -0.2941083794, 2.20
 67076919\

3- Conformer 1 $\Delta G_{\text{gas}} = 0.0$ kcal/mol

C, -0.578197
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 82855\C, -1.7898074685, 1.8757060418, -4.0698285999\C, -1.355373647, 1.4749
 403615, -1.7216970819\C, -1.0082964723, -0.2893934244, -3.3253409218\C, -1.
 4145144496, 0.5618505784, -4.3531453335\C, -1.7601573231, 2.327160155, -2.7
 503424634\O, -1.800022462, -1.15614692, 1.6682644966\C, -0.8714574463, -0.3
 836118344, 1.5278086981\N, -0.2387157117, -0.1097808898, 0.3652310363\C, -0
 .3685914555, 0.4668970473, 2.758334348\Cl, 1.4348247275, 0.6310025047, 2.76
 53290391\Cl, -0.8897996096, -0.2954235148, 4.2769682741\Cl, -1.1067203146,
 2.1131158177, 2.6165936315\C, 0.5555513023, -1.7497598551, -1.2694107137\C
 , 0.3890218791, -3.0728711212, -1.375828691\C, 1.8854695245, -1.103796775, -
 1.4864273129\O, 2.1390252278, 0.0406935209, -1.1482249781\O, 2.7833245633,
 -1.9114223691, -2.0778578036\C, 4.0944348461, -1.3480607434, -2.2635368163
 \H, 0.6054210326, 0.4518782796, 0.3385995341\H, -1.4467551009, -1.426589471
 3, -0.6247383492\H, -0.5746198412, -3.5348239451, -1.1786305197\H, 1.207989
 7307, -3.7275367867, -1.6533626258\H, 4.6793131839, -2.1302774262, -2.74735
 91528\H, 4.5338805467, -1.0764291384, -1.3003644574\H, 4.0402258523, -0.458
 4589425, -2.8957639533\H, -0.7189215042, -1.3099372753, -3.559813751\H, -1.

4358678873, 0.1959211201, -5.3763320466\H, -2.1035160277, 2.5406387712, -4.8699393529\H, -2.0526252465, 3.3472876923, -2.5160285464\H, -1.3408710428, 1.8365505442, -0.6987767824\\

3 - Conformer 2 $\Delta G_{\text{gas}}=1.0$ kcal/mol

C, 1.0169630
082, 0.6482962925, -0.5097836221\C, 0.3016989687, 1.8663860677, -1.1029167506\C, -0.9175788799, 4.1310287315, -2.2331180603\C, -0.8976453607, 2.3630084087, -0.5775486343\C, 0.880539528, 2.5172605271, -2.1991146749\C, 0.2780000359, 3.6423799898, -2.7617586159\C, -1.5027135523, 3.486861388, -1.1418616298\O, 0.4727255202, -1.7113617888, -1.9720607591\C, -0.0697189396, -1.5130704809, -0.9017018481\N, 0.1039347115, -0.4274173249, -0.1185394954\C, -1.0165078881, -2.6137101871, -0.2842092204\Cl, -0.065358225, -3.5027266841, 0.9743094838\Cl, -1.5409033828, -3.7451522605, -1.5501664915\Cl, -2.4748799771, -1.8765780557, 0.495735991\C, 1.9328596528, 1.030082734, 0.6519766707\C, 3.2642290924, 1.0631780971, 0.5196802932\C, 1.281870377, 1.3605149043, 1.9551050397\O, 0.1151429922, 1.1044120426, 2.2157374157\O, 2.1083996036, 1.9520280507, 2.8326150442\C, 1.5421369495, 2.2410815289, 4.1240412184\H, -0.3811518132, -0.3169990454, 0.7643299855\H, 1.645161234, 0.2224595878, -1.2951244187\H, 3.7431470018, 0.7883813451, -0.4160851969\H, 3.9091835259, 1.3634464211, 1.3378200716\H, 2.3455462343, 2.7089847195, 4.6927146493\H, 1.2088867091, 1.3206221489, 4.6099810022\H, 0.6929643113, 2.9212148219, 4.0231813943\H, 1.8060881658, 2.1344292313, -2.6235304864\H, 0.7374704344, 4.1294473969, -3.6176926876\H, -1.392945713, 5.0040943125, -2.6720140075\H, -2.4361119727, 3.8578903716, -0.7267820078\H, -1.3613170346, 1.8733045237, 0.2719608536\\

3 - Conformer 3 $\Delta G_{\text{gas}}=0.8$ kcal/mol

C, 0.037927
6831, -0.1582114511, -1.312999658\C, 0.8516322369, -1.4561435778, -1.3282746777\C, 2.3451598924, -3.8315078197, -1.4669648509\C, 0.819105778, -2.3771445813, -0.2740011975\C, 1.6401524793, -1.7399024546, -2.4499788486\C, 2.3819641383, -2.9188101801, -2.5221281737\C, 1.5636072487, -3.5555354312, -0.3439998298\O, 1.5581653502, 2.1000060866, -0.543428345\C, 0.7974390732, 1.5738163619, 0.2462225659\N, 0.0176126934, 0.5005347908, -0.0057081613\C, 0.6974313513, 2.1122250334, 1.7259960104\Cl, 1.5754754676, 0.9499941643, 2.7977713046\Cl, -1.0291191925, 2.2199292066, 2.265724791\Cl, 1.4463424204, 3.7195240484, 1.8422751183\C, -1.3818137117, -0.3667820129, -1.8374424621\C, -1.7572392088, 0.0589415669, -3.0494247346\C, -2.3463661716, -1.0630408259, -0.9342546393\O, -2.1517479235, -1.2402435261, 0.2596235385\O, -3.4684683948, -1.4628688636, -1.5541710202\C, -4.4536285177, -2.0922411427, -0.7144725681\H, -0.6276310489, 0.129980107, 0.6824236166\H, 0.5332421582, 0.5475893316, -1.9831152868\H, -1.0684789319, 0.5978961359, -3.6941926816\H, -2.75739018, -0.1175633799, -3.4289588918\H, -4.7802176572, -1.4068369928, 0.0716623242\H, -4.0417453237, -2.994280082, -0.2555972262\H, -5.2814527373, -2.3409987961, -1.3782897555\H, 1.6819266976, -1.0274379537, -3.2709591981\H, 2.9947599861, -3.1182412808, -3.3971636478\H, 2.9259330765, -4.7485975622, -1.5170152733\H, 1.5326820009, -4.258618909, 0.484174748\H, 0.2133793988, -2.1763707645, 0.6030227625\\

3 - Conformer 4 $\Delta G_{\text{gas}}=0.7$ kcal/mol

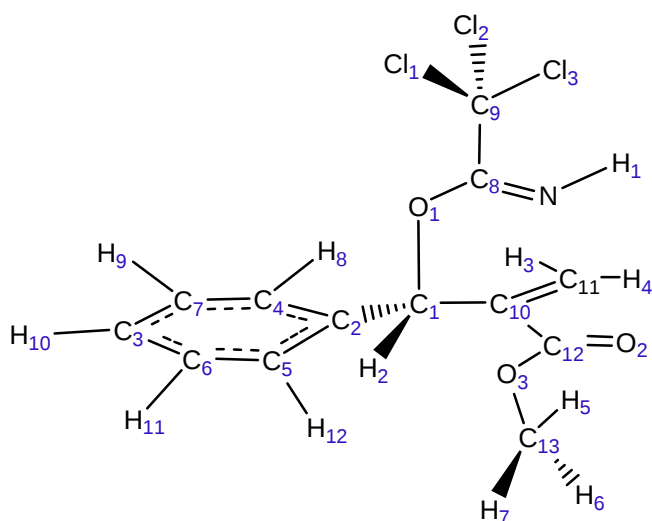
C, 0.5716284
13, 0.2708705015, -1.1605602515\C, -0.6473650238, 0.0660838312, -2.065501464\C, -2.8188360918, -0.2934912152, -3.8113919963\C, -0.4390009704, -0.322628727, -3.3943639723\C, -1.9584915885, 0.2731752174, -1.6191319806\C, -3.035

8103772,0.0918357748,-2.4875145697\C,-1.515045634,-0.5009937977,-4.263771472\0,1.5818151825,-2.1542769477,-0.1019314696\C,0.9115435128,-1.4128862015,0.5906246175\N,0.3781936327,-0.2354670842,0.1994855702\C,0.5837277456,-1.795546212,2.0867695723\C1,1.4249665814,-3.2931429951,2.5355127819\C1,-1.2028850566,-2.0288943684,2.2528847097\C1,1.1069710075,-0.4574519023,3.1913786036\C,1.0294642205,1.7284663317,-1.1362805455\C,2.1254873234,2.135254045,-1.7877400704\C,0.2052702583,2.6900435065,-0.3442806695\0,-0.6423789199,2.3496021805,0.468385465\0,0.4968144336,3.9771071545,-0.5924895687\C,-0.2335307558,4.9425508092,0.1862461766\H,-0.149196647,0.3531984325,0.8341813465\H,1.3904127757,-0.3215284241,-1.5743519393\H,2.7474177403,1.4323063084,-2.3351364055\H,2.4304928417,3.1756511634,-1.7922061236\H,-1.3059337326,4.8493554303,-0.0012070309\H,0.1324073814,5.9147825506,-0.1433896678\H,-0.0417300728,4.7976858626,1.2523846226\H,-2.1406439212,0.5758599137,-0.5936574106\H,-4.0481608509,0.2511433689,-2.1256500841\H,-3.6601497194,-0.4365886821,-4.4841270597\H,-1.3344650645,-0.8109417958,-5.2895890831\H,0.5740490298,-0.4971993025,-3.7501794345\

COMPLETE REFERENCE 9

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ELF ANALYSIS



	basin	$N(\Omega_i)$	$\sigma^2[N(\Omega_i)]$	$\lambda[N(\Omega_i)]$	Contribution Analysis (%)
1	C(C1)	2.08	0.25	0.12	22 (34.8) 33 (30.4) 34 (30.4) 36 (4.3)
2	C(C2)	2.09	0.26	0.12	33 (30.4) 35 (34.8) 36 (34.8)
3	C(C3)	2.09	0.26	0.12	30 (28.0) 37 (32.0) 38 (32.0) 39 (4.0) 40 (4.0)
4	C(C4)	2.09	0.26	0.12	32 (30.4) 35 (30.4) 37 (4.3) 39 (34.8)
5	C(C5)	2.09	0.26	0.12	28 (30.4) 36 (30.4) 38 (4.3) 40 (34.8)
6	C(C6)	2.09	0.26	0.12	29 (30.4) 38 (34.8) 40 (34.8)
7	C(C7)	2.09	0.26	0.12	31 (30.4) 37 (34.8) 39 (34.8)
8	O(O1)	2.13	0.34	0.16	41 (45.2) 42 (19.4) 43 (35.5)
9	C(C8)	2.09	0.25	0.12	21 (4.3) 41 (4.3) 42 (26.1) 43 (4.3) 44 (34.8) 45 (21.7) 46 (4.3)
10	C(N)	2.11	0.30	0.14	21 (25.0) 44 (28.6) 46 (46.4)
11	C(C9)	2.08	0.24	0.12	45 (30.4) 47 (17.4) 48 (17.4) 49 (17.4) 50 (4.3) 51 (4.3) 57 (4.3) 58 (4.3)
12	C(Cl1)	10.06	0.55	0.05	48 (11.1) 50 (33.3) 51 (31.5) 52 (24.1)
13	C(Cl2)	10.06	0.55	0.05	49 (11.1) 53 (29.6) 54 (29.6) 55 (29.6)
14	C(Cl3)	10.07	0.55	0.05	47 (11.1) 56 (24.1) 57 (31.5) 58 (33.3)
15	C(C10)	2.09	0.26	0.12	23 (4.2) 24 (4.2) 34 (25.0) 59 (20.8) 60 (25.0) 61 (20.8)
16	C(C11)	2.09	0.25	0.12	23 (29.2) 24 (29.2) 34 (4.2) 59 (16.7) 61 (20.8)
17	C(C12)	2.09	0.25	0.12	60 (29.2) 62 (29.2) 63 (8.3) 64 (20.8) 65 (8.3) 66 (4.2)
18	C(O2)	2.13	0.34	0.16	60 (3.1) 62 (21.9) 65 (37.5) 66 (37.5)
19	C(O3)	2.13	0.34	0.16	63 (67.7) 64 (16.1) 67 (16.1)
20	C(C13)	2.09	0.25	0.12	25 (28.0) 26 (28.0) 27 (28.0) 63 (4.0) 67 (12.0)

21	V(H1,N)	2.00	0.80	0.40	10 (8.9) 44 (27.8) 46 (49.4)
22	V(H2,C1)	2.12	0.69	0.33	1 (12.7) 33 (28.6) 34 (27.0) 35 (4.8) 36 (3.2) 46 (9.5) 65 (3.2)
23	V(H3,C11)	2.11	0.66	0.31	16 (11.3) 24 (30.6) 34 (4.8) 43 (3.2) 59 (19.4) 60 (3.2) 61 (22.6)
24	V(H4,C11)	2.10	0.64	0.30	16 (11.9) 23 (32.2) 34 (3.4) 59 (20.3) 60 (3.4) 61 (23.7) 63 (3.4)
25	V(H5,C13)	2.03	0.63	0.31	20 (11.7) 26 (31.7) 27 (31.7) 63 (8.3) 67 (13.3)
26	V(H6,C13)	2.03	0.62	0.31	20 (11.7) 25 (31.7) 27 (31.7) 63 (10.0) 67 (13.3)
27	V(H7,C13)	2.03	0.63	0.31	20 (11.5) 25 (31.1) 26 (31.1) 63 (8.2) 66 (3.3) 67 (13.1)
28	V(H8,C5)	2.14	0.68	0.32	5 (11.1) 29 (4.8) 33 (3.2) 35 (3.2) 36 (31.7) 38 (3.2) 40 (36.5)
29	V(H9,C6)	2.13	0.65	0.31	6 (10.9) 28 (4.7) 30 (4.7) 36 (3.1) 37 (3.1) 38 (32.8) 40 (37.5)
30	V(H10,C3)	2.13	0.64	0.30	3 (11.3) 29 (4.8) 31 (4.8) 37 (35.5) 38 (35.5) 39 (3.2) 40 (3.2)
31	V(H11,C7)	2.13	0.65	0.31	7 (10.9) 30 (4.7) 32 (4.7) 35 (3.1) 37 (32.8) 38 (3.1) 39 (37.5)
32	V(H12,C4)	2.14	0.66	0.31	4 (11.1) 31 (4.8) 33 (3.2) 35 (31.7) 36 (3.2) 37 (3.2) 39 (36.5)
33	V(C1,C2)	2.37	1.14	0.48	1 (6.4) 2 (6.4) 22 (16.5) 34 (14.7) 35 (18.3) 36 (20.2)
34	V(C1,C10)	2.26	1.09	0.48	1 (6.6) 15 (5.7) 22 (16.0) 33 (15.1) 49 (13.2) 60 (14.2) 61 (14.2)
35	V(C2,C4)	2.59	1.24	0.48	2 (6.6) 4 (5.8) 32 (16.5) 33 (16.5) 36 (19.8) 39 (20.7)
36	V(C2,C5)	2.70	1.29	0.48	2 (6.3) 5 (5.6) 28 (15.9) 33 (17.5) 35 (19.0) 40 (20.6)
37	V(C3,C7)	2.68	1.27	0.47	3 (6.3) 7 (6.3) 30 (17.5) 31 (16.7) 38 (19.8) 39 (22.2)
38	V(C3,C6)	2.69	1.27	0.47	3 (6.3) 6 (6.3) 29 (16.7) 30 (17.5) 37 (19.8) 40 (22.2)
39	V(C4,C7)	2.87	1.34	0.47	4 (6.1) 7 (6.1) 31 (18.3) 32 (17.6) 35 (19.1) 37 (21.4)
40	V(C5,C6)	2.88	1.35	0.47	5 (6.1) 6 (6.1) 28 (17.4) 29 (18.2) 36 (19.7) 38 (21.2)
41	V(O1)	3.16	1.36	0.43	8 (10.9) 42 (30.2) 43 (42.6) 44 (3.9) 45 (3.9) 46 (3.1)
42	V(O1,C8)	2.02	1.17	0.58	8 (5.4) 9 (5.4) 41 (34.8) 43 (27.7) 44 (12.5) 45 (9.8) 46 (3.6)
43	V(O1)	2.46	1.23	0.50	8 (9.2) 41 (45.8) 42 (25.8) 44 (3.3)
44	V(C8,N)	2.69	1.35	0.50	9 (6.1) 10 (6.1) 21 (16.7) 41 (3.8) 42 (10.6) 43 (3.0) 45 (12.9) 46 (37.9)
45	V(C8,C9)	2.17	1.06	0.49	9 (4.9) 11 (6.8) 41 (4.9) 42 (10.7) 44 (16.5) 46 (3.9) 47 (10.7) 48 (9.7) 49 (9.7)
46	V(N)	3.05	1.36	0.45	10 (10.0) 21 (30.0) 22 (4.6) 41 (3.1) 42 (3.1) 44 (38.5) 45 (3.1)
47	V(C9,Cl3)	1.50	0.93	0.62	11 (4.4) 14 (6.7) 45 (12.2) 48 (8.9) 49 (7.8) 56 (14.4) 57 (18.9) 58 (18.9)
48	V(C9,Cl1)	1.48	0.93	0.63	11 (4.5) 12 (6.7) 45 (11.2) 47 (9.0) 49 (7.9) 50 (19.1) 51 (19.1) 52 (14.6)
49	V(C9,Cl2)	1.46	0.92	0.63	11 (4.5) 13 (6.7) 45 (11.2) 47 (7.9) 48 (7.9) 53 (18.0) 54

					(18.0) 55 (18.0)
50	V(C11)	2.35	1.14	0.49	12 (16.1) 48 (15.2) 51 (32.1) 52 (27.7)
51	V(C11)	2.30	1.12	0.49	12 (15.3) 48 (15.3) 50 (32.4) 52 (27.9)
52	V(C11)	1.75	0.97	0.55	12 (14.0) 45 (2.2) 47 (1.1) 48 (14.0) 49 (1.1) 50 (33.3) 51 (33.3)
53	V(C12)	2.18	1.10	0.50	13 (14.8) 49 (14.8) 54 (30.6) 55 (30.6)
54	V(C12)	2.10	1.07	0.51	13 (15.4) 49 (15.4) 53 (31.7) 55 (30.8)
55	V(C12)	2.14	1.09	0.51	13 (14.8) 49 (14.8) 53 (30.6) 54 (29.6)
56	V(C13)	1.75	0.97	0.55	14 (14.0) 47 (14.0) 57 (33.3) 38 (33.3)
57	V(C13)	2.29	1.12	0.49	14 (15.3) 47 (15.3) 56 (27.9) 58 (32.4)
58	V(C13)	2.33	1.14	0.49	14 (16.1) 47 (15.2) 56 (27.7) 57 (32.1)
59	V(C10,C11)	1.55	0.93	0.60	15 (5.6) 16 (4.4) 23 (13.3) 24 (13.3) 34 (15.6) 60 (14.4) 61 (26.7)
60	V(C10,C12)	2.24	1.07	0.48	15 (5.7) 17 (6.7) 34 (14.3) 59 (12.4) 61 (13.3) 62 (14.3) 63 (6.7) 64 (9.5) 65 (5.7) 66 (3.8)
61	V(C10,C11)	1.75	1.00	0.57	15 (5.1) 16 (5.1) 23 (14.3) 24 (14.3) 34 (15.3) 59 (24.5) 60 (14.3)
62	V(C12,O2)	2.39	1.32	0.55	17 (5.4) 18 (5.4) 60 (11.5) 63 (3.8) 64 (8.5) 65 (31.5) 66 (30.8)
63	V(O3)	4.56	1.54	0.34	19 (13.7) 25 (3.3) 26 (3.9) 27 (3.3) 60 (4.6) 62 (3.3) 64 (32.7) 67 (26.8)
64	V(C12,O3)	1.68	1.00	0.60	17 (5.1) 19 (5.1) 60 (10.2) 62 (11.2) 63 (51.0) 66 (3.1) 67 (9.2)
65	V(O2)	2.68	1.21	0.45	18 (10.1) 60 (5.0) 62 (34.5) 66 (41.2)
66	V(O2)	2.66	1.20	0.45	18 (10.3) 60 (3.4) 62 (34.2) 65 (41.9)
67	V(O3,C13)	1.34	0.85	0.63	19 (5.9) 20 (3.5) 25 (9.4) 26 (9.4) 27 (9.4) 63 (48.2) 64 (10.6)

	basin	$N(\Omega_i)$	$\sigma^2[N(\Omega_i)]$	$\lambda[N(\Omega_i)]$	Contribution Analysis (%)
1	C(C1)	2.09	0.25	0.12	22 (31.8) 33 (31.8) 34 (27.3) 36 (9.1)
2	C(C2)	2.09	0.26	0.12	34 (25.0) 37 (33.3) 38 (33.3) 41 (4.2) 42 (4.2)
3	C(C3)	2.09	0.26	0.12	30 (28.0) 39 (32.0) 40 (32.0) 41 (4.0) 41 (4.0)
4	C(C4)	2.09	0.26	0.12	32 (29.2) 38 (33.3) 39 (4.2) 41 (33.3)
5	C(C5)	2.09	0.26	0.12	28 (30.4) 37 (34.8) 42 (34.8)
6	C(C6)	2.09	0.26	0.12	29 (28.0) 37 (4.0) 39 (4.0) 40 (32.0) 42 (32.0)
7	C(C7)	2.09	0.26	0.12	31 (29.2) 39 (33.3) 40 (4.2) 41 (33.3)
8	C(O1)	2.13	0.34	0.16	36 (78.1) 43 (18.8) 44 (3.1)
9	C(C8)	2.09	0.25	0.12	21 (4.2) 36 (8.3) 43 (20.8) 44 (37.5) 45 (25.0) 46 (4.2)
10	C(N)	2.11	0.30	0.14	21 (25.9) 44 (33.3) 46 (40.7)
11	C(C9)	2.08	0.25	0.12	45 (30.4) 47 (17.4) 48 (17.4) 49 (17.4) 52 (4.3) 53 (4.3) 55 (4.3) 58 (4.3)
12	C(C11)	10.06	0.55	0.05	48 (11.3) 50 (28.3) 51 (28.3) 52 (32.1)

13	C(Cl2)	10.06	0.55	0.05	49 (11.1) 53 (31.5) 54 (27.8) 55 (29.6)
14	C(Cl3)	10.06	0.55	0.05	47 (11.1) 56 (27.8) 57 (27.8) 58 (33.3)
15	C(C10)	2.09	0.26	0.12	33 (26.1) 35 (13.0) 59 (30.4) 60 (30.4)
16	C(C11)	2.09	0.25	0.12	23 (30.4) 24 (30.4) 46 (4.3) 60 (34.8)
17	C(C12)	2.09	0.25	0.12	59 (31.8) 61 (31.8) 62 (18.2) 63 (9.1) 64 (4.5) 65 (4.5)
18	C(O2)	2.12	0.34	0.16	59 (3.0) 61 (21.2) 63 (39.4) 65 (36.4)
19	C(O3)	2.12	0.34	0.16	62 (16.1) 64 (71.0) 66 (12.9)
20	C(C13)	2.09	0.26	0.12	25 (28.0) 26 (28.0) 27 (28.0) 64 (4.0) 66 (12.0)
21	V(H1,N)	2.01	0.79	0.39	10 (9.0) 44 (32.1) 45 (2.6) 46 (42.3)
22	V(H2,C1)	2.09	0.67	0.32	1 (11.3) 33 (27.4) 34 (25.8) 36 (17.7) 37 (3.2) 38 (3.2) 59 (3.2) 64 (3.2)
23	V(H3,C11)	2.12	0.66	0.31	16 (11.3) 24 (30.6) 33 (3.2) 35 (3.2) 46 (11.3) 59 (3.2) 60 (30.6)
24	V(H4,C11)	2.11	0.65	0.31	16 (11.1) 23 (30.2) 33 (3.2) 35 (3.2) 46 (9.5) 59 (3.2) 60 (31.7) 63 (3.2)
25	V(H5,C13)	2.04	0.63	0.31	20 (11.3) 26 (30.6) 27 (30.6) 64 (9.7) 65 (3.2) 66 (12.9)
26	V(H6,C13)	2.04	0.63	0.31	20 (11.3) 25 (30.6) 27 (30.6) 64 (9.7) 65 (3.2) 66 (12.9)
27	V(H7,C13)	2.03	0.61	0.30	20 (11.7) 25 (31.7) 26 (31.7) 64 (10.0) 66 (13.3)
28	V(H8,C5)	2.12	0.66	0.31	5 (11.1) 29 (3.2) 34 (3.2) 36 (3.2) 37 (33.3) 38 (3.2) 40 (3.2) 42 (36.5)
29	V(H9,C6)	2.11	0.64	0.30	6 (11.5) 28 (3.3) 30 (3.3) 37 (3.3) 39 (3.3) 40 (34.4) 42 (37.7)
30	V(H10,C3)	2.12	0.64	0.30	3 (11.5) 29 (3.3) 31 (3.3) 39 (36.1) 40 (36.1) 41 (3.3) 42 (3.3)
31	V(H11,C7)	2.11	0.64	0.30	7 (11.5) 30 (3.3) 32 (3.3) 38 (3.3) 39 (36.1) 40 (3.3) 41 (36.1)
32	V(H12,C4)	2.13	0.67	0.31	4 (10.8) 31 (3.1) 34 (3.1) 37 (3.1) 38 (33.8) 39 (3.1) 41 (33.8)
33	V(C1,C10)	2.25	1.12	0.50	1 (6.3) 15 (5.4) 22 (15.2) 34 (13.4) 35 (10.7) 36 (8.0) 59 (13.4) 60 (15.2)
34	V(C1,C2)	2.12	1.04	0.49	1 (5.9) 2 (5.9) 22 (15.8) 33 (14.9) 36 (8.9) 37 (17.8) 38 (18.8)
35	V(C10)	0.74	0.57	0.77	15 (5.6) 23 (3.7) 24 (3.7) 33 (22.2) 59 (22.2) 60 (25.9)
36	V(O1)	5.64	1.62	0.29	8 (15.9) 22 (7.0) 33 (5.7) 34 (5.7) 43 (39.5) 44 (5.7) 45 (4.5) 46 (3.2)
37	V(C2,C5)	2.78	1.32	0.47	2 (6.2) 5 (6.2) 28 (16.2) 34 (13.8) 38 (21.5) 42 (21.5)
38	V(C2,C4)	2.82	1.34	0.48	2 (6.1) 4 (6.1) 32 (16.8) 34 (14.5) 37 (21.4) 41 (20.6)
39	V(C3,C7)	2.82	1.32	0.47	3 (6.1) 7 (6.1) 30 (16.8) 31 (16.8) 40 (20.6) 41 (21.4)
40	V(C3,C6)	2.74	1.29	0.47	3 (6.3) 6 (6.3) 29 (16.4) 30 (17.2) 39 (21.1) 42 (21.9)
41	V(C4,C7)	2.79	1.31	0.47	4 (6.1) 7 (6.1) 31 (16.8) 32 (16.8) 38 (20.6) 39 (21.4)
42	V(C5,C6)	2.85	1.33	0.47	5 (6.0) 6 (6.0) 28 (17.3) 29 (17.3) 37 (21.1) 40 (21.1)
43	V(O1,C8)	1.84	1.09	0.59	8 (5.8) 9 (4.8) 36 (59.6) 44 (13.5) 45 (9.6)

44	V(C8,N)	2.92	1.43	0.49	9 (6.4) 10 (6.4) 21 (17.7) 36 (6.4) 43 (9.9) 45 (13.5) 46 (32.6)
45	V(C8,C9)	2.21	1.07	0.48	9 (5.8) 11 (6.8) 36 (6.8) 43 (9.7) 44 (18.4) 46 (3.9) 47 (9.7) 48 (9.7) 49 (9.7)
46	V(N)	2.71	1.33	0.49	10 (8.6) 21 (25.8) 23 (5.5) 24 (4.7) 36 (3.9) 44 (35.9) 45 (3.1) 60 (6.3)
47	V(C9,Cl3)	1.46	0.92	0.63	11 (4.5) 14 (6.8) 45 (11.4) 48 (8.0) 49 (8.0) 56 (17.0) 57 (17.0) 58 (19.3)
48	V(C9,Cl1)	1.46	0.92	0.63	11 (4.4) 12 (6.7) 47 (7.8) 49 (8.9) 50 (16.7) 51 (16.7) 52 (18.9)
49	V(C9,Cl2)	1.49	0.93	0.62	11 (4.4) 13 (6.6) 45 (11.0) 47 (7.7) 48 (8.8) 53 (18.7) 54 (16.5) 55 (17.6)
50	V(Cl1)	2.03	1.05	0.52	12 (14.7) 48 (14.7) 51 (30.4) 52 (33.3)
51	V(Cl1)	2.07	1.06	0.51	12 (14.7) 48 (14.7) 50 (30.4) 52 (33.3)
52	V(Cl1)	2.32	1.13	0.49	12 (15.0) 48 (15.0) 50 (30.1) 51 (30.1)
53	V(Cl2)	2.24	1.11	0.50	13 (15.5) 49 (15.5) 54 (29.1) 55 (30.9)
54	V(Cl2)	1.95	1.02	0.52	13 (14.7) 49 (14.7) 53 (31.4) 55 (31.4)
55	V(Cl2)	2.20	1.10	0.50	13 (14.8) 49 (14.8) 53 (31.5) 54 (29.6)
56	V(Cl3)	2.08	1.07	0.51	14 (14.3) 47 (14.3) 57 (29.5) 58 (32.4)
57	V(Cl3)	1.96	1.03	0.53	14 (14.9) 47 (14.9) 56 (30.7) 58 (32.7)
58	V(Cl3)	2.37	1.15	0.49	14 (15.9) 47 (15.0) 56 (30.1) 57 (29.2)
59	V(C10,C12)	2.45	1.19	0.49	15 (6.0) 17 (6.0) 33 (12.9) 35 (10.3) 60 (15.5) 61 (13.8) 62 (9.5) 63 (5.2) 64 (6.0) 65 (4.3)
60	V(C10,C11)	2.56	1.26	0.49	15 (5.7) 16 (6.5) 23 (15.4) 24 (16.3) 33 (13.8) 35 (11.4) 46 (6.5) 59 (14.6)
61	V(C12,O2)	2.31	1.30	0.56	17 (5.5) 18 (5.5) 59 (12.5) 62 (7.8) 63 (30.5) 64 (3.9) 65 (31.3)
62	V(C12,O3)	1.62	0.98	0.60	17 (4.2) 19 (5.2) 59 (11.5) 61 (10.4) 64 (51.0) 65 (3.1) 66 (8.3)
63	V(O2)	2.71	1.21	0.45	18 (10.8) 59 (5.0) 61 (32.5) 65 (42.5)
64	V(O3)	4.61	1.55	0.34	19 (14.3) 25 (3.9) 26 (3.9) 27 (3.9) 59 (4.5) 61 (3.2) 62 (31.8) 66 (26.6)
65	V(O2)	2.71	1.22	0.45	18 (9.8) 59 (4.1) 61 (32.8) 63 (41.8)
66	V(O3,C13)	1.33	0.85	0.64	19 (4.8) 20 (3.6) 25 (9.6) 26 (9.6) 27 (9.6) 62 (9.6) 64 (49.4)