Supplementary material for

Nondegenerate equilibrium in (2-propyl)cycloalkyl cations. Comparison of (2-propyl)cyclopentyl and (2-propyl)cyclohexyl cation using ^{13}C-NMR spectroscopy, equilibrium isotope effects and quantum chemical calculations

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Supplementary material:
redundant coordinates for structures
1A, 1B, 1TS, 2A, 2B1, 2B2 and 2TS

and van´t Hoff plot for equilibrium **1A** / **1B**

Redundant internal coordinates for **1A**
optimized at the B3LYP/6-31G(d)level

H,0,0.7992745616,1.8325810392,-0.0498091983
C,0,1.0224288207,1.0203311978,-0.7488503197
C,0,2.3104487947,0.2950220155,-0.3205377942
C,0,-0.0680124579,-0.0691927679,-0.7138939632
H,0,1.0792361105,1.4589406959,-1.7494009832
C,0,1.8403879211,-0.604372791,0.8273263511
C,0,0.4950847021,-1.2004113434,0.3733048663
H,0,3.0995065052,0.9903904151,-0.0224136115
H,0,2.7000797457,-0.3099722739,-1.1478765407
C,0,-1.3451360365,0.1220684262,-0.0810280404
H,0,-0.1665850308,-0.5892471697,-1.6687236976
H,0,2.5353162087,-1.4173193221,1.0658154145
H,0,1.7041982309,-0.0176808108,1.7431059365
H,0,-0.1725619034,-1.4141638309,1.2153159144
H,0,0.5825668964,-2.1210327824,-0.2077323962
C,0,-2.5051834241,-0.6963672711,-0.503164749
C,0,-1.5519812886,1.11983648,0.9959984766
H,0,-3.0789564402,-1.0719389034,0.3510964071
H,0,-0.6482505639,1.3197480444,1.5768982424
H,0,-2.3871828039,0.8668656831,1.6527432996
H,0,-1.8060113218,2.0693822343,0.4921533133
H,0,-2.2419483256,-1.5060815387,-1.1864759971
H,0,-3.1869040585,-0.0119551566,-1.0396250675

Redundant internal coordinates for **1A**
optimized at the MP2/6-31G(d)level

H,0.6057638215,-1.3193937123,-1.4742151118
C,0.0982484979,-1.6034205149,-0.5485735029
C,1.1172443783,-1.9377829043,0.5480895537
C,-0.7135004155,-0.4510247678,0.0209002124
H,-0.5712471797,-2.4353388363,-0.7841859579
C,1.5792731353,-0.563712532,1.0231257546
C,0.3167521702,0.2910057103,1.1568255544
H,1.9372718778,-2.5613164755,0.1832952209
H,0.6280846987,-2.4773448967,1.3663517382
C,-0.7625074999,0.8584093889,-0.5015480998
H,-1.6064541215,-0.7505163532,0.5700310309
H,2.095189052,-0.5786711987,1.9893033604
H,2.2655751964,-0.1135009503,0.2985804981
H,0.5322485787,1.3633006817,1.0589393553
H,-0.247085857,0.1707091015,2.0846766446
C,-1.857549599,1.7787765571,-0.0851598006
C,0.1703696238,1.3414207146,-1.5571429855
H,-1.4959804659,2.795821659,0.0852468836
H,1.1128957871,0.7963458253,-1.5890022636
H,0.3583508699,2.4132871487,-1.4694113771
H,-0.3413399485,1.1732020282,-2.5157884773
H,-2.4040731283,1.4169989093,0.7874474602
H,-2.5591809279,1.8243871574,-0.9303691214

Redundant internal coordinates for **1B**
optimized at the B3LYP/6-31G(d)level

H,0,-0.2077764415,2.0492172032,0.2458281342
C,0,-0.6378911995,1.0674724479,0.4763109775
C,0,-2.1550826218,0.8807747415,0.241937645
C,0,0.0290721348,-0.0473765809,-0.2269093355
H,0,-0.3897444913,0.8978272116,1.5453230475
C,0,-2.2973184162,-0.6381487855,0.0194240385
C,0,-0.9859333102,-0.9983734836,-0.7115338424
H,0,-2.4579428537,1.4348263075,-0.6535258974
H,0,-2.7506234235,1.2531485251,1.0774510444
C,0,1.4734837753,-0.2365144353,-0.3779241773
H,0,1.6512513101,-0.8894998781,-1.2422065427
H,0,-2.3457314445,-1.1737754563,0.9741528873
H,0,-3.1818274899,-0.9098961896,-0.559566861
H,0,-1.0732299416,-0.7092779397,-1.7838239055
H,0,-0.6620375539,-2.0450844611,-0.7268991072
C,0,1.8833498082,-1.091276839,0.8926982197
C,0,2.3169160918,1.0441164132,-0.4701135713
H,0,1.3170943749,-2.0221513795,0.9760707303
H,0,2.0211168641,1.6587437043,-1.3259859768
H,0,3.3676429292,0.7718338365,-0.6022276964
H,0,2.2411335235,1.6475107368,0.439784044
H,0,1.7708037394,-0.5080798021,1.8102831483
H,0,2.9402933253,-1.3393832882,0.7620032258

Redundant internal coordinates for **1B**
optimized at the MP2/6-31G(d)level

H,0.1832361066,-1.0038706707,-1.7988153961
C,0.6289239312,-0.8243869198,-0.8142710425
C,2.1318024429,-0.4994363208,-0.7564116384
C,-0.0389432166,0.2388202636,-0.0474898804
H,0.4179801733,-1.7418213986,-0.2258439132
C,2.2714610411,0.2458570866,0.5764281438
C,0.9686263374,1.0575365544,0.6328441664
H,2.400687681,0.1531354452,-1.5935245653
H,2.7515911623,-1.395520686,-0.820463643
C,-1.473884535,0.4197124158,0.0931895779
H,-1.6774985717,1.4578581161,0.3825775624
H,2.3079377495,-0.4553002598,1.4168522628
H,3.1585859867,0.8794506293,0.6293318629
H,1.0493217989,1.9175674053,-0.0710563307
H,0.6469829143,1.4869009547,1.5874265245
C,-1.8002671385,-0.4584580195,1.3623830515
C,-2.3283889422,-0.009828806,-1.0970837959
H,-1.2050115729,-0.1817994379,2.234996261
H,-2.0690549404,0.5517824691,-1.9980666409
H,-3.3790988148,0.1849966191,-0.8707249976
H,-2.2217316452,-1.0781905611,-1.3005396961
H,-1.666777676,-1.5192723765,1.1417732103
H,-2.8531298736,-0.2748137738,1.5885460053

Redundant internal coordinates for **1TS**
optimized at the B3LYP/6-31G(d)level

C,0,1.0645151408,-0.4123098881,-0.9859208371
C,0,0.6552657178,1.9874620691,-1.1600270351
C,0,-0.0621736768,-0.0186684803,-0.0237514278
C,0,1.7557187083,0.9281467077,-1.3335856859
C,0,-0.116979255,1.5025335832,0.0807565067
C,0,-0.791370398,-0.9239659329,0.7791939826
C,0,-1.7600951707,-0.4544026225,1.8286951863
C,0,-0.5573702328,-2.4076522931,0.6880000905
H,0,1.7379149384,-1.1429074681,-0.5273100377
H,0,0.6496562291,-0.8813321961,-1.8863953719
H,0,-0.0091485756,2.0029260856,-2.0323982438
H,0,1.0497323144,2.9975353437,-1.0283897127
H,0,2.1846204147,0.9141477998,-2.3379647476
H,0,2.5735074111,1.1149399242,-0.628735405
H,0,0.4218636932,1.7752853772,1.0000170472
H,0,-1.1287986051,1.9062277607,0.1696952588
H,0,-2.6819307282,-1.0426994837,1.8122456349
H,0,-1.2827702197,-0.6367102498,2.8018318168
H,0,-1.997244107,0.60767857,1.766249807
H,0,-1.4916171744,-2.9647784058,0.7973999322
H,0,-0.0524934186,-2.7133960302,-0.2292712728
H,0,0.0862730965,-2.6849966648,1.534738337
H,0,-1.1846302696,-0.458779221,-0.4518777239

Redundant internal coordinates for **1TS**
optimized at the MP2/6-31G(d)level

C 2.3342966665,-0.3946986538,0.2029098131
C 0.984503689,-1.1178125671,0.2322655595
C 1.9948983674,1.0013284289,0.7273880609
C -0.0005697106,-0.0188673524,-0.1753346982
C -1.3980813855,-0.2037820251,-0.2861724819
C 0.6589402686,1.3521846924,0.0477896636
C -2.3063033197,0.9619267172,-0.4645406395
C -2.0122539303,-1.5560293871,-0.2277226334
H 2.7101051027,-0.3401216189,-0.8250670349
H 3.088266395,-0.9072134704,0.8048542319
H 0.9447362154,-2.0028338763,-0.4079362308
H 0.7400360579,-1.4312035299,1.2547103847
H 2.7669298022,1.7438257639,0.5133087332
H 1.86081853,0.967321195,1.8136389572
H -0.2693342224,-0.1547323786,-1.3319464964
H 0.8313981595,1.861721942,-0.9060821581
H 0.0303666351,2.0039531771,0.6606063375
H -3.1756467358,0.709966073,-1.0741644306
H -1.8015310097,1.8406742746,-0.8662836012
H -2.6691363844,1.2199517566,0.5417140918
H -2.7880354679,-1.6793988693,-0.9868916522
H -2.5124683129,-1.609347207,0.7510050598
H -1.2890886367,-2.3680623496,-0.2809620561

Redundant internal coordinates for **2A**
optimized at the B3LYP/6-31G(d)level

C,0,0.2817898115,-0.3310320258,-1.6614415556
C,0,0.252194695,-0.4349596116,-0.2165881886
C,0,1.553916626,-0.4999231149,-2.3908337852
C,0,-0.939363617,-0.0451784026,-2.4405755352
C,0,-1.0512614618,-0.8649206233,0.4814132598
C,0,0.62446596,1.0893504255,0.2043453829
H,0,1.1055802452,-1.0294341557,0.132563952
H,0,-0.738524275,0.2767262631,-3.4638436249
H,0,1.4473718227,-1.4092837193,-3.0095856426
H,0,2.4224704871,-0.6239697818,-1.7419347133
H,0,1.712225329,0.3122320775,-3.1122684252
H,0,-1.600938348,0.6639711397,-1.9313015213
H,0,-1.5134467658,-0.9892684487,-2.479333003
C,0,0.7370091975,1.1385294064,1.7393763758
C,0,-0.9084175779,-0.7704377782,2.0071685996
H,0,-1.883850732,-0.2299217844,0.1540615066
H,0,-0.1715231314,1.7543364286,-0.1470272142
H,0,-1.2927726667,-1.892194703,0.1823905052
H,0,1.5647860114,1.3965598226,-0.2615468572
C,0,-0.5293880235,0.6494611486,2.4494019597
H,0,1.6058696433,0.5478711931,2.0555629041
H,0,-0.1473343473,-1.4854533095,2.3480769396
H,0,0.9493073137,2.1830361135,2.0010669288
H,0,-1.8516992765,-1.0752073732,2.4720306703
H,0,-1.3592546814,1.3368161402,2.2346235029
H,0,-0.3739402872,0.6778475522,3.5328650126

Redundant internal coordinates for **2A**
optimized at the MP2/6-31G(d)level

C,0,0.2825096851,-0.322781608,-1.6171685193
C,0,0.2350890087,-0.4952383918,-0.1992580719
C,0,1.5560710703,-0.4863324254,-2.343720158
C,0,-0.9214206669,0.016328982,-2.3981712546
C,0,-1.0593096199,-0.8934477624,0.5034236259
C,0,0.5933523429,1.0540530409,0.1421011044
H,0,1.0947205968,-1.0676841016,0.1666634455
H,0,-0.6889607471,0.4962462451,-3.3497176902
H,0,1.4243444949,-1.3659490413,-2.9952529004
H,0,2.4085158585,-0.6634476682,-1.6878425732
H,0,1.7438603498,0.3560267835,-3.0178493724
H,0,-1.6498718016,0.5997459092,-1.8327804004
H,0,-1.4068649966,-0.9516507647,-2.6146741855
C,0,0.7380643876,1.1279658271,1.6707854354
C,0,-0.8952285686,-0.7616621726,2.01725183
H,0,-1.8881239824,-0.2584121715,0.1709038269
H,0,-0.2263906766,1.6959088147,-0.194654856
H,0,-1.3078753691,-1.9247864121,0.2272020605
H,0,1.5196935524,1.3729332151,-0.3440238921
C,0,-0.5184054147,0.6673292535,2.4020638765
H,0,1.6043504266,0.5326142714,1.980668704
H,0,-0.1231650442,-1.4596786451,2.364963422
H,0,0.964756259,2.1740771942,1.9090783995
H,0,-1.8280935137,-1.0563587276,2.5075165588
H,0,-1.3487909289,1.3444320844,2.1637134595
H,0,-0.3564378239,0.7386945544,3.4822387838

Redundant internal coordinates for **2B1**
optimized at the B3LYP/6-31G(d)level

H,0,-1.5836221235,0.5886132437,-1.5988515547
C,0,-1.4499966407,0.1400069598,-0.6116502676
C,0,-0.1463419731,0.4477510974,-0.0112143859
C,0,-1.4678363916,-1.4481740848,-0.7302269283
H,0,-2.2777449158,0.4205767016,0.0487418246
C,0,-1.2481309673,-2.0904377936,0.6385273769
C,0,0.052631102,0.0024072064,1.3711693222
H,0,-0.6978567316,-1.7648766417,-1.4430412278
C,0,0.9152650419,1.0630674399,-0.8218243992
H,0,-2.4382092542,-1.7082602418,-1.1635029412
C,0,0.0413510649,-1.5914319672,1.2890248892
H,0,-2.1043624388,-1.8836368931,1.2925486853
H,0,-0.7926872957,0.2918104064,2.0051877184
H,0,-1.194614023,-3.1798103013,0.5227223912
H,0,0.9892094604,0.3433873236,1.8134398276
C,0,0.6420205139,2.6079207106,-0.5895162492
H,0,0.7067818268,0.8770154858,-1.8826693488
C,0,2.371010999,0.7117695564,-0.4885398899
H,0,0.9204318095,-1.9291674699,0.7294287504
H,0,0.818689131,2.8905515854,0.4516951511
H,0,0.1553107222,-1.9456652379,2.3178092334
H,0,3.027643432,1.2319929982,-1.1917234386
H,0,2.5610573732,-0.3611717859,-0.5895052876
H,0,2.6573512927,1.025838703,0.5195808544
H,0,-0.3670149659,2.9071731464,-0.8836143278
H,0,1.3598002062,3.1383542284,-1.222743118

Redundant internal coordinates for **2B1**
optimized at the MP2/6-31G(d)level

H,-1.6125209032,0.6152729969,-1.5811261355
C,-1.4739732048,0.1604480939,-0.5977216999
C,-0.1770597793,0.4570036786,-0.0026349073
C,-1.4158500235,-1.4185635243,-0.7410777196
H,-2.3094642355,0.4007427869,0.0657637991
C,-1.1957159165,-2.0619193038,0.619715021
C,0.0161483044,0.0529998035,1.3829374243
H,-0.6186112783,-1.6931557236,-1.4409464981
C,0.8927198351,1.0144086211,-0.8241843884
H,-2.3658513373,-1.7137741103,-1.1965940008
C,0.0722758567,-1.530880424,1.2714944733
H,-2.0595027305,-1.8744262057,1.267876058
H,-0.846300692,0.303806184,2.0072510484
H,-1.1159234539,-3.1485646079,0.5015883559
H,0.9382518616,0.4227914138,1.8318179187
C,0.6461968972,2.5510463313,-0.5659153053
H,0.6741199506,0.8372507093,-1.8836525388
C,2.3332384624,0.6360144873,-0.4953013992
H,0.9595731372,-1.8267089424,0.7026822726
H,0.857266415,2.8123378562,0.4732980002
H,0.2028079686,-1.8968491168,2.2942746763
H,2.9981581362,1.1607472118,-1.1855585481
H,2.5044510326,-0.4361891064,-0.6182365568
H,2.6159068105,0.9269195684,0.5189027476
H,-0.3646378079,2.8698743885,-0.8289543066
H,1.3543945365,3.0765781159,-1.2122552848

Redundant internal coordinates for **2B2**
optimized at the B3LYP/6-31G(d)level

C,0,-0.1627641949,-0.1418333875,-1.8077578506
C,0,-0.1946035004,-0.234552429,-0.3421038242
C,0,1.1163533796,-0.0251808049,1.849044513
C,0,-1.3049678154,0.6797809651,1.7846318574
H,0,1.8150962787,-0.9647904216,-2.3210712097
C,0,-1.4501697584,0.0678047211,0.3727033331
C,0,0.9898174302,-0.642184043,0.4357391488
C,0,-0.2186338861,-0.0288488815,2.5993587187
H,0,-0.0985694265,0.470388703,3.5662121009
H,0,1.4878527085,1.0016614252,1.7449129871
H,0,-2.1453710628,0.6165418491,-0.2729435051
H,0,1.9062800273,-0.5528751341,-0.1554495827
H,0,0.6405772293,-0.9399474318,-3.6361909134
H,0,1.8819840888,-0.5811007763,2.3975884423
H,0,-2.2760044412,0.6258893904,2.2849724452
H,0,-1.0647944148,1.7448655344,1.6782050342
H,0,-1.8998779494,-0.9452017695,0.4676866054
H,0,0.8316007376,-1.7383724282,0.5352739932
C,0,0.7582902445,-1.1110925322,-2.5624688364
C,0,0.29097905,1.3617083174,-2.0303549241
H,0,-1.1879222297,-0.20917535,-2.1916336413
H,0,1.313584464,1.5257409251,-1.6808653937
H,0,-0.379229003,2.0833165448,-1.55647713
H,0,0.2609331092,1.5236734642,-3.1121466582
H,0,0.4935402153,-2.1534014414,-2.3588991855
H,0,-0.5254860265,-1.0608246377,2.8180727968

Redundant internal coordinates for **2B2**
optimized at the MP2/6-31G(d)level

C,0,-0.1710362029,-0.1679122083,-1.7943571607
C,0,-0.216354846,-0.2999726309,-0.350688941
C,0,1.1175915837,0.0073011491,1.7829181383
C,0,-1.2859685135,0.7171357576,1.7177182317
H,0,1.821705779,-0.9060709446,-2.3184318262
C,0,-1.4656791866,0.0022604127,0.3666668233
C,0,0.9578580873,-0.7140634501,0.43026128
C,0,-0.1964188575,0.0551752177,2.553768014
H,0,-0.0568269319,0.6112537631,3.4859455713
H,0,1.4814821504,1.024122045,1.5955169312
H,0,-2.1894202053,0.4927506853,-0.2922630399
H,0,1.8705664627,-0.7015296416,-0.1698997156
H,0,0.6681589691,-0.8268365827,-3.6492246762
H,0,1.8961897398,-0.5064803791,2.3536429646
H,0,-2.2470307341,0.7138755767,2.2394900767
H,0,-1.0315544998,1.7665876985,1.5290952975
H,0,-1.8726288613,-1.0129971344,0.554841417
H,0,0.7437814279,-1.7859588438,0.6231893518
C,0,0.775301792,-1.0623624105,-2.5877971109
C,0,0.2949193844,1.3477480066,-1.8531206412
H,0,-1.1848711213,-0.1963785964,-2.2077469147
H,0,1.3151453961,1.4618134936,-1.4816823313
H,0,-0.3752349235,2.0285724564,-1.3239293189
H,0,0.27563258,1.6031374592,-2.9162024241
H,0,0.527610557,-2.117886621,-2.4504312633
H,0,-0.50398523,-0.9598334971,2.8358780989

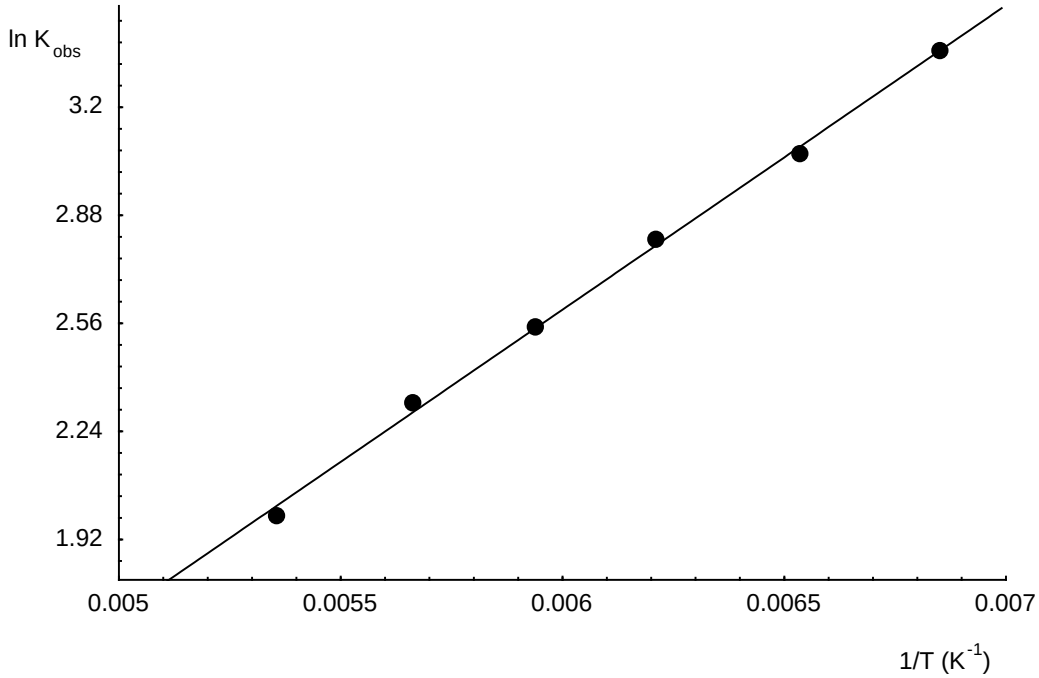
Redundant internal coordinates for **2TS**
optimized at the B3LYP/6-31G(d)level

C,0,2.5452550886,-0.3350256715,-0.6986927291
C,0,1.520901828,-1.4694470171,-0.8024329637
C,0,1.859352202,1.0314412358,-0.7945469618
C,0,0.4000963688,-1.3302149762,0.247961927
C,0,-0.2502616717,0.0440016176,0.2474963023
C,0,0.7436736573,1.195728063,0.2587730229
C,0,-1.6507129817,0.2208345343,0.4227284977
C,0,-2.2986405618,1.5669594897,0.6064875681
C,0,-2.5991048112,-0.9476588252,0.5492995821
H,0,3.0866304864,-0.4113607505,0.2543229705
H,0,3.2934446164,-0.4333058738,-1.4918503877
H,0,2.0006982035,-2.4436889188,-0.6658725131
H,0,1.0735691512,-1.4801378842,-1.8061406628
H,0,2.5817661296,1.8421403596,-0.6569785473
H,0,1.4287004368,1.1647610168,-1.79680407
H,0,-0.3283937913,-2.1358903551,0.147926331
H,0,0.8306338994,-1.4292278411,1.2564140641
H,0,-1.008016072,0.165067636,-0.7903217663
H,0,0.2578690096,2.1662752627,0.1507576453
H,0,1.185255366,1.177932313,1.2665488254
H,0,-3.1767288732,1.6654616632,-0.0385108093
H,0,-1.641402898,2.4215134425,0.4610882012
H,0,-2.6659319108,1.5934268127,1.6420519152
H,0,-3.6101322697,-0.6593827088,0.2546877506
H,0,-2.6284944172,-1.2341003123,1.6097112774
H,0,-2.3028217769,-1.8291945644,-0.0194756975

Redundant internal coordinates for **2TS**
optimized at the MP2/6-31G(d)level

C 2.5365220807,-0.3432651425,-0.6478903843
C 1.5136242248,-1.4661004456,-0.787334866
C 1.8659863269,1.0201472703,-0.7827409232
C 0.3753911789,-1.32122624,0.2279401777
C -0.2673180587,0.0561245119,0.171526367
C 0.7334286264,1.2008295197,0.234043838
C -1.6523152087,0.2289552291,0.433190335
C -2.2955506373,1.5626560647,0.600274967
C -2.5687972529,-0.9477118068,0.5750408048
H 3.032076041,-0.4153961843,0.3288846446
H 3.3183911431,-0.4523872268,-1.4057911142
H 1.9858669447,-2.4431057631,-0.6449198866
H 1.0951077364,-1.465677499,-1.8026489285
H 2.5922918404,1.8263719679,-0.6401072442
H 1.4626891688,1.1384519788,-1.7973710415
H -0.3540923869,-2.1233685251,0.1022526036
H 0.7737052244,-1.4147064213,1.2479539648
H -0.9056506579,0.1602341548,-0.8589960087
H 0.2609694793,2.1750681069,0.0995065847
H 1.1413816768,1.1821479847,1.2537358724
H -3.2185256568,1.6227540547,0.0179999947
H -1.6574582068,2.414507013,0.382622629
H -2.588837994,1.6118907002,1.6590338787
H -3.6128640743,-0.641312515,0.5139067571
H -2.3876007538,-1.3892116118,1.5636394628
H -2.3832772049,-1.7287139799,-0.1640040648

Van’t Hoff plot for 1A/1B equilibrium



	VAR1 1/T (K^{-1})	VAR2 ln K_{obs}
1	.006852	3.3663
2	.006534	3.0625
3	.006209	2.8069
4	.005940	2.5503
5	.005664	2.3263
6	.005355	1.9900

Regression Summary for Dependent Variable: VAR2
R= .99994579 R^2= .99909250 Adjusted R^2= .99861562
F(1,4)=2093.0 p<.00000 Std.Error of estimate: .02443

	BETA	St. Err. of BETA	B	St. Err. of B	t(4)	p-level
Intercpt			-2.8098	.12049	-23.3192	.000020
VAR1	.999946	.021837	901.707219	.70981	45.7491	.000001

From the slope (901.707) and the intercept (-2.8098) of the van't Hoff’s plot, the enthalpy $\Delta H°$=-1.80±0.4 kcal/mol and entropy $\Delta S°$=5.7±0.3 cal K^{-1} mol^{-1} for the reaction **1A→1B** were obtained.