**Supplementary Information**

**A DFT study on the reaction mechanism of Hydrazones with *α*-Oxo-ketenes; competition between stepwise 1,3-dipolar cycloaddition and Diels-Alder pathways**

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**B3LYP/6-311+G(d,p)**

**In2-B**

C -0.65920000 1.14100000 -0.40480000

C -1.34070000 2.12040000 -1.33750000

H -1.04260000 1.97970000 -2.38060000

H -2.43190000 1.99560000 -1.30590000

C -0.94070000 3.52650000 -0.79900000

C -0.70840000 3.26150000 0.70590000

H -1.64110000 3.37060000 1.27580000

H 0.02960000 3.92050000 1.17050000

C 0.02800000 -1.38520000 1.39090000

H 0.75620000 -2.02650000 1.88550000

C -1.13350000 -0.99180000 2.16010000

H -0.86260000 -0.69190000 3.16730000

C -2.44470000 -1.01870000 1.84700000

H -3.10300000 -0.63000000 2.62060000

C -0.39860000 -0.15240000 -0.82560000

O -0.58060000 -0.72990000 -1.89220000

N 0.35840000 -1.06100000 0.18470000

N 1.47240000 -1.74560000 -0.37100000

H 1.13690000 -2.08610000 -1.27140000

C 2.66050000 -0.96160000 -0.54130000

C 2.97650000 0.10810000 0.29720000

C 3.55830000 -1.36460000 -1.53490000

C 4.19690000 0.76370000 0.13450000

H 2.27700000 0.44580000 1.05310000

C 4.77370000 -0.70520000 -1.68080000

H 3.30610000 -2.19410000 -2.18770000

C 5.10150000 0.36290000 -0.84550000

H 4.43390000 1.59880000 0.78400000

H 5.46310000 -1.02470000 -2.45410000

H 6.04730000 0.87850000 -0.96270000

C -0.27850000 1.79770000 0.81850000

O 0.27630000 1.34290000 1.83040000

C 0.37730000 3.97580000 -1.45620000

H 1.16690000 3.23240000 -1.31310000

H 0.24480000 4.11900000 -2.53310000

H 0.72440000 4.92260000 -1.02990000

C -2.03080000 4.57350000 -1.05510000

H -1.74360000 5.55110000 -0.65400000

H -2.21220000 4.69570000 -2.12820000

H -2.97650000 4.28280000 -0.58710000

C -3.14790000 -1.51660000 0.66270000

C -4.39730000 -0.95170000 0.34990000

C -2.67100000 -2.56420000 -0.14030000

C -5.11940000 -1.38370000 -0.75580000

H -4.79190000 -0.15760000 0.97500000

C -3.40020000 -3.00520000 -1.23790000

H -1.73770000 -3.05470000 0.10780000

C -4.62100000 -2.41220000 -1.55510000

H -6.07280000 -0.92450000 -0.99070000

H -3.01450000 -3.81370000 -1.84770000

H -5.18530000 -2.75620000 -2.41430000

**In-A,B**

C -0.73520000 1.30350000 0.69130000

C -1.05170000 2.70720000 1.16440000

H -1.91480000 2.73370000 1.83570000

H -0.20950000 3.13660000 1.72480000

C -1.29790000 3.51990000 -0.14210000

C -0.42600000 2.77300000 -1.17730000

H 0.59740000 3.17200000 -1.19540000

H -0.80490000 2.82020000 -2.20150000

C 0.43540000 -1.67550000 0.55410000

H 0.42290000 -2.73940000 0.33410000

C 1.66230000 -0.96180000 0.45160000

C 2.77780000 -1.62280000 0.05810000

C -0.97640000 0.21860000 1.52150000

O -1.43290000 0.14620000 2.65940000

N -0.70740000 -1.18910000 0.93830000

N -1.75050000 -2.12530000 1.14660000

H -2.05350000 -1.97560000 2.10800000

C -2.85330000 -2.02680000 0.23900000

C -2.70060000 -1.56650000 -1.07000000

C -4.09640000 -2.49390000 0.67810000

C -3.79730000 -1.58400000 -1.93120000

H -1.74840000 -1.17680000 -1.41130000

C -5.17940000 -2.51020000 -0.19420000

H -4.21200000 -2.84500000 1.69840000

C -5.03640000 -2.05640000 -1.50540000

H -3.67400000 -1.21860000 -2.94460000

H -6.13920000 -2.87310000 0.15590000

H -5.88210000 -2.06600000 -2.18280000

C -0.34510000 1.32060000 -0.69790000

O 0.02220000 0.39280000 -1.42970000

C -2.78070000 3.41540000 -0.54350000

H -3.09450000 2.37180000 -0.63750000

H -3.42050000 3.89060000 0.20660000

H -2.96140000 3.90910000 -1.50380000

C -0.90460000 4.99350000 0.01080000

H -1.06360000 5.54480000 -0.92190000

H -1.50150000 5.47990000 0.78950000

H 0.15010000 5.09570000 0.28510000

H 1.66610000 0.08790000 0.70860000

H 2.67700000 -2.67790000 -0.18870000

C 4.12050000 -1.08390000 -0.08330000

C 5.15930000 -1.95510000 -0.45810000

C 4.42960000 0.27210000 0.13760000

C 6.46300000 -1.49410000 -0.60070000

H 4.93470000 -3.00140000 -0.63680000

C 5.73110000 0.73030000 -0.00570000

H 3.64840000 0.96900000 0.41490000

C 6.75230000 -0.14980000 -0.37390000

H 7.25080000 -2.17990000 -0.88950000

H 5.95450000 1.77690000 0.16580000

H 7.76730000 0.21410000 -0.48540000

In-C

C 0.91330000 1.87260000 -0.37750000

C 0.36460000 1.99950000 0.86150000

C -0.36760000 3.30120000 1.02880000

H -0.16200000 3.75180000 2.00490000

H -1.44860000 3.11150000 0.99070000

C 0.11470000 4.16990000 -0.16460000

C 0.60730000 3.11130000 -1.19870000

H -0.17240000 2.89830000 -1.94240000

H 1.48350000 3.45370000 -1.75320000

C 1.86830000 0.88420000 -0.90090000

C -0.29070000 -1.00440000 -0.44540000

H -0.22570000 -0.75400000 -1.50670000

C 3.07800000 -1.18680000 -0.16490000

C 4.35590000 -0.61190000 -0.23850000

H 4.46750000 0.43900000 -0.45890000

C 5.48200000 -1.40460000 -0.05210000

H 6.46250000 -0.94590000 -0.11490000

C 5.36590000 -2.76920000 0.21540000

H 6.25100000 -3.37780000 0.35930000

C 4.09800000 -3.33740000 0.29060000

H 3.98550000 -4.39620000 0.49570000

C 2.95960000 -2.55860000 0.09570000

H 1.97940000 -3.01070000 0.15440000

C -1.56060000 -1.42380000 0.08490000

H -1.58320000 -1.67640000 1.13950000

C -2.66280000 -1.50010000 -0.69270000

H -2.55760000 -1.22320000 -1.74000000

C -4.00540000 -1.91470000 -0.29800000

C -4.33850000 -2.29600000 1.01520000

H -3.58270000 -2.28920000 1.79140000

C -5.63270000 -2.68340000 1.33390000

H -5.87110000 -2.97400000 2.35070000

C -6.62740000 -2.69910000 0.35280000

H -7.63670000 -3.00210000 0.60680000

C -6.31560000 -2.32340000 -0.95200000

H -7.08130000 -2.33230000 -1.71920000

C -5.01870000 -1.93530000 -1.27210000

H -4.78010000 -1.64320000 -2.28960000

C -0.99910000 5.05940000 -0.72820000

H -1.86020000 4.46340000 -1.04600000

H -0.64480000 5.62440000 -1.59620000

H -1.34650000 5.78140000 0.01790000

C 1.30260000 5.03950000 0.28450000

H 1.00010000 5.73930000 1.07020000

H 1.69610000 5.62220000 -0.55360000

H 2.11760000 4.42380000 0.67620000

N 1.89740000 -0.40980000 -0.31510000

N 0.75260000 -0.92870000 0.31470000

H 0.62400000 0.26680000 1.64990000

O 2.67220000 1.17510000 -1.77440000

O 0.37490000 1.17960000 1.91970000

Ts1-A,B

C -0.81730000 1.25340000 0.56310000

C -1.06480000 2.64770000 1.13970000

H -1.91280000 2.67810000 1.82930000

H -0.18560000 3.00250000 1.69240000

C -1.30610000 3.53870000 -0.11440000

C -0.44620000 2.84510000 -1.19210000

H 0.59190000 3.20140000 -1.15680000

H -0.80240000 2.99030000 -2.21450000

C 0.58500000 -2.11040000 0.21810000

H 0.67950000 -3.19760000 0.17210000

C 1.78260000 -1.32010000 0.13570000

C 2.99420000 -1.91260000 0.06200000

C -1.05580000 0.18870000 1.35550000

O -1.42250000 -0.26480000 2.37690000

N -0.59300000 -1.60290000 0.34250000

N -1.62000000 -2.54480000 0.51350000

H -1.65580000 -2.87120000 1.47310000

C -2.88570000 -2.19510000 -0.00200000

C -2.99830000 -1.40300000 -1.14960000

C -4.03750000 -2.71530000 0.60160000

C -4.26020000 -1.13800000 -1.67740000

H -2.10580000 -1.00300000 -1.61550000

C -5.28900000 -2.45140000 0.05660000

H -3.95070000 -3.32480000 1.49600000

C -5.40960000 -1.65950000 -1.08590000

H -4.34030000 -0.52260000 -2.56680000

H -6.17370000 -2.86000000 0.53220000

H -6.38630000 -1.45250000 -1.50740000

C -0.42910000 1.35310000 -0.83850000

O -0.11940000 0.47600000 -1.63230000

C -2.79130000 3.48100000 -0.51500000

H -3.12350000 2.45080000 -0.67140000

H -3.42130000 3.92150000 0.26390000

H -2.96500000 4.03520000 -1.44250000

C -0.88780000 4.99230000 0.13530000

H -1.04200000 5.60390000 -0.75930000

H -1.47560000 5.43650000 0.94530000

H 0.16910000 5.06030000 0.41080000

H 1.66540000 -0.24530000 0.12470000

H 3.02610000 -3.00050000 0.08270000

C 4.29670000 -1.26160000 -0.03950000

C 5.45520000 -2.05670000 -0.00210000

C 4.45010000 0.13020000 -0.17960000

C 6.72130000 -1.48700000 -0.09100000

H 5.35520000 -3.13240000 0.09940000

C 5.71370000 0.69770000 -0.27050000

H 3.57650000 0.76880000 -0.22900000

C 6.85500000 -0.10670000 -0.22480000

H 7.60130000 -2.11910000 -0.05820000

H 5.81310000 1.77150000 -0.38180000

H 7.83940000 0.34150000 -0.29700000

**Ts1’-B**

C -0.51370000 1.19710000 -0.31930000

C -1.20370000 2.20480000 -1.23950000

H -0.89120000 2.11310000 -2.28340000

H -2.29230000 2.06870000 -1.21450000

C -0.82040000 3.58990000 -0.64090000

C -0.66350000 3.27560000 0.86170000

H -1.63260000 3.32240000 1.37610000

H 0.01900000 3.94280000 1.39270000

C 0.07920000 -1.68800000 1.83250000

H 0.61730000 -2.50180000 2.32800000

C -1.08480000 -1.10460000 2.51330000

H -0.83000000 -0.59560000 3.43870000

C -2.37260000 -1.15800000 2.14470000

H -3.07240000 -0.62290000 2.78230000

C -0.28140000 -0.03960000 -0.80230000

O -0.28650000 -0.81840000 -1.68230000

N 0.54250000 -1.25800000 0.72520000

N 1.63220000 -2.02220000 0.21440000

H 1.27970000 -2.54400000 -0.58380000

C 2.77860000 -1.26490000 -0.14480000

C 3.10500000 -0.07790000 0.51730000

C 3.63560000 -1.77130000 -1.13040000

C 4.28560000 0.58770000 0.18890000

H 2.43660000 0.32740000 1.26720000

C 4.81220000 -1.10020000 -1.44210000

H 3.37990000 -2.69130000 -1.64690000

C 5.14620000 0.08440000 -0.78370000

H 4.53000000 1.50990000 0.70460000

H 5.46780000 -1.50220000 -2.20660000

H 6.06300000 0.60710000 -1.02980000

C -0.17550000 1.82590000 0.94910000

O 0.38100000 1.36480000 1.93740000

C 0.52910000 4.05180000 -1.22030000

H 1.31030000 3.30310000 -1.06020000

H 0.45010000 4.22860000 -2.29740000

H 0.85480000 4.98380000 -0.74840000

C -1.89800000 4.64390000 -0.91970000

H -1.62660000 5.60920000 -0.48060000

H -2.03030000 4.79530000 -1.99600000

H -2.86370000 4.34410000 -0.50140000

C -2.99260000 -1.84090000 0.99750000

C -4.18130000 -1.31580000 0.46500000

C -2.48020000 -3.01960000 0.43410000

C -4.81130000 -1.92030000 -0.61820000

H -4.60660000 -0.41830000 0.90210000

C -3.11400000 -3.62970000 -0.64320000

H -1.59400000 -3.47890000 0.85570000

C -4.27730000 -3.07900000 -1.17950000

H -5.72160000 -1.49020000 -1.02060000

H -2.70330000 -4.54190000 -1.06110000

H -4.76880000 -3.55530000 -2.02010000

**Ts1-C**

C 0.73920000 1.91360000 -0.82880000

C 0.47170000 1.71090000 0.58010000

C 0.45860000 3.08960000 1.23780000

H 0.92680000 3.04150000 2.22360000

H -0.59290000 3.36460000 1.39180000

C 1.14960000 4.05350000 0.25160000

C 0.81780000 3.41770000 -1.12920000

H -0.14560000 3.78890000 -1.50030000

H 1.57280000 3.66150000 -1.88100000

C 0.84550000 1.08160000 -1.88800000

C -0.75250000 -1.98670000 -1.03750000

H -0.57480000 -2.30280000 -2.05930000

C 2.51060000 -0.97720000 -0.26920000

C 3.64790000 -0.33310000 -0.79880000

H 3.58010000 0.11660000 -1.78250000

C 4.83540000 -0.28710000 -0.08380000

H 5.69620000 0.21400000 -0.51370000

C 4.93370000 -0.88530000 1.17600000

H 5.86440000 -0.85120000 1.73010000

C 3.82350000 -1.54470000 1.69830000

H 3.88880000 -2.03440000 2.66410000

C 2.62720000 -1.60170000 0.98800000

H 1.79470000 -2.15740000 1.40320000

C -2.01020000 -2.18090000 -0.40050000

H -2.10310000 -1.82700000 0.62250000

C -3.05640000 -2.78250000 -1.02140000

H -2.90900000 -3.10810000 -2.04890000

C -4.37760000 -3.05030000 -0.47150000

C -4.75880000 -2.69750000 0.83830000

H -4.05520000 -2.19790000 1.49360000

C -6.03340000 -2.98130000 1.30900000

H -6.30570000 -2.70110000 2.32040000

C -6.96500000 -3.62310000 0.48890000

H -7.95900000 -3.84240000 0.86140000

C -6.60680000 -3.97820000 -0.81020000

H -7.32180000 -4.47620000 -1.45520000

C -5.33000000 -3.69510000 -1.28280000

H -5.05750000 -3.97500000 -2.29510000

C 0.61600000 5.48750000 0.35230000

H -0.46650000 5.52070000 0.19660000

H 1.08390000 6.13420000 -0.39680000

H 0.82790000 5.91510000 1.33720000

C 2.67150000 4.03930000 0.48220000

H 2.91410000 4.41800000 1.47970000

H 3.18070000 4.67260000 -0.25070000

H 3.08130000 3.02910000 0.39790000

N 1.37100000 -1.00930000 -1.07630000

N 0.25350000 -1.39570000 -0.43650000

H 0.12110000 -0.98270000 0.50500000

O 0.86860000 0.84490000 -3.02830000

O 0.23020000 0.68290000 1.21560000

**Ts2-A**

C -0.38790000 1.15260000 -0.68470000

C -0.70110000 1.12370000 0.69500000

C 0.46950000 -1.39070000 -0.10460000

C -0.61300000 2.56070000 -1.21240000

C -1.43350000 3.29400000 -0.12000000

C -1.08720000 2.50210000 1.18010000

H 0.41520000 -2.20830000 -0.81430000

H 0.37410000 3.02010000 -1.35530000

H -0.25470000 2.98290000 1.71180000

C -0.89160000 -0.03970000 1.46830000

O 0.04030000 0.23080000 -1.43810000

O -1.35170000 -0.18420000 2.59030000

N -1.54360000 -2.31900000 0.68070000

N -0.57840000 -1.28820000 0.70440000

C -1.05990000 4.77710000 -0.01100000

H -1.28680000 5.31290000 -0.93860000

H -1.61730000 5.26230000 0.79670000

H 0.00730000 4.90210000 0.19690000

C -2.93640000 3.15460000 -0.42170000

H -3.53440000 3.62770000 0.36310000

H -3.18970000 3.63300000 -1.37350000

H -3.23500000 2.10410000 -0.48070000

C -2.83020000 -2.01450000 0.14390000

C -2.96790000 -1.30610000 -1.05220000

C -3.96300000 -2.52700000 0.78250000

C -4.23600000 -1.11520000 -1.59600000

H -2.09300000 -0.91000000 -1.55270000

C -5.22330000 -2.34440000 0.22120000

H -3.85770000 -3.06160000 1.72120000

C -5.36800000 -1.63510000 -0.96990000

H -4.33530000 -0.56140000 -2.52290000

H -6.09460000 -2.74600000 0.72630000

H -6.35050000 -1.48590000 -1.40210000

H -1.61690000 -2.67040000 1.63010000

C 1.77160000 -0.85720000 0.21480000

H 1.83670000 -0.15910000 1.03960000

C 2.85830000 -1.25130000 -0.47880000

H 2.70690000 -1.95150000 -1.29770000

C 4.24410000 -0.84820000 -0.26050000

C 5.24700000 -1.42880000 -1.05570000

C 4.62730000 0.09610000 0.70980000

C 6.58480000 -1.08590000 -0.88810000

H 4.96820000 -2.15580000 -1.81130000

C 5.96230000 0.43780000 0.87660000

H 3.87870000 0.56790000 1.33490000

C 6.94700000 -0.15150000 0.07970000

H 7.34240000 -1.54600000 -1.51190000

H 6.23980000 1.16770000 1.62850000

H 7.98810000 0.11930000 0.21330000

H -1.09620000 2.54170000 -2.19330000

H -1.92790000 2.47420000 1.87880000

**Ts2-B**

C -0.33950000 0.57240000 -0.43250000

C -1.16960000 1.56960000 -1.21100000

H -0.81180000 1.68480000 -2.23630000

H -2.21270000 1.22880000 -1.26690000

C -1.09490000 2.90080000 -0.40330000

C -0.92240000 2.39640000 1.04560000

H -1.89830000 2.19350000 1.50840000

H -0.38860000 3.08230000 1.70740000

C 0.55890000 -2.48190000 -0.29640000

H 1.12630000 -3.39090000 -0.46110000

C -0.79930000 -2.52160000 -0.07430000

H -1.30830000 -3.44000000 -0.34710000

C -1.52630000 -1.45670000 0.48390000

H -1.04390000 -0.93890000 1.29870000

C 0.65800000 -0.17030000 -1.13150000

O 1.05490000 0.03470000 -2.27100000

N 1.29310000 -1.35210000 -0.46850000

N 2.61460000 -1.62140000 -0.90750000

H 2.65130000 -1.42430000 -1.90550000

C 3.64910000 -0.94430000 -0.20110000

C 3.47700000 -0.45480000 1.09540000

C 4.89910000 -0.84100000 -0.82410000

C 4.55760000 0.12840000 1.75690000

H 2.50610000 -0.50060000 1.57280000

C 5.96770000 -0.25950000 -0.15110000

H 5.03170000 -1.22060000 -1.83230000

C 5.80540000 0.22760000 1.14640000

H 4.41170000 0.51170000 2.76080000

H 6.93000000 -0.18440000 -0.64540000

H 6.63880000 0.68210000 1.66910000

C -0.18420000 1.06210000 0.94530000

O 0.37150000 0.51640000 1.89250000

C 0.15260000 3.69650000 -0.82810000

H 1.06400000 3.10000000 -0.72810000

H 0.07570000 4.01120000 -1.87290000

H 0.26900000 4.59300000 -0.21110000

C -2.35110000 3.75820000 -0.58980000

H -2.29410000 4.67850000 0.00050000

H -2.47440000 4.04590000 -1.63900000

H -3.25070000 3.21590000 -0.28300000

C -2.97180000 -1.33180000 0.39540000

C -3.67000000 -0.62910000 1.39590000

C -3.70250000 -1.87980000 -0.67580000

C -5.05290000 -0.50300000 1.34220000

H -3.11640000 -0.20060000 2.22430000

C -5.08410000 -1.74720000 -0.73050000

H -3.17680000 -2.39310000 -1.47290000

C -5.76320000 -1.06250000 0.27940000

H -5.57840000 0.03010000 2.12610000

H -5.63470000 -2.17010000 -1.56290000

H -6.84160000 -0.96060000 0.23420000

**Ts2-C**

C 0.83080000 1.57560000 -0.32020000

C 0.33970000 1.62600000 1.01210000

C -0.71200000 2.72650000 1.09820000

H -0.66360000 3.23550000 2.06420000

H -1.70650000 2.26590000 1.02320000

C -0.42730000 3.65150000 -0.11150000

C 0.22220000 2.68120000 -1.14820000

H -0.54640000 2.29310000 -1.83290000

H 0.97100000 3.18070000 -1.76990000

C 2.05430000 0.90390000 -0.75450000

C 0.03200000 -0.86060000 -0.40730000

H 0.19140000 -0.85960000 -1.47900000

C 3.46920000 -1.13960000 -0.14510000

C 4.70890000 -0.50420000 -0.30660000

H 4.75030000 0.54920000 -0.53530000

C 5.88150000 -1.24420000 -0.19270000

H 6.83220000 -0.73860000 -0.32050000

C 5.85020000 -2.61020000 0.08410000

H 6.77090000 -3.17490000 0.17210000

C 4.61780000 -3.23700000 0.24680000

H 4.56920000 -4.29810000 0.46460000

C 3.43420000 -2.51370000 0.13090000

H 2.48170000 -3.00960000 0.26230000

C -1.28630000 -0.98210000 0.11830000

H -1.39140000 -0.97340000 1.19770000

C -2.36260000 -1.08630000 -0.70100000

H -2.17710000 -1.09210000 -1.77330000

C -3.76120000 -1.19400000 -0.31760000

C -4.19640000 -1.16830000 1.02200000

H -3.47860000 -1.06060000 1.82620000

C -5.54530000 -1.27380000 1.32820000

H -5.86430000 -1.25040000 2.36380000

C -6.49270000 -1.40670000 0.30930000

H -7.54530000 -1.48760000 0.55460000

C -6.08010000 -1.43290000 -1.02150000

H -6.80980000 -1.53440000 -1.81640000

C -4.72880000 -1.32720000 -1.33060000

H -4.40970000 -1.34700000 -2.36750000

C -1.69500000 4.31870000 -0.65600000

H -2.44310000 3.57300000 -0.94300000

H -1.47080000 4.92600000 -1.53920000

H -2.14790000 4.97730000 0.09220000

C 0.59730000 4.72630000 0.29440000

H 0.19570000 5.37060000 1.08310000

H 0.85720000 5.35870000 -0.55990000

H 1.52040000 4.27320000 0.66720000

N 2.24720000 -0.42200000 -0.23860000

N 1.11940000 -0.99340000 0.35990000

H 0.98740000 -0.59300000 1.33210000

O 2.87340000 1.37850000 -1.52450000

O 0.65170000 0.89810000 1.99100000

**Tr-rotate-B**

C -1.13060000 1.75990000 0.07940000

C -2.20210000 2.33290000 -0.82510000

H -2.02550000 2.10130000 -1.87960000

H -3.18810000 1.91750000 -0.57510000

C -2.17650000 3.86550000 -0.54770000

C -1.68080000 3.93560000 0.91440000

H -2.52060000 3.86680000 1.61920000

H -1.12870000 4.84630000 1.16050000

C 0.49080000 -0.26220000 1.98220000

H 1.40180000 -0.67710000 2.41510000

C -0.69410000 -0.08210000 2.82480000

H -0.66080000 0.83590000 3.40470000

C -1.73040000 -0.92380000 2.95050000

H -2.51350000 -0.59890000 3.63030000

C -0.56190000 0.53470000 -0.21750000

O -0.71140000 -0.25720000 -1.13860000

N 0.58710000 0.04860000 0.74110000

N 1.77890000 -0.35370000 0.07570000

H 1.44950000 -0.91000000 -0.71300000

C 2.62090000 0.71470000 -0.37820000

C 2.70500000 1.93340000 0.29590000

C 3.43920000 0.46310000 -1.48360000

C 3.61740000 2.89220000 -0.14400000

H 2.05330000 2.14910000 1.13470000

C 4.34920000 1.42630000 -1.90560000

H 3.36510000 -0.48400000 -2.00840000

C 4.44460000 2.64670000 -1.23710000

H 3.67360000 3.84060000 0.37820000

H 4.97970000 1.22300000 -2.76380000

H 5.15100000 3.39810000 -1.56950000

C -0.80830000 2.69730000 1.12620000

O -0.00700000 2.59650000 2.06620000

C -1.15050000 4.54290000 -1.47470000

H -0.16240000 4.08390000 -1.37730000

H -1.45710000 4.45810000 -2.52180000

H -1.05270000 5.60700000 -1.23670000

C -3.55420000 4.50920000 -0.74010000

H -3.52400000 5.58200000 -0.52310000

H -3.90150000 4.38930000 -1.77170000

H -4.29960000 4.05360000 -0.08090000

C -1.98920000 -2.21500000 2.29920000

C -3.31080000 -2.69010000 2.27470000

C -0.98950000 -3.01430000 1.72230000

C -3.62800000 -3.90140000 1.66910000

H -4.09580000 -2.09410000 2.72820000

C -1.30370000 -4.22920000 1.12410000

H 0.04850000 -2.70410000 1.75370000

C -2.62470000 -4.67510000 1.08920000

H -4.65690000 -4.24220000 1.65230000

H -0.51580000 -4.83170000 0.68680000

H -2.86760000 -5.62100000 0.61900000

**M06-2X/6-31G(d,p)**

**In-A,B**

C -0.67838700 1.10368900 0.80783600

C -1.09253900 2.45799500 1.33110700

H -1.98073800 2.39986200 1.96994700

H -0.29610000 2.92550000 1.92866400

C -1.34914800 3.28844700 0.04778100

C -0.33557100 2.69064500 -0.94315400

H 0.65593400 3.14763500 -0.80971900

H -0.61113500 2.79794900 -1.99644900

C 0.47960300 -1.81569400 0.42729800

H 0.47878800 -2.85268300 0.09493800

C 1.70043600 -1.06772500 0.41125300

C 2.82142100 -1.66588400 -0.03663500

C -0.97745300 -0.03960800 1.53364000

O -1.52834900 -0.21100600 2.61201300

N -0.66001100 -1.38427900 0.85328900

N -1.70925700 -2.32052700 0.93337200

H -2.00394600 -2.27980400 1.91118100

C -2.81734300 -1.98306300 0.08986400

C -2.63895600 -1.28732300 -1.10445900

C -4.08242700 -2.43170600 0.46785000

C -3.74585800 -1.04303300 -1.91429300

H -1.65478500 -0.92954200 -1.39605300

C -5.17442100 -2.18576400 -0.35475200

H -4.20714200 -2.96811900 1.40446700

C -5.01237700 -1.48874000 -1.54981800

H -3.60729600 -0.49464600 -2.84070700

H -6.15707200 -2.53437200 -0.05393000

H -5.86712000 -1.29091100 -2.18761000

C -0.22479200 1.21497800 -0.55509100

O 0.20211300 0.34717800 -1.32433700

C -2.77022500 3.01644800 -0.45705700

H -2.93944900 1.94211900 -0.59173000

H -3.51114600 3.38834600 0.25808700

H -2.94352400 3.51365300 -1.41761200

C -1.15098600 4.78350000 0.27422000

H -1.31643700 5.34699700 -0.65039300

H -1.85448300 5.15754800 1.02592600

H -0.13592400 4.99680900 0.62553000

H 1.68227400 -0.04462100 0.76699300

H 2.77396000 -2.71332200 -0.33570900

C 4.12401600 -1.01713800 -0.16052500

C 5.28432800 -1.80073300 -0.20151000

C 4.23689900 0.37776700 -0.25259500

C 6.53534100 -1.20359100 -0.29272700

H 5.19902900 -2.88272800 -0.14782900

C 5.48736900 0.97139100 -0.35195800

H 3.33749300 0.98552400 -0.28653300

C 6.63828600 0.18343800 -0.36459200

H 7.42894700 -1.81835200 -0.31265600

H 5.56715200 2.05040300 -0.43220600

H 7.61419500 0.65122500 -0.44473900

**In-C**

C 0.89289000 1.75273700 -0.35163600

C 0.26246100 1.83574700 0.84678600

C -0.57584200 3.07997300 0.95054900

H -0.50433200 3.52854600 1.94725500

H -1.62968500 2.81396600 0.78670400

C -0.02535100 3.98561100 -0.17296200

C 0.56392000 2.97064000 -1.18681000

H -0.17287200 2.72350200 -1.96489000

H 1.45122500 3.36015000 -1.69499900

C 1.94771800 0.83349700 -0.82634800

C -0.18915900 -1.02813400 -0.45413400

H -0.12835000 -0.71537300 -1.50144800

C 3.17204900 -1.24826000 -0.18466200

C 4.44640600 -0.67247200 -0.26187000

H 4.55506800 0.38491900 -0.45742400

C 5.56909400 -1.47501100 -0.10789600

H 6.55158200 -1.01833800 -0.17366100

C 5.45114000 -2.84240300 0.13033400

H 6.33668300 -3.45779100 0.24847600

C 4.18369500 -3.40713100 0.20963300

H 4.06895400 -4.47079300 0.39282800

C 3.04781800 -2.62120200 0.04774700

H 2.06245400 -3.06641200 0.10869000

C -1.47463900 -1.42003800 0.08117600

H -1.49326300 -1.71769800 1.12573500

C -2.57760400 -1.39427300 -0.68679700

H -2.46473900 -1.07409500 -1.72309400

C -3.94173000 -1.75022100 -0.29159500

C -4.27474900 -2.15463500 1.00960400

H -3.50741900 -2.21211100 1.77496600

C -5.58384600 -2.48202700 1.33166900

H -5.82731100 -2.79174300 2.34270900

C -6.58564900 -2.41229000 0.36326100

H -7.60841700 -2.66838200 0.61987000

C -6.26936500 -2.01150200 -0.93103400

H -7.04319400 -1.95269700 -1.68934700

C -4.95770900 -1.68313700 -1.25340700

H -4.71004300 -1.37053500 -2.26431600

C -1.09990600 4.87312800 -0.79276500

H -1.92686100 4.27401600 -1.18761300

H -0.68464600 5.46175700 -1.61744000

H -1.50817200 5.57136300 -0.05444600

C 1.10876300 4.84881100 0.38787900

H 0.73937500 5.51649300 1.17341100

H 1.55167700 5.46323000 -0.40232400

H 1.89887700 4.22157300 0.81337400

N 1.98925200 -0.47245300 -0.29966200

N 0.85329700 -1.02293000 0.29918000

O 2.79763400 1.20736400 -1.61508300

O 0.25668000 1.02783000 1.90880900

H 0.63022600 0.15235800 1.67917500

**Ts1-A,B**

C -0.74123100 1.08554700 0.60043300

C -1.06103100 2.46448000 1.16269600

H -1.94790700 2.47152400 1.80476800

H -0.22040000 2.85692200 1.75107600

C -1.26631100 3.32390200 -0.10955000

C -0.25893300 2.70644200 -1.09071800

H 0.75172900 3.09765000 -0.90651100

H -0.49353300 2.86791600 -2.14613300

C 0.59910800 -2.28804100 0.14706000

H 0.69447600 -3.37678700 0.08678700

C 1.79579800 -1.47705700 0.13386400

C 3.01739600 -2.02586700 0.03998100

C -1.09392300 0.00832100 1.32486600

O -1.56064600 -0.53819600 2.24903500

N -0.56421200 -1.75539600 0.21142300

N -1.63517700 -2.63422900 0.28725500

H -1.64984700 -3.15294800 1.15878500

C -2.88103000 -2.08625500 -0.06861500

C -2.95227600 -1.10177900 -1.05849100

C -4.04844500 -2.57089500 0.52474800

C -4.19641800 -0.60444000 -1.43392800

H -2.03651600 -0.75012500 -1.52558200

C -5.28323000 -2.07162300 0.12997100

H -3.98453200 -3.33229700 1.29779600

C -5.36549700 -1.08272500 -0.84763800

H -4.24984300 0.15886100 -2.20466600

H -6.18580400 -2.45276700 0.59705100

H -6.33073800 -0.69250100 -1.15157300

C -0.23756400 1.21041000 -0.76669600

O 0.15336300 0.35445000 -1.54166400

C -2.68978400 3.11821400 -0.63754300

H -2.90639000 2.05364900 -0.78065200

H -3.42438000 3.51941500 0.06810100

H -2.82440400 3.62881500 -1.59666500

C -1.00931600 4.80353100 0.15693600

H -1.13911700 5.39180900 -0.75738200

H -1.70863700 5.18936800 0.90626200

H 0.00850300 4.96759800 0.52542600

H 1.65233200 -0.40398800 0.18321300

H 3.11054900 -3.11229200 0.03991000

C 4.26740600 -1.26639500 -0.06785700

C 5.48053200 -1.86678100 0.28866500

C 4.27950200 0.05319200 -0.54200200

C 6.67418400 -1.15877900 0.20632500

H 5.48110400 -2.89461700 0.64177100

C 5.47284700 0.75784200 -0.62713700

H 3.35122900 0.50780600 -0.87722000

C 6.67270700 0.15688900 -0.24873800

H 7.60604700 -1.63522300 0.49339100

H 5.47090300 1.77587500 -1.00308400

H 7.60422500 0.70906300 -0.31990200

**Ts1’-B**

C -0.56855400 1.02006500 -0.09388300

C -1.31709000 1.95930400 -1.02815800

H -1.03044800 1.84503000 -2.07913400

H -2.40292600 1.79541300 -0.96389400

C -0.95472500 3.36385600 -0.48502800

C -0.82584200 3.11183500 1.02404900

H -1.81755700 3.09377600 1.49910900

H -0.20947400 3.84087100 1.55636800

C 0.06945000 -1.70652200 2.28065300

H 0.57867200 -2.50211300 2.83328900

C -1.13853400 -1.08626200 2.84569700

H -1.02606700 -0.67299500 3.84456700

C -2.31869700 -0.99054100 2.22266300

H -3.10948600 -0.44069400 2.73067400

C -0.27682700 -0.21282700 -0.54162700

O -0.20409500 -1.08498000 -1.31456100

N 0.55371800 -1.31730100 1.16980300

N 1.63221300 -2.08960200 0.69790000

H 1.25898300 -2.85898700 0.14671700

C 2.58016000 -1.34163500 -0.03743200

C 2.81714700 -0.00138200 0.27622800

C 3.32274100 -1.97153100 -1.03847200

C 3.79087900 0.69918100 -0.43160300

H 2.24396400 0.47365800 1.06806500

C 4.29657200 -1.26121600 -1.72765100

H 3.13103400 -3.01473500 -1.27600800

C 4.53454100 0.07972400 -1.43130300

H 3.97234800 1.74168100 -0.18774200

H 4.86669700 -1.75736100 -2.50676600

H 5.29382000 0.63284400 -1.97361200

C -0.23477000 1.70534600 1.15192300

O 0.38281400 1.32045800 2.12971600

C 0.40256500 3.79327500 -1.05141000

H 1.16789400 3.03409900 -0.85603300

H 0.33953000 3.93827800 -2.13484900

H 0.73000300 4.73540400 -0.60000800

C -2.02227400 4.39717900 -0.82914400

H -1.75843500 5.38040900 -0.42602300

H -2.13004800 4.49741200 -1.91457100

H -2.99509200 4.11058100 -0.41619500

C -2.68096200 -1.55144600 0.90534600

C -3.48162400 -0.79135000 0.04491500

C -2.26542500 -2.82071700 0.48888000

C -3.81393000 -1.26243100 -1.21932400

H -3.82208400 0.18908100 0.36892600

C -2.61264300 -3.30096000 -0.76895200

H -1.68080300 -3.43869000 1.16507100

C -3.37704100 -2.51963900 -1.63100100

H -4.41910400 -0.65112300 -1.88132000

H -2.28618100 -4.28888800 -1.07769900

H -3.63950800 -2.89223200 -2.61565400

**Ts1-C**

C 0.68022700 1.90529200 -0.83753700

C 0.43167600 1.68616000 0.57450900

C 0.49290200 3.05394600 1.25628900

H 0.96970800 2.96639300 2.23699800

H -0.54197400 3.38264100 1.42827200

C 1.22200800 3.99620500 0.27435300

C 0.82139100 3.40970700 -1.11188800

H -0.13367400 3.83718600 -1.44737400

H 1.56702500 3.63551300 -1.88099400

C 0.73646100 1.08224000 -1.90997000

C -0.75878200 -2.03409300 -1.05305500

H -0.56261400 -2.39884600 -2.05661400

C 2.48130100 -0.93023000 -0.28656500

C 3.60169300 -0.26412000 -0.83008100

H 3.52717500 0.13482300 -1.83693800

C 4.77454200 -0.13078700 -0.09763600

H 5.62228600 0.38686400 -0.53835000

C 4.87372300 -0.66309900 1.19308500

H 5.79287100 -0.56138200 1.76166400

C 3.78131300 -1.34464100 1.72989900

H 3.84942700 -1.78408500 2.72147400

C 2.60064200 -1.48851600 1.00340100

H 1.78098700 -2.05937800 1.42790500

C -2.02481500 -2.20616500 -0.42419900

H -2.13426400 -1.79951500 0.57918100

C -3.06107400 -2.84774800 -1.02728800

H -2.89891900 -3.22100600 -2.03794300

C -4.38748100 -3.09779700 -0.48068800

C -4.77747900 -2.71271800 0.81963900

H -4.07254700 -2.20394500 1.46957200

C -6.05914000 -2.97845900 1.28693200

H -6.33744400 -2.67332800 2.29144900

C -6.98871800 -3.63524600 0.47387800

H -7.98858200 -3.84082800 0.84384100

C -6.62103700 -4.02455600 -0.81502000

H -7.33438900 -4.53540100 -1.45500000

C -5.33775800 -3.75943000 -1.28445200

H -5.05716100 -4.06520200 -2.28900400

C 0.78163600 5.45858700 0.41605500

H -0.30177700 5.56441400 0.29190300

H 1.26971000 6.09047200 -0.33460600

H 1.04702400 5.85321600 1.40309300

C 2.74543600 3.88077400 0.46888400

H 3.03404400 4.21056500 1.47291500

H 3.27793800 4.50681200 -0.25572800

H 3.08996200 2.84964600 0.34141800

N 1.35953000 -1.04216400 -1.11199800

N 0.23578500 -1.40430200 -0.46600800

H 0.08621700 -0.93573000 0.45176800

O 0.71222300 0.82715200 -3.05307200

O 0.15526900 0.65651100 1.20252700

**Ts2-B**

C -0.27153200 0.49476000 -0.52683400

C -1.02395200 1.53001300 -1.33021800

H -0.55672900 1.71601300 -2.30228100

H -2.05553000 1.19034900 -1.51484600

C -1.04277400 2.79192700 -0.43338000

C -1.07413100 2.18517000 0.97706500

H -2.10391900 1.91492600 1.25705900

H -0.66941500 2.82826600 1.76373700

C 0.54257200 -2.67644500 -0.57518100

H 1.11663400 -3.57302500 -0.79724200

C -0.84418700 -2.69016900 -0.42493800

H -1.41039600 -3.50067500 -0.87091500

C -1.42812900 -1.67515800 0.30802800

H -0.79741200 -1.23152200 1.07111100

C 0.69070500 -0.28648700 -1.20195000

O 1.14064500 -0.13108500 -2.32295500

N 1.26494600 -1.55286000 -0.54798900

N 2.62198100 -1.76976900 -0.86951500

H 2.70965800 -1.60492000 -1.87253300

C 3.53079700 -0.93374700 -0.15922400

C 3.19080700 -0.31454200 1.04147100

C 4.81635100 -0.79261700 -0.68725700

C 4.14978100 0.45019900 1.70303700

H 2.18945500 -0.41177400 1.44986600

C 5.76034400 -0.02954400 -0.01397200

H 5.06993100 -1.28433000 -1.62259000

C 5.43270800 0.59754500 1.18671600

H 3.87754100 0.93775800 2.63387300

H 6.75585900 0.07806100 -0.43290600

H 6.17041400 1.19638100 1.70997800

C -0.28381200 0.88442700 0.87308900

O 0.17279800 0.29215800 1.85158100

C 0.26214000 3.57092200 -0.62513800

H 1.13242900 2.92687600 -0.45620600

H 0.32931300 3.96820400 -1.64291100

H 0.31960200 4.41158300 0.07445800

C -2.24228700 3.68787900 -0.72241800

H -2.24918700 4.56247900 -0.06334000

H -2.21540900 4.04736900 -1.75674300

H -3.18146200 3.14354700 -0.57661800

C -2.85150600 -1.38824500 0.39421200

C -3.32529400 -0.67169100 1.50398400

C -3.74969700 -1.76708800 -0.61368400

C -4.67459200 -0.35944000 1.61264700

H -2.61864200 -0.37174600 2.27464100

C -5.09692200 -1.45174000 -0.50295100

H -3.38014900 -2.28849700 -1.49201200

C -5.56073400 -0.75114900 0.61058900

H -5.03599600 0.18934500 2.47604200

H -5.78760400 -1.74372400 -1.28712600

H -6.61441300 -0.50436500 0.69288500

Ts2-C

C 1.04804300 1.61465600 -0.10406800

C 0.47867900 1.54088600 1.18499100

C -0.48893900 2.69284600 1.37665100

H -0.06292900 3.35994200 2.13702200

H -1.44784500 2.33445400 1.76987900

C -0.60443300 3.38796100 0.00074200

C 0.65633200 2.90861000 -0.76919500

H 0.45359400 2.80229500 -1.84217900

H 1.48204800 3.62874700 -0.68204400

C 2.31150100 0.96908200 -0.50659400

C 0.17923100 -0.62434400 -0.46102300

H 0.35256500 -0.52994800 -1.53061500

C 3.54844300 -1.23083400 -0.19422700

C 4.82912500 -0.70340000 -0.40285600

H 4.95455000 0.35157500 -0.59523800

C 5.92853800 -1.55389500 -0.37324600

H 6.91585600 -1.13265900 -0.53490800

C 5.78383800 -2.91811600 -0.13993800

H 6.65143800 -3.56871300 -0.11978900

C 4.50866200 -3.43340900 0.06608700

H 4.37004100 -4.49412700 0.25030100

C 3.39514500 -2.60223800 0.03859800

H 2.40504000 -3.00994600 0.20191900

C -1.16225200 -0.73019600 0.05167300

H -1.26483700 -0.76069500 1.13349800

C -2.22478400 -0.76347300 -0.77563100

H -2.03821700 -0.74715000 -1.85005700

C -3.63164900 -0.81025000 -0.38212900

C -4.04364700 -0.65851400 0.95065200

H -3.30956400 -0.48597800 1.73130000

C -5.39001700 -0.71121100 1.27907100

H -5.69703000 -0.59036400 2.31261300

C -6.34871900 -0.91103700 0.28497800

H -7.40119000 -0.94915600 0.54637000

C -5.95394500 -1.05322700 -1.04185300

H -6.69597300 -1.20292200 -1.81888300

C -4.60493800 -0.99935400 -1.37208100

H -4.29413900 -1.10883500 -2.40758100

C -1.86050200 2.89812000 -0.72510100

H -1.82990500 1.81244000 -0.85508700

H -1.93963300 3.35896100 -1.71540100

H -2.76436800 3.14783500 -0.15908000

C -0.64569500 4.90967700 0.12611400

H -1.53356800 5.23292800 0.68022000

H -0.67618600 5.37963000 -0.86281500

H 0.23870700 5.28430700 0.65080900

N 2.39366200 -0.41183800 -0.20485200

N 1.21163700 -0.94622800 0.31507700

H 1.04123600 -0.52065600 1.33236900

O 3.20660100 1.54896800 -1.09169700

O 0.68539200 0.67279500 2.08293700

Ts2-A

C -0.37255100 0.99289500 -0.58715700

C -0.59639000 0.95399200 0.82614200

C 0.58096000 -1.56002700 -0.01534800

C -0.82474800 2.35817200 -1.09073900

C -1.73404000 2.91614600 0.02058900

C -1.13617800 2.27951200 1.30197300

H 0.52294400 -2.37845800 -0.72910800

H 0.07286700 2.97910200 -1.22139300

H -0.34149200 2.92160200 1.70875900

C -0.76018200 -0.21314200 1.58155800

O 0.10335200 0.13388700 -1.35919400

O -1.24608100 -0.42177100 2.68183200

N -1.53359800 -2.33617200 0.62524500

N -0.45332000 -1.43566700 0.76956700

C -1.73707100 4.44045600 0.07041100

H -2.14728300 4.86375500 -0.85275300

H -2.34982000 4.79792200 0.90494900

H -0.72336500 4.83274600 0.20323600

C -3.15738700 2.38689300 -0.17739300

H -3.81789500 2.75062300 0.61687400

H -3.56737600 2.71347200 -1.13971700

H -3.17101200 1.29181600 -0.15462100

C -2.68734400 -1.72154000 0.02199700

C -2.65629000 -1.39890200 -1.33510400

C -3.83663000 -1.49467800 0.77453100

C -3.78815000 -0.86098700 -1.93590600

H -1.74559300 -1.55330900 -1.90445000

C -4.97465700 -0.97892000 0.15818200

H -3.82822800 -1.70328400 1.84064400

C -4.95354900 -0.66255600 -1.19633700

H -3.76250200 -0.60451700 -2.99006200

H -5.87111200 -0.80704100 0.74496100

H -5.83716300 -0.25098200 -1.67273800

H -1.76162300 -2.60399300 1.58203000

C 1.86958800 -0.95584300 0.24758900

H 1.91785800 -0.18077100 1.00456700

C 2.94469800 -1.38097800 -0.43514500

H 2.80154000 -2.16368100 -1.18005700

C 4.32093200 -0.90401900 -0.28588100

C 5.34174500 -1.57001900 -0.97569600

C 4.65681500 0.19510300 0.51817700

C 6.66490000 -1.16041600 -0.85986500

H 5.08931600 -2.41906300 -1.60514900

C 5.97740700 0.60429300 0.63317200

H 3.88014500 0.73935500 1.04569500

C 6.98571400 -0.07262800 -0.05345200

H 7.44438100 -1.68838600 -1.39912100

H 6.22420900 1.45815500 1.25545800

H 8.01701600 0.25230800 0.03775200

H -1.30942200 2.26746200 -2.06788600

H -1.88768500 2.15407300 2.08917300