**Supporting informations**

**Comparative computational studies of 1, 4-diformyl-piperazine and 1, 4-dithionyl-piperazine**

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| **Atoms** | **X** | **Y** | **Z** |
| N | 1.35144000 | -0.27113200 | -0.24176700 |
| C | 0.37923500 | -1.35254600 | -0.36922700 |
| C | 2.66049800 | -0.48421000 | 0.08114400 |
| C | -0.84766600 | -1.07347700 | 0.50883200 |
| H | 0.06436400 | -1.44414100 | -1.41824600 |
| H | 0.85291300 | -2.29297600 | -0.07199100 |
| N | -1.35144100 | 0.27113400 | 0.24177000 |
| H | -1.65379000 | -1.77949100 | 0.30097900 |
| H | -0.57001300 | -1.15387100 | 1.56939900 |
| C | -0.37923700 | 1.35254800 | 0.36923100 |
| C | 0.84766700 | 1.07347800 | -0.50882700 |
| H | -0.85291300 | 2.29297800 | 0.07199300 |
| H | -0.06436700 | 1.44414300 | 1.41825000 |
| H | 0.57001400 | 1.15387600 | -1.56939500 |
| H | 1.65378900 | 1.77949200 | -0.30097100 |
| C | -2.66049700 | 0.48420800 | -0.08115100 |
| O | -3.51434800 | -0.38565500 | -0.18693300 |
| O | 3.51435000 | 0.38565200 | 0.18692700 |
| H | 2.88303200 | -1.55471000 | 0.24710700 |
| H | -2.88303400 | 1.55470800 | -0.24711100 |
| **B3LYP/6-31++G(d,p)** | **chaise-tr.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| N | 1.32881500 | -0.28003200 | -0.28725500 |
| C | 0.35058900 | -1.35036700 | -0.38206300 |
| C | 2.62279000 | -0.48628500 | 0.07973700 |
| C | -0.82957100 | -1.06079200 | 0.54627000 |
| H | -0.01057600 | -1.42582100 | -1.41644400 |
| H | 0.83061200 | -2.29556500 | -0.11235900 |
| N | -1.32882200 | 0.28003400 | 0.28728300 |
| H | -1.65034700 | -1.76105600 | 0.38199100 |
| H | -0.49927900 | -1.12644400 | 1.59188500 |
| C | -0.35059500 | 1.35037000 | 0.38208700 |
| C | 0.82956500 | 1.06079500 | -0.54624600 |
| H | -0.83061800 | 2.29556700 | 0.11238300 |
| H | 0.01056900 | 1.42582400 | 1.41646900 |
| H | 0.49927200 | 1.12644500 | -1.59186000 |
| H | 1.65034100 | 1.76105800 | -0.38196700 |
| C | -2.62279700 | 0.48628800 | -0.07971100 |
| O | -3.46154900 | -0.38506900 | -0.20649200 |
| O | 3.46157000 | 0.38506100 | 0.20640900 |
| H | 2.84480400 | -1.55462000 | 0.25536600 |
| H | -2.84478400 | 1.55461200 | -0.25543900 |
| **M062X/6-31++G(d,p)** | **dif-chai-m06.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| N | -1.31857100 | -0.28254100 | -0.29691300 |
| C | -0.82295500 | 1.06094900 | -0.55661200 |
| C | -2.61570200 | -0.49463900 | 0.07515300 |
| C | 0.33830000 | 1.35384100 | 0.38845700 |
| H | -0.47750100 | 1.12273600 | -1.59402800 |
| H | -1.64937800 | 1.75468000 | -0.40855400 |
| N | 1.31981800 | 0.28313000 | 0.30120400 |
| H | 0.82165000 | 2.29740100 | 0.12996500 |
| H | -0.03627900 | 1.42310900 | 1.41510500 |
| C | 0.82397600 | -1.06027100 | 0.56100200 |
| C | -0.33709500 | -1.35329200 | -0.38424600 |
| H | 1.65031600 | -1.75414800 | 0.41321500 |
| H | 0.47828900 | -1.12159900 | 1.59832100 |
| H | 0.03778500 | -1.42262900 | -1.41081800 |
| H | -0.82049200 | -2.29683400 | -0.12576700 |
| C | 2.61475600 | 0.49409200 | -0.07906700 |
| O | 3.46800500 | -0.38571400 | -0.21630300 |
| O | -3.47047100 | 0.38443900 | 0.20749400 |
| H | -2.83080000 | -1.55970600 | 0.24753400 |
| H | 2.82972700 | 1.55899000 | -0.25266200 |
| **MP2/6-31++G(d,p)** | **dif-chai-mp2.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| N | -1.31675000 | -0.28817300 | -0.32411400 |
| C | -0.82068600 | 1.05767700 | -0.57318800 |
| C | -2.61483500 | -0.49049200 | 0.07910300 |
| C | 0.33317000 | 1.35658000 | 0.38959900 |
| H | -0.45710800 | 1.12929000 | -1.61623600 |
| H | -1.66271000 | 1.75125300 | -0.42983100 |
| N | 1.31654100 | 0.28809300 | 0.32333000 |
| H | 0.82377700 | 2.30981400 | 0.13085500 |
| H | -0.06371200 | 1.43600900 | 1.42000600 |
| C | 0.82048300 | -1.05772300 | 0.57249700 |
| C | -0.33335000 | -1.35663400 | -0.39032100 |
| H | 1.66249400 | -1.75132500 | 0.42920100 |
| H | 0.45689600 | -1.12929300 | 1.61555800 |
| H | 0.06356400 | -1.43604300 | -1.42071100 |
| H | -0.82396700 | -2.30987200 | -0.13160900 |
| C | 2.61504500 | 0.49056000 | -0.07842600 |
| O | 3.45620500 | -0.38598000 | -0.21958100 |
| O | -3.45583000 | 0.38608500 | 0.22106100 |
| H | -2.81654000 | -1.57361000 | 0.25844600 |
| H | 2.81680000 | 1.57369100 | -0.25762000 |
| **MP2/ccpvdz** | **dif-chai-mp2dz.tif** | | |

* + 1. **1,4-dithionyl-piperazine**

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| **Atoms** | **X** | **Y** | **Z** |
| N | -1.32655000 | -0.39971500 | -0.27707200 |
| C | -0.91712500 | 0.97176200 | -0.57482800 |
| C | -2.59785600 | -0.74455200 | 0.01279500 |
| C | 0.24210800 | 1.38319900 | 0.34063100 |
| H | -0.60346600 | 1.02910700 | -1.62594200 |
| H | -1.78119400 | 1.62259900 | -0.42829800 |
| N | 1.32642600 | 0.39962500 | 0.27638900 |
| H | 0.62949700 | 2.35973400 | 0.03970500 |
| H | -0.11684300 | 1.45770800 | 1.37597300 |
| C | 0.91698000 | -0.97185000 | 0.57414300 |
| C | -0.24222100 | -1.38326400 | -0.34137800 |
| H | 1.78105500 | -1.62269400 | 0.42768900 |
| H | 0.60325600 | -1.02920800 | 1.62524200 |
| H | 0.11676500 | -1.45765900 | -1.37671200 |
| H | -0.62959500 | -2.35983100 | -0.04054900 |
| C | 2.59789200 | 0.74456400 | -0.01266000 |
| S | 3.93278300 | -0.23333600 | -0.11253700 |
| S | -3.93261700 | 0.23344200 | 0.11349100 |
| H | -2.69677100 | -1.81769900 | 0.19443600 |
| H | 2.69683900 | 1.81771900 | -0.19424200 |
| **B3LYP/6-31++G(d,p)** | **chaise-tr-dithio.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| N | -1.28387600 | 0.41945200 | 0.36435700 |
| C | -0.87561800 | -0.94751400 | 0.65675300 |
| C | -2.53444300 | 0.75073100 | 0.00656700 |
| C | 0.18759300 | -1.38198600 | -0.35377100 |
| H | -0.45805800 | -0.97962200 | 1.67120900 |
| H | -1.75655500 | -1.58878000 | 0.60532100 |
| N | 1.28387100 | -0.41945800 | -0.36433200 |
| H | 0.58049800 | -2.36832900 | -0.09654700 |
| H | -0.25921400 | -1.43043600 | -1.35496000 |
| C | 0.87560900 | 0.94751200 | -0.65673200 |
| C | -0.18759100 | 1.38198100 | 0.35379600 |
| H | 1.75655100 | 1.58877300 | -0.60531000 |
| H | 0.45804500 | 0.97961000 | -1.67118700 |
| H | 0.25921600 | 1.43041800 | 1.35498600 |
| H | -0.58050000 | 2.36832600 | 0.09658800 |
| C | 2.53444200 | -0.75072500 | -0.00654600 |
| S | 3.85020000 | 0.23234300 | 0.13358600 |
| S | -3.85019500 | -0.23233700 | -0.13362600 |
| H | -2.62893400 | 1.82012000 | -0.19996800 |
| H | 2.62895600 | -1.82012300 | 0.19993800 |
| **M062X/6-31++G(d,p)** | **dith-chai-m06.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| N | -1.21612600 | -0.46184400 | -0.49095200 |
| C | -0.81671000 | 0.91091400 | -0.77150000 |
| C | -2.45523300 | -0.77179500 | -0.03535500 |
| C | 0.10038500 | 1.39512100 | 0.35093400 |
| H | -0.27830000 | 0.92931700 | -1.72345100 |
| H | -1.71599200 | 1.52011600 | -0.84550400 |
| N | 1.21609900 | 0.46183000 | 0.49087100 |
| H | 0.49420900 | 2.38882500 | 0.13564400 |
| H | -0.45743600 | 1.43063400 | 1.29085600 |
| C | 0.81669100 | -0.91093000 | 0.77140400 |
| C | -0.10040700 | -1.39512900 | -0.35103200 |
| H | 1.71597800 | -1.52012700 | 0.84539200 |
| H | 0.27829000 | -0.92935200 | 1.72336100 |
| H | 0.45740600 | -1.43063000 | -1.29096000 |
| H | -0.49422500 | -2.38883800 | -0.13574800 |
| C | 2.45523600 | 0.77179800 | 0.03536400 |
| S | 3.74059900 | -0.23391800 | -0.16039100 |
| S | -3.74056900 | 0.23393500 | 0.16052000 |
| H | -2.54356600 | -1.83341100 | 0.19478700 |
| H | 2.54357400 | 1.83341600 | -0.19476100 |
| **MP2/6-31++G(d,p)** | **dith-chai-mp2.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| N | -1.24750000 | -0.44532000 | -0.43795200 |
| C | -0.84966700 | 0.92811200 | -0.72157100 |
| C | -2.50047400 | -0.76755900 | -0.02108600 |
| C | 0.13892400 | 1.39275200 | 0.35465400 |
| H | -0.36203400 | 0.95981200 | -1.71329700 |
| H | -1.75713200 | 1.55067100 | -0.73098700 |
| N | 1.24797000 | 0.44572300 | 0.43938100 |
| H | 0.53895500 | 2.39126000 | 0.11630600 |
| H | -0.37832000 | 1.43870100 | 1.33070200 |
| C | 0.85000900 | -0.92763300 | 0.72322300 |
| C | -0.13846600 | -1.39235200 | -0.35306800 |
| H | 1.75739600 | -1.55029300 | 0.73284700 |
| H | 0.36223300 | -0.95904400 | 1.71487600 |
| H | 0.37895200 | -1.43836300 | -1.32903100 |
| H | -0.53855200 | -2.39083900 | -0.11473000 |
| C | 2.50044300 | 0.76745200 | 0.02060600 |
| S | 3.80100300 | -0.23484200 | -0.15019700 |
| S | -3.80159600 | 0.23426600 | 0.14815600 |
| H | -2.57807500 | -1.84666900 | 0.19935100 |
| H | 2.57815800 | 1.84653400 | -0.19992600 |
| **MP2/ccpvdz** | **dith-chai-mp2dz.tif** | | |

* 1. **Skew conformers**
     1. **1,4-diformyl-piperazine**

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| **Atoms** | **X** | **Y** | **Z** |
| C | 0.29821500 | 1.47511800 | 0.55360200 |
| C | -1.06126600 | 0.85267800 | 0.95536400 |
| C | -0.29795100 | -1.47425600 | 0.55529600 |
| C | 1.06136000 | -0.85128300 | 0.95670400 |
| H | -1.09601900 | 0.67092800 | 2.03632700 |
| H | -1.88458500 | 1.51899900 | 0.69488900 |
| H | 0.66272800 | 2.11552400 | 1.36930200 |
| H | -0.66272100 | -2.11378000 | 1.37156900 |
| H | -0.18088800 | -2.09646100 | -0.33673900 |
| H | 1.88477800 | -1.51791300 | 0.69731900 |
| H | 1.09584600 | -0.66815600 | 2.03744400 |
| H | 0.18147300 | 2.09636800 | -0.33914200 |
| N | -1.25729000 | -0.40808700 | 0.25424600 |
| N | 1.25758400 | 0.40864100 | 0.25403400 |
| C | -2.16542200 | -0.50875000 | -0.75913100 |
| H | -2.13635300 | -1.49604300 | -1.25561800 |
| C | 2.16521100 | 0.50757400 | -0.76006200 |
| H | 2.13594300 | 1.49405200 | -1.25816700 |
| O | -2.94436500 | 0.37224000 | -1.09918700 |
| O | 2.94397200 | -0.37397600 | -1.09903500 |
| **B3LYP/6-31++G(d,p)** | **dif-twist.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| C | 0.08208600 | 0.74891200 - | -1.49237300 |
| C | -1.18198000 | 1.10187000 | -0.66621000 |
| C | -0.08231600 | 0.74981900 | 1.49201900 |
| C | 1.18174400 | 1.10235300 | 0.66565300 |
| H | -1.20842600 | 2.16965000 | -0.42654700 |
| H | -2.08890400 | 0.84048500 | -1.21162000 |
| H | 0.39210500 | 1.60698300 | -2.10019300 |
| H | -0.39241500 | 1.60824400 | 2.09929300 |
| H | 0.12782900 | -0.09016000 | 2.15975100 |
| H | 2.08868200 | 0.84131800 | 1.21120900 |
| H | 1.20814200 | 2.16999600 | 0.42537500 |
| H | -0.12802500 | -0.09150300 | -2.15956500 |
| N | -1.15020800 | 0.35692200 | 0.58058600 |
| N | 1.15001400 | 0.35667100 | -0.58069800 |
| C | -1.64665300 | -0.91535200 | 0.57903100 |
| H | -1.41430700 | -1.46901600 | 1.50554500 |
| C | 1.64682900 | -0.91545400 | -0.57854700 |
| H | 1.41453900 | -1.46963700 | -1.50476200 |
| O | -2.29870800 | -1.39680100 | -0.32801100 |
| O | 2.29919300 | -1.39624800 | 0.32862000 |
| **M062X/6-31++G(d,p)** | **dif-twist-m06.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| C | 0.06172300 | 0.75142300 - | -1.49568700 |
| C | -1.18447200 | 1.11183300 | -0.65258600 |
| C | -0.06168700 | 0.75127800 | 1.49574000 |
| C | 1.18450700 | 1.11176200 | 0.65267100 |
| H | -1.19758900 | 2.17520100 | -0.40620900 |
| H | -2.10125300 | 0.86307800 | -1.18265200 |
| H | 0.36801100 | 1.60198100 | -2.11134100 |
| H | -0.36796200 | 1.60177700 | 2.11148300 |
| H | 0.15799000 | -0.09212200 | 2.15078900 |
| H | 2.10128700 | 0.86296000 | 1.18271600 |
| H | 1.19762400 | 2.17515100 | 0.40638600 |
| H | -0.15795900 | -0.09190700 | -2.15082500 |
| N | -1.13955100 | 0.36027900 | 0.59177200 |
| N | 1.13958200 | 0.36031900 | -0.59175600 |
| C | -1.62961100 | -0.91948500 | 0.58932000 |
| H | -1.39131800 | -1.46866800 | 1.51114200 |
| C | 1.62955600 | -0.91948000 | -0.58937800 |
| H | 1.39130600 | -1.46856300 | -1.51127100 |
| O | -2.29942700 | -1.40790300 | -0.32439900 |
| O | 2.29937100 | -1.40798000 | 0.32429700 |
| **MP2/6-31++G(d,p)** | **dif-twist-mp2.tif** | | |

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| **Atoms** | **X** | **Y** | **Z** |
| C | 0.04916600 | 0.72939100 | -1.49569700 |
| C | -1.18728100 | 1.11426600 | -0.64214100 |
| C | -0.04900600 | 0.72868600 | 1.49596300 |
| C | 1.18744400 | 1.11392000 | 0.64257800 |
| H | -1.18636300 | 2.19112400 | -0.40348500 |
| H | -2.11802000 | 0.86914300 | -1.17257300 |
| H | 0.33689900 | 1.56794600 | -2.15710300 |
| H | -0.33668800 | 1.56693100 | 2.15778500 |
| H | 0.18805700 | -0.14583900 | 2.12333400 |
| H | 2.11817600 | 0.86854600 | 1.17290400 |
| H | 1.18654500 | 2.19088300 | 0.40439900 |
| H | -0.18792300 | -0.14481300 | -2.12350600 |
| N | -1.14669000 | 0.36508300 | 0.60470100 |
| N | 1.14683200 | 0.36530100 | -0.60460700 |
| C | -1.64696900 | -0.92003900 | 0.58480600 |
| H | -1.39049000 | -1.47775000 | 1.51572600 |
| C | 1.64684400 | -0.91993600 | -0.58517700 |
| H | 1.39030200 | -1.47724500 | -1.51632000 |
| O | -2.32340600 | -1.38725800 | -0.32148400 |
| O | 2.32307200 | -1.38766000 | 0.32100800 |
| **MP2/ccpvdz** | **dif-twist-mp2dz.tif** | | |

1. **1,4-dithionyl-piperazine**

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| **Atoms** | **X** | **Y** | **Z** |
| C | -0.21599900 | -1.47027400 | 0.44289000 |
| C | 1.06632600 | -0.81373000 | 0.97053500 |
| C | 0.21601700 | 1.47031900 | 0.44282800 |
| C | -1.06632900 | 0.81380500 | 0.97046500 |
| H | 1.00973300 | -0.65327100 | 2.05410800 |
| H | 1.92864000 | -1.45197300 | 0.77113900 |
| H | -0.52691200 | -2.26666700 | 1.13202300 |
| H | 0.52691600 | 2.26673400 | 1.13194300 |
| H | 0.02661900 | 1.91817900 | -0.53763700 |
| H | -1.92863500 | 1.45203600 | 0.77100100 |
| H | -1.00977500 | 0.65341200 | 2.05405000 |
| H | -0.02656900 | -1.91816500 | -0.53755400 |
| N | 1.28758700 | 0.46470400 | 0.30177200 |
| N | -1.28757300 | -0.46466900 | 0.30177200 |
| C | 2.39755700 | 0.73869700 | -0.41017700 |
| H | 2.36183500 | 1.73923800 | -0.84932000 |
| C | -2.39755500 | -0.73872600 | -0.41013500 |
| H | -2.36182300 | -1.73929300 | -0.84921800 |
| S | -3.72234700 | 0.22508000 | -0.66886900 |
| S | 3.72233300 | -0.22514400 | -0.66886700 |
| **B3LYP/6-31++G(d,p)** | **dith-twist.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| C | 0.10301900 | 1.06998600 | 1.48866000 |
| C | 1.24536500 | 1.43296200 | 0.50713200 |
| C | -0.10311600 | 1.06975500 | -1.48874200 |
| C | -1.24545000 | 1.43289500 | -0.50726100 |
| H | 1.21183000 | 2.49276900 | 0.23622100 |
| H | 2.21952500 | 1.20525600 | 0.94008000 |
| H | -0.14983700 | 1.93222900 | 2.11628000 |
| H | 0.14972300 | 1.93189300 | -2.11651500 |
| H | -0.40507200 | 0.23804800 | -2.12891300 |
| H | -2.21961600 | 1.20515800 | -0.94018000 |
| H | -1.21188500 | 2.49273700 | -0.23649300 |
| H | 0.40496000 | 0.23839000 | 2.12898300 |
| N | 1.06123700 | 0.65345700 | -0.70647600 |
| N | -1.06132900 | 0.65355200 | 0.70645400 |
| C | 1.59169200 | -0.57519300 | -0.83184500 |
| H | 1.23447100 | -1.09265300 | -1.72530900 |
| C | -1.59167300 | -0.57513600 | 0.83191400 |
| H | -1.23442700 | -1.09249300 | 1.72542800 |
| S | -2.66740800 | -1.30731300 | -0.18022300 |
| S | 2.66753000 | -1.30718800 | 0.18031200 |
| **M062X/6-31++G(d,p)** | **dith-twist-m06.tif** | | |
| **Atoms** | **X** | **Y** | **Z** |
| C | -0.16425800 | 1.10816800 | -1.48472300 |
| C | -1.26449400 | 1.46233700 | -0.45542300 |
| C | 0.16423500 | 1.10821000 | 1.48470800 |
| C | 1.26447100 | 1.46235200 | 0.45540000 |
| H | -1.22424600 | 2.51795400 | -0.18066100 |
| H | -2.25467700 | 1.23434800 | -0.84469400 |
| H | 0.06995800 | 1.97388100 | -2.11068300 |
| H | -0.06998500 | 1.97394000 | 2.11064200 |
| H | 0.48698700 | 0.28580600 | 2.12156100 |
| H | 2.25465400 | 1.23437000 | 0.84467600 |
| H | 1.22422500 | 2.51796200 | 0.18061100 |
| H | -0.48700900 | 0.28574300 | -2.12155100 |
| N | -1.02410600 | 0.67919000 | 0.74594300 |
| N | 1.02408300 | 0.67917300 | -0.74594400 |
| C | -1.48519200 | -0.59428100 | 0.84311400 |
| H | -1.08810100 | -1.10742800 | 1.71781700 |
| C | 1.48519900 | -0.59428700 | -0.84310300 |
| H | 1.08811100 | -1.10745500 | -1.71779400 |
| S | 2.54138900 | -1.34475600 | 0.16724500 |
| S | -2.54136000 | -1.34478600 | -0.16723000 |
| **MP2/6-31++G(d,p)** | **dith-twist-mp2.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| C | -0.15153000 | 1.05780900 | -1.48787700 |
| C | -1.25535100 | 1.44679200 | -0.47073600 |
| C | 0.15152300 | 1.05782600 | 1.48787200 |
| C | 1.25534500 | 1.44679700 | 0.47072700 |
| H | -1.19717400 | 2.51499700 | -0.20306000 |
| H | -2.25441200 | 1.22691500 | -0.87369100 |
| H | 0.07138000 | 1.90611600 | -2.16104900 |
| H | -0.07138800 | 1.90614100 | 2.16103300 |
| H | 0.47981800 | 0.19614200 | 2.08858300 |
| H | 2.25440500 | 1.22692200 | 0.87368300 |
| H | 1.19716800 | 2.51500000 | 0.20303900 |
| H | -0.47982600 | 0.19611800 | -2.08857800 |
| N | -1.04361700 | 0.66356000 | 0.73744000 |
| N | 1.04361000 | 0.66355200 | -0.73744100 |
| C | -1.55945200 | -0.59135900 | 0.84036200 |
| H | -1.16979900 | -1.11697500 | 1.72868800 |
| C | 1.55945300 | -0.59136300 | -0.84035700 |
| H | 1.16980100 | -1.11698700 | -1.72867800 |
| S | 2.65188600 | -1.30322000 | 0.17236900 |
| S | -2.65187600 | -1.30322900 | -0.17236300 |
| **MP2/ccpvdz** | **dith-twist-mp2dz.tif** | | |

* 1. **Axial/equatorial exchange**
     1. **1,4-dithionyl-piperazine**

**aa high energy point**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.16695600 | 0.41203700 | 0.73358400 |
| C | 0.11416800 | 1.40292200 | 0.39953300 |
| C | 2.29579800 | 0.50421200 | -0.05724800 |
| C | -0.67383800 | 0.97264500 | -0.86361200 |
| H | -0.56268200 | 1.49224400 | 1.25304800 |
| H | 0.58096900 | 2.37960200 | 0.23894300 |
| N | -1.15823300 | -0.42079000 | -0.73300600 |
| H | -1.53370600 | 1.62664000 | -1.01453600 |
| H | -0.02872300 | 1.02323500 | -1.74756900 |
| C | -0.03294300 | -1.34437900 | -0.44715800 |
| C | 0.58240800 | -0.93894300 | 0.89464700 |
| H | -0.42074900 | -2.36862100 | -0.41261300 |
| H | 0.69860300 | -1.28738800 | -1.25361500 |
| H | -0.16910100 | -0.90269400 | 1.68754600 |
| H | 1.38088700 | -1.62431000 | 1.18879900 |
| C | -2.28281300 | -0.54710200 | 0.05979000 |
| O | -3.04289500 | 0.35970200 | 0.36282900 |
| O | 3.03562300 | -0.42483400 | -0.34386200 |
| H | 2.50895800 | 1.54290300 | -0.37070000 |
| H | -2.47402800 | -1.59542300 | 0.35919800 |
| **B3LYP/6-31++G(d,p)** | **MAX1-aa.tif** | | |

**ae high energy point**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.55280900 | 0.44656900 | 0.44801100 |
| C | 0.57500100 | 1.53505200 | 0.60762000 |
| C | 2.08762500 | 0.28610400 | -0.81283700 |
| C | -0.76972800 | 1.14374800 | -0.01587600 |
| H | 0.47864800 | 1.74895900 | 1.67652600 |
| H | 0.94673500 | 2.44111100 | 0.11986600 |
| N | -1.21234800 | -0.22032100 | 0.35306900 |
| H | -1.55537000 | 1.84118100 | 0.28350200 |
| H | -0.69037300 | 1.21127700 | -1.11094900 |
| C | -0.19655800 | -1.29437200 | 0.50318200 |
| C | 1.07025000 | -0.74336400 | 1.15404000 |
| H | -0.62315100 | -2.08973300 | 1.12177800 |
| H | 0.07022600 | -1.71729700 | -0.47291500 |
| H | 0.89178200 | -0.46209700 | 2.19633100 |
| H | 1.84802700 | -1.50966100 | 1.12942900 |
| C | -2.40613100 | -0.58508100 | -0.22237900 |
| O | -3.18162600 | 0.18287700 | -0.77230800 |
| O | 2.49982600 | -0.76758800 | -1.27229900 |
| H | 2.16629500 | 1.24165300 | -1.36386900 |
| H | -2.62439900 | -1.66396500 | -0.11290000 |
| **B3LYP/6-31++G(d,p)** | **MAX2-ae.tif** | | |

**ee high energy point**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.39161100 | -0.25667100 | -0.21678300 |
| C | -0.48922600 | -1.30545100 | 0.28214200 |
| C | -2.73808300 | -0.50633100 | -0.07088600 |
| C | 0.92314000 | -1.07231200 | -0.20996900 |
| H | -0.49060500 | -1.32470100 | 1.38326100 |
| H | -0.85175800 | -2.27302500 | -0.07673200 |
| N | 1.40239900 | 0.24078900 | 0.24104300 |
| H | 1.60103000 | -1.83016200 | 0.18488100 |
| H | 0.95664900 | -1.13219500 | -1.30866100 |
| C | 0.53408200 | 1.38099500 | -0.10217900 |
| C | -0.97331300 | 1.12239300 | 0.06643900 |
| H | 0.81031900 | 2.23852800 | 0.51698500 |
| H | 0.71515500 | 1.65992300 | -1.15201300 |
| H | -1.27176400 | 1.36730000 | 1.09713700 |
| H | -1.53001400 | 1.79598800 | -0.58657800 |
| C | 2.75823500 | 0.44245500 | 0.09995100 |
| O | 3.58083700 | -0.43660600 | -0.10134800 |
| O | -3.60313700 | 0.35201000 | 0.00331200 |
| H | -2.97450700 | -1.58631600 | -0.06358200 |
| H | 3.04937000 | 1.50211800 | 0.22677200 |
| **B3LYP/6-31++G(d,p)** | **MAX3-ee.tif** | | |

**minimum**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.33790900 | 0.28213200 | 0.30936400 |
| C | 0.35396500 | 1.35825800 | 0.38349900 |
| C | 2.63019300 | 0.48495400 | -0.08120400 |
| C | -0.82959100 | 1.06752600 | -0.55141200 |
| H | -0.00950600 | 1.45111500 | 1.41593500 |
| H | 0.83590500 | 2.30063200 | 0.10614000 |
| N | -1.33652300 | -0.28053800 | -0.30704500 |
| H | -1.64932300 | 1.76831600 | -0.38250100 |
| H | -0.50275900 | 1.14572700 | -1.59751900 |
| C | -0.34930400 | -1.35367700 | -0.38431300 |
| C | 0.82645900 | -1.06331100 | 0.55903900 |
| H | -0.83045600 | -2.29900200 | -0.11550700 |
| H | 0.02030600 | -1.43880100 | -1.41515200 |
| H | 0.49098300 | -1.13453100 | 1.60274900 |
| H | 1.64595700 | -1.76670100 | 0.39994800 |
| C | -2.62998900 | -0.48919900 | 0.07651300 |
| O | -3.47779700 | 0.38240100 | 0.21326800 |
| O | 3.47481500 | -0.38983100 | -0.21728700 |
| H | 2.85100000 | 1.55330000 | -0.26260600 |
| H | -2.84835900 | -1.55908100 | 0.25169500 |
| **B3LYP/6-31++G(d,p)** | **MINI.tif** | | |

* + 1. **1,4-dithionyl-piperazine**

**aa high energy point**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.07199600 | 0.58898000 | -0.74428800 |
| C | 0.06412800 | 1.43264300 | -0.28366100 |
| C | -2.23304000 | 0.79097600 | -0.05795800 |
| C | 0.70688400 | 0.83445800 | 0.99715600 |
| H | 0.80641500 | 1.48522600 | -1.08301200 |
| H | -0.29780000 | 2.44493300 | -0.08537100 |
| N | 1.06908100 | -0.58531300 | 0.77127300 |
| H | 1.60640500 | 1.39126800 | 1.26215800 |
| H | -0.00208100 | 0.87280700 | 1.83018300 |
| C | -0.14577800 | -1.34710600 | 0.37044400 |
| C | -0.59396700 | -0.79478400 | -0.98492900 |
| H | 0.11375200 | -2.40862000 | 0.30203800 |
| H | -0.91838600 | -1.22926100 | 1.12897500 |
| H | 0.22936500 | -0.76198400 | -1.70098000 |
| H | -1.41902700 | -1.37782100 | -1.40018700 |
| C | 2.20875300 | -0.81502900 | 0.05673600 |
| S | 3.49017100 | 0.19276000 | -0.21612100 |
| S | -3.49548800 | -0.25625800 | 0.15092400 |
| H | -2.30795600 | 1.81144900 | 0.32515700 |
| H | 2.25291500 | -1.84466400 | -0.31142100 |
| **B3LYP/6-31++G(d,p)** | **S-MAX1-aa.tif** | | |

**ae high energy point**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.53769800 | 0.99914200 | 0.04571000 |
| C | 0.44371200 | 1.83962000 | -0.47336700 |
| C | 2.10261400 | 0.11802000 | -0.82417500 |
| C | -0.85045500 | 1.02201400 | -0.57580500 |
| H | 0.33174200 | 2.69830300 | 0.19479500 |
| H | 0.70376100 | 2.21805100 | -1.46553300 |
| N | -1.11253200 | 0.15112500 | 0.59208900 |
| H | -1.71267400 | 1.68181000 | -0.70354700 |
| H | -0.81084600 | 0.38800400 | -1.47262900 |
| C | 0.01630700 | -0.36152100 | 1.42071800 |
| C | 1.19457900 | 0.60731900 | 1.41537700 |
| H | -0.34659000 | -0.50440400 | 2.44280700 |
| H | 0.35209500 | -1.32675300 | 1.02840100 |
| H | 0.97070300 | 1.52003200 | 1.97406200 |
| H | 2.05666100 | 0.11868800 | 1.87537700 |
| C | -2.21451800 | -0.63423100 | 0.52721800 |
| S | -3.44739400 | -0.56816600 | -0.57447600 |
| S | 2.91899700 | -1.27465700 | -0.47272000 |
| H | 2.02670000 | 0.46113800 | -1.85916700 |
| H | -2.24679000 | -1.36890700 | 1.33618700 |
| **B3LYP/6-31++G(d,p)** | **S-MAX2-ae.tif** | | |

**ee high energy point**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.38139000 | -0.37160200 | -0.13680300 |
| C | -0.37001700 | -1.32327700 | 0.34799300 |
| C | -2.67904300 | -0.76203200 | -0.06484400 |
| C | 1.00498800 | -0.98803700 | -0.18697100 |
| H | -0.34966400 | -1.31733400 | 1.44822800 |
| H | -0.65703700 | -2.32508800 | 0.01822600 |
| N | 1.39899100 | 0.36067100 | 0.22488600 |
| H | 1.74630200 | -1.68791700 | 0.20215500 |
| H | 1.02542300 | -1.06346000 | -1.28482600 |
| C | 0.41860500 | 1.43522000 | -0.03753900 |
| C | -1.07384100 | 1.05002700 | 0.05528100 |
| H | 0.60773500 | 2.25423200 | 0.66070000 |
| H | 0.60746900 | 1.81819200 | -1.05025600 |
| H | -1.47165300 | 1.34212200 | 1.03828500 |
| H | -1.63862100 | 1.62587800 | -0.67995000 |
| C | 2.70962900 | 0.70618700 | 0.14161900 |
| S | 4.01364600 | -0.27653100 | -0.11206300 |
| S | -4.02204500 | 0.20100300 | -0.06068700 |
| H | -2.78169500 | -1.84912800 | -0.02771700 |
| H | 2.86099600 | 1.77894800 | 0.28932700 |
| **B3LYP/6-31++G(d,p)** | **S-MAX3-ee.tif** | | |

**minimum**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.30783600 | 0.41502000 | 0.33979600 |
| C | 0.21408100 | 1.39017300 | 0.34716700 |
| C | 2.56936400 | 0.74813000 | -0.00162300 |
| C | -0.89612300 | 0.96299600 | -0.62373200 |
| H | -0.19573300 | 1.46390300 | 1.36288300 |
| H | 0.60729300 | 2.36920500 | 0.06225600 |
| N | -1.30618700 | -0.41111900 | -0.33766100 |
| H | -1.77232500 | 1.60631700 | -0.52326800 |
| H | -0.52954100 | 1.01512000 | -1.65735400 |
| C | -0.20923700 | -1.38282900 | -0.34926900 |
| C | 0.89272100 | -0.95678200 | 0.63024300 |
| H | -0.60064800 | -2.36524500 | -0.07333200 |
| H | 0.20544600 | -1.44760400 | -1.36353100 |
| H | 0.51620600 | -1.00274000 | 1.66042500 |
| H | 1.76847200 | -1.60228300 | 0.54038500 |
| C | -2.56762300 | -0.75053400 | -0.00158000 |
| S | -3.89878800 | 0.22943300 | 0.12689800 |
| S | 3.89662100 | -0.23737600 | -0.12823300 |
| H | 2.66694700 | 1.81801500 | -0.20229700 |
| H | -2.66208300 | -1.82181500 | 0.19300700 |
| **B3LYP/6-31++G(d,p)** | **S-MINI.tif** | | |

* 1. **About C-N bond rotation**
     1. **1,4-diformyl-piperazine**

**Conformer Cis**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.37707700 | 0.19060800 | 0.25151000 |
| C | 0.62522300 | 1.42356500 | 0.44577000 |
| C | 2.70710300 | 0.17802100 | -0.05722600 |
| C | -0.62521600 | 1.42356100 | -0.44576000 |
| H | 0.32178100 | 1.51165900 | 1.49910400 |
| H | 1.26676500 | 2.27590100 | 0.20165100 |
| N | -1.37707100 | 0.19060600 | -0.25148900 |
| H | -1.26675600 | 2.27590000 | -0.20164900 |
| H | -0.32177300 | 1.51164800 | -1.49909500 |
| C | -0.62639700 | -1.05094100 | -0.44136400 |
| C | 0.62640000 | -1.05093600 | 0.44139900 |
| H | -1.28788500 | -1.88116100 | -0.18831400 |
| H | -0.33608600 | -1.14027500 | -1.49728000 |
| H | 0.33608800 | -1.14025400 | 1.49731600 |
| H | 1.28788700 | -1.88116000 | 0.18836000 |
| C | -2.70711000 | 0.17802400 | 0.05719000 |
| O | -3.38843900 | -0.82523800 | 0.21443500 |
| O | 3.38843000 | -0.82524300 | -0.21446700 |
| H | 3.12431900 | 1.19766000 | -0.15895300 |
| H | -3.12432100 | 1.19766400 | 0.15892600 |
| **B3LYP/6-31++G(d,p)** | **dif-cis.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.34902700 | 0.19363600 | -0.29960900 |
| C | -0.59929300 | 1.42533700 | -0.47331700 |
| C | -2.66982900 | 0.17755500 | 0.05026300 |
| C | 0.59931300 | 1.42535200 | 0.47332900 |
| H | -0.24508100 | 1.49749500 | -1.50771100 |
| H | -1.25608800 | 2.27281800 | -0.26902700 |
| N | 1.34904500 | 0.19364300 | 0.29966900 |
| H | 1.25611000 | 2.27282500 | 0.26901000 |
| H | 0.24510200 | 1.49754700 | 1.50772100 |
| C | 0.59683900 | -1.04281200 | 0.47370700 |
| C | -0.59682500 | -1.04282800 | -0.47360500 |
| H | 1.27230700 | -1.87232800 | 0.27082700 |
| H | 0.24545600 | -1.10704200 | 1.50862700 |
| H | -0.24544100 | -1.10709800 | -1.50852300 |
| H | -1.27229600 | -1.87233500 | -0.27069700 |
| C | 2.66981800 | 0.17754700 | -0.05031600 |
| O | 3.34372500 | -0.83727200 | -0.23865300 |
| O | -3.34376400 | -0.83725600 | 0.23854300 |
| H | -3.08673800 | 1.19124700 | 0.14955900 |
| H | 3.08672000 | 1.19123500 | -0.14968700 |
| **MP2/6-31++G(d,p)** | **dif-cis-mp2.tif** | | |

**Conformer Tran**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | 1.35148000 | 0.27116500 | 0.24176000 |
| C | 0.37929800 | 1.35262800 | 0.36923000 |
| C | 2.66055700 | 0.48420700 | -0.08100200 |
| C | -0.84765000 | 1.07348200 | -0.50868400 |
| H | 0.06456200 | 1.44428000 | 1.41827400 |
| H | 0.85297100 | 2.29302600 | 0.07187000 |
| N | -1.35142000 | -0.27114000 | -0.24149600 |
| H | -1.65378000 | 1.77949100 | -0.30084000 |
| H | -0.57006600 | 1.15380400 | -1.56927200 |
| C | -0.37924400 | -1.35260100 | -0.36899900 |
| C | 0.84770700 | -1.07345900 | 0.50891700 |
| H | -0.85291300 | -2.29300300 | -0.07164200 |
| H | -0.06450700 | -1.44424800 | -1.41804400 |
| H | 0.57012600 | -1.15379600 | 1.56950400 |
| H | 1.65383200 | -1.77946900 | 0.30106800 |
| C | -2.66050000 | -0.48417900 | 0.08125500 |
| O | -3.51449600 | 0.38563400 | 0.18637800 |
| O | 3.51431100 | -0.38571600 | -0.18717400 |
| H | 2.88303400 | 1.55464500 | -0.24745700 |
| H | -2.88320100 | -1.55471900 | 0.24675700 |
| **B3LYP/6-31++G(d,p)** | **dif-tr.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.31276900 | 0.28978000 | 0.31240200 |
| C | -0.82352000 | -1.05488700 | 0.56667900 |
| C | -2.60682800 | 0.49478500 | -0.07866100 |
| C | 0.32899400 | -1.35589200 | -0.38634200 |
| H | -0.47110200 | -1.12371500 | 1.60026900 |
| H | -1.65755900 | -1.73904500 | 0.42270900 |
| N | 1.31267600 | -0.28973800 | -0.31205300 |
| H | 0.81073500 | -2.30019400 | -0.12903500 |
| H | -0.05559300 | -1.43081300 | -1.40807600 |
| C | 0.82343700 | 1.05492900 | -0.56634800 |
| C | -0.32909000 | 1.35594400 | 0.38665600 |
| H | 1.65747900 | 1.73908300 | -0.42237700 |
| H | 0.47102400 | 1.12376300 | -1.59994300 |
| H | 0.05548800 | 1.43088000 | 1.40838900 |
| H | -0.81084000 | 2.30023700 | 0.12933900 |
| C | 2.60690000 | -0.49482500 | 0.07838700 |
| O | 3.45210200 | 0.38511900 | 0.21536900 |
| O | -3.45190600 | -0.38521400 | -0.21606000 |
| H | -2.81614400 | 1.56109400 | -0.25816700 |
| H | 2.81624000 | -1.56115400 | 0.25774300 |
| **MP2/6-31++G(d,p)** | **dif-tr-mp2.tif** | | |

**Transition state ST1**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.39267900 | 0.03142900 | 0.49592200 |
| C | -0.81771500 | 1.23585700 | -0.14174000 |
| C | -2.78003300 | -0.14203900 | 0.14961600 |
| C | 0.59829100 | 1.45122400 | 0.39596200 |
| H | -0.79358700 | 1.13769400 | -1.23896400 |
| H | -1.44047800 | 2.10023300 | 0.11249200 |
| N | 1.40307000 | 0.25291700 | 0.19522400 |
| H | 1.07498800 | 2.29015600 | -0.12050300 |
| H | 0.54654600 | 1.68882200 | 1.46771000 |
| C | 0.82935400 | -0.98994700 | 0.70426500 |
| C | -0.58962100 | -1.17014700 | 0.16596000 |
| H | 1.47704100 | -1.80944500 | 0.38735100 |
| H | 0.80674200 | -0.95876900 | 1.80207300 |
| H | -0.56179200 | -1.34584200 | -0.92074800 |
| H | -1.05224200 | -2.04092200 | 0.64200100 |
| C | 2.62515600 | 0.27510600 | -0.40928900 |
| O | 3.34839900 | -0.69658700 | -0.58411400 |
| O | -3.19453400 | -0.33026000 | -0.96993200 |
| H | -3.46424700 | -0.08886200 | 1.01578500 |
| H | 2.91078000 | 1.29095500 | -0.74148800 |
| **B3LYP/6-31++G(d,p)** | **TS1-dif.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.38172800 | 0.04519800 | 0.52522500 |
| C | -0.81303100 | 1.22700400 | -0.15264200 |
| C | -2.75468500 | -0.14668600 | 0.13129000 |
| C | 0.58635500 | 1.46371300 | 0.39511700 |
| H | -0.76894700 | 1.08185800 | -1.24081700 |
| H | -1.44801300 | 2.08986500 | 0.06039200 |
| N | 1.38649100 | 0.26528200 | 0.21628400 |
| H | 1.06831700 | 2.29022000 | -0.12985300 |
| H | 0.52167100 | 1.71163600 | 1.45966200 |
| C | 0.82396000 | -0.96135800 | 0.75949900 |
| C | -0.57837700 | -1.15512500 | 0.20653100 |
| H | 1.48140600 | -1.78085100 | 0.47310400 |
| H | 0.78378500 | -0.89234100 | 1.85107800 |
| H | -0.53271000 | -1.32797200 | -0.87692800 |
| H | -1.04859100 | -2.02023800 | 0.67863300 |
| C | 2.58514300 | 0.26699500 | -0.43576100 |
| O | 3.29864500 | -0.72245600 | -0.61915900 |
| O | -3.12115700 | -0.36252500 | -1.01312400 |
| H | -3.46862000 | -0.08252400 | 0.96335800 |
| H | 2.86226000 | 1.26957500 | -0.79513500 |
| **MP2/6-31++G(d,p)** | **TS1-dif-mp2.tif** | | |

**Transition state ST2**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.38267200 | -0.01049900 | 0.17242900 |
| C | -0.74153000 | 1.23729100 | -0.28966600 |
| C | -2.67244000 | -0.16477900 | -0.43785700 |
| C | 0.59546600 | 1.41508900 | 0.43343500 |
| H | -0.56896800 | 1.23038900 | -1.38241100 |
| H | -1.40059600 | 2.07732700 | -0.04920800 |
| N | 1.43117500 | 0.23719400 | 0.24516800 |
| H | 1.12080700 | 2.29185700 | 0.04290500 |
| H | 0.40741400 | 1.57183100 | 1.50412000 |
| C | 0.81182000 | -1.03695900 | 0.59728000 |
| C | -0.52969000 | -1.18390000 | -0.12154000 |
| H | 1.49969300 | -1.83382100 | 0.30931900 |
| H | 0.65198800 | -1.07806400 | 1.68268200 |
| H | -0.35372400 | -1.29810500 | -1.20706800 |
| H | -1.03976000 | -2.08140600 | 0.24103800 |
| C | 2.70897600 | 0.30149700 | -0.22743800 |
| O | 3.45026600 | -0.65661700 | -0.39989600 |
| O | -3.70692000 | -0.21548300 | 0.17623300 |
| H | -2.66128400 | -0.23831900 | -1.55053400 |
| H | 3.02253400 | 1.33881000 | -0.45001000 |
| **B3LYP/6-31++G(d,p)** | **TS2-dif.tif** | | |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.36350900 | -0.00397400 | 0.20027900 |
| C | -0.72205400 | 1.22819300 | -0.29267500 |
| C | -2.62301500 | -0.17774800 | -0.46628800 |
| C | 0.58783700 | 1.42822300 | 0.45669400 |
| H | -0.51648000 | 1.17749100 | -1.37506400 |
| H | -1.39349500 | 2.06726700 | -0.10071400 |
| N | 1.42251300 | 0.25140600 | 0.29817500 |
| H | 1.12248300 | 2.29619500 | 0.06756900 |
| H | 0.37473500 | 1.59105500 | 1.51749300 |
| C | 0.80774700 | -1.01126400 | 0.67560500 |
| C | -0.50440800 | -1.17330500 | -0.07570000 |
| H | 1.50730000 | -1.80793400 | 0.42781500 |
| H | 0.61551600 | -1.01504600 | 1.75232000 |
| H | -0.29480100 | -1.27898100 | -1.15268600 |
| H | -1.02370600 | -2.06852200 | 0.27070000 |
| C | 2.66322100 | 0.29434800 | -0.26930400 |
| O | 3.38429300 | -0.68381600 | -0.48041100 |
| O | -3.69336300 | -0.22559000 | 0.10868400 |
| H | -2.55774700 | -0.26939400 | -1.56981400 |
| H | 2.96974700 | 1.32040700 | -0.52297100 |
| **MP2/6-31++G(d,p)** | **TS2-dif-mp2.tif** | | |

* + 1. **1,4-dithionyl-piperazine**

**Conformer Cis**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.37927500 | 0.41612600 | -0.31055800 |
| C | -0.60224300 | 1.64344400 | -0.47606300 |
| C | -2.70374000 | 0.43413000 | -0.05351600 |
| C | 0.60225000 | 1.64345600 | 0.47605200 |
| H | -0.24920000 | 1.71305900 | -1.51441800 |
| H | -1.24396700 | 2.50434800 | -0.27092600 |
| N | 1.37928100 | 0.41613300 | 0.31058100 |
| H | 1.24397500 | 2.50435400 | 0.27089100 |
| H | 0.24920800 | 1.71309900 | 1.51440500 |
| C | 0.60394800 | -0.81677600 | 0.47087900 |
| C | -0.60394300 | -0.81678800 | -0.47082500 |
| H | 1.26324500 | -1.65942200 | 0.25631700 |
| H | 0.26642600 | -0.88929300 | 1.51326400 |
| H | -0.26642100 | -0.88933200 | -1.51320800 |
| H | -1.26324200 | -1.65942700 | -0.25624100 |
| C | 2.70374600 | 0.43412900 | 0.05353100 |
| S | 3.73163400 | -0.85003800 | -0.14516400 |
| S | -3.73164400 | -0.85003200 | 0.14513200 |
| H | -3.08967700 | 1.45417700 | 0.02206600 |
| H | 3.08967200 | 1.45417400 | -0.02213800 |
| **B3LYP/6-31++G(d,p)** | **dith-cis.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.27600200 | 0.42125700 | -0.55391000 |
| C | -0.49134600 | 1.64911600 | -0.58721600 |
| C | -2.57266400 | 0.42808800 | -0.15439600 |
| C | 0.49134600 | 1.64911600 | 0.58721000 |
| H | 0.06371100 | 1.69321300 | -1.52924800 |
| H | -1.16518800 | 2.50512000 | -0.53311700 |
| N | 1.27600000 | 0.42125600 | 0.55390700 |
| H | 1.16519000 | 2.50511900 | 0.53311000 |
| H | -0.06371200 | 1.69321500 | 1.52924200 |
| C | 0.47873800 | -0.80116300 | 0.59399800 |
| C | -0.47874000 | -0.80116100 | -0.59400500 |
| H | 1.15720200 | -1.65145500 | 0.56300000 |
| H | -0.09033200 | -0.81774600 | 1.52745800 |
| H | 0.09033000 | -0.81774100 | -1.52746500 |
| H | -1.15720400 | -1.65145400 | -0.56300900 |
| C | 2.57267000 | 0.42808600 | 0.15442100 |
| S | 3.52174700 | -0.86093800 | -0.21539800 |
| S | -3.52174700 | -0.86093800 | 0.21539800 |
| H | -2.97377400 | 1.44083100 | -0.11152000 |
| H | 2.97376800 | 1.44083200 | 0.11150700 |
| **MP2/6-31++G(d,p)** | **dith-cis-mp2.tif** | | |

**Conformer Tran**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.32647400 | -0.39982700 | -0.27692200 |
| C | -0.91705900 | 0.97169200 | -0.57469400 |
| C | -2.59763500 | -0.74469000 | 0.01264400 |
| C | 0.24186900 | 1.38332400 | 0.34093000 |
| H | -0.60325600 | 1.02890600 | -1.62577500 |
| H | -1.78122400 | 1.62249200 | -0.42844700 |
| N | 1.32646800 | 0.39978600 | 0.27686000 |
| H | 0.62923400 | 2.35987000 | 0.04004700 |
| H | -0.11713800 | 1.45763500 | 1.37624400 |
| C | 0.91706200 | -0.97169600 | 0.57462900 |
| C | -0.24190400 | -1.38334200 | -0.34099200 |
| H | 1.78119700 | -1.62253100 | 0.42836400 |
| H | 0.60325000 | -1.02894000 | 1.62570900 |
| H | 0.11711900 | -1.45768100 | -1.37630000 |
| H | -0.62923400 | -2.35989100 | -0.04006900 |
| C | 2.59763200 | 0.74470100 | -0.01263600 |
| S | 3.93260600 | -0.23338800 | -0.11303100 |
| S | -3.93258500 | 0.23341800 | 0.11311600 |
| H | -2.69702000 | -1.81777200 | 0.19426800 |
| H | 2.69699300 | 1.81778300 | -0.19425600 |
| **B3LYP/6-31++G(d,p)** | **dith-tra.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.21612600 | -0.46184400 | -0.49095200 |
| C | -0.81671000 | 0.91091400 | -0.77150000 |
| C | -2.45523300 | -0.77179500 | -0.03535500 |
| C | 0.10038500 | 1.39512100 | 0.35093400 |
| H | -0.27830000 | 0.92931700 | -1.72345100 |
| H | -1.71599200 | 1.52011600 | -0.84550400 |
| N | 1.21609900 | 0.46183000 | 0.49087100 |
| H | 0.49420900 | 2.38882500 | 0.13564400 |
| H | -0.45743600 | 1.43063400 | 1.29085600 |
| C | 0.81669100 | -0.91093000 | 0.77140400 |
| C | -0.10040700 | -1.39512900 | -0.35103200 |
| H | 1.71597800 | -1.52012700 | 0.84539200 |
| H | 0.27829000 | -0.92935200 | 1.72336100 |
| H | 0.45740600 | -1.43063000 | -1.29096000 |
| H | -0.49422500 | -2.38883800 | -0.13574800 |
| C | 2.45523600 | 0.77179800 | 0.03536400 |
| S | 3.74059900 | -0.23391800 | -0.16039100 |
| S | -3.74056900 | 0.23393500 | 0.16052000 |
| H | -2.54356600 | -1.83341100 | 0.19478700 |
| H | 2.54357400 | 1.83341600 | -0.19476100 |
| **MP2/6-31++G(d,p)** | **dith-tra-mp2.tif** | | |

**Transition state ST1**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.40719700 | 0.31080100 | 0.67995800 |
| C | -0.90669400 | 1.30217600 | -0.29346800 |
| C | -2.80163300 | 0.02823500 | 0.52449100 |
| C | 0.52144200 | 1.69760000 | 0.08435700 |
| H | -0.93056900 | 0.90332300 | -1.32073500 |
| H | -1.54817900 | 2.18807100 | -0.25490000 |
| N | 1.37943800 | 0.51510000 | 0.16937000 |
| H | 0.93240100 | 2.38037400 | -0.66418200 |
| H | 0.51377300 | 2.20851700 | 1.05694500 |
| C | 0.87101300 | -0.54028500 | 1.04596500 |
| C | -0.56187400 | -0.90490800 | 0.66196500 |
| H | 1.53210200 | -1.40352100 | 0.95033500 |
| H | 0.90216800 | -0.18395500 | 2.08434000 |
| H | -0.57803700 | -1.38618900 | -0.32870400 |
| H | -0.95864600 | -1.61551800 | 1.39304900 |
| C | 2.57457000 | 0.45146700 | -0.44782200 |
| S | 3.69792100 | -0.76874200 | -0.39970600 |
| S | -3.52446300 | -0.65265200 | -0.76682000 |
| H | -3.40085600 | 0.31773200 | 1.39285600 |
| H | 2.77388700 | 1.34644700 | -1.04280800 |
| **B3LYP/6-31++G(d,p)** | **TS1-dith.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.37515200 | 0.55279800 | 0.60021200 |
| C | -0.85830200 | 1.21046400 | -0.61246800 |
| C | -2.73439700 | 0.11980300 | 0.43161300 |
| C | 0.51745600 | 1.78580200 | -0.30490100 |
| H | -0.78245900 | 0.50416000 | -1.45269700 |
| H | -1.54560700 | 2.01203700 | -0.89080100 |
| N | 1.39396300 | 0.71890900 | 0.16046700 |
| H | 0.95416200 | 2.23816500 | -1.19592800 |
| H | 0.43328500 | 2.54547400 | 0.47740500 |
| C | 0.88626200 | 0.00130800 | 1.32145400 |
| C | -0.48741500 | -0.56083900 | 0.99197800 |
| H | 1.59127300 | -0.79210200 | 1.56288200 |
| H | 0.81405500 | 0.69906600 | 2.16009500 |
| H | -0.39716500 | -1.30564400 | 0.18838100 |
| H | -0.91464100 | -1.04596800 | 1.87148400 |
| C | 2.43100700 | 0.27001700 | -0.58353300 |
| S | 3.38749200 | -1.03920000 | -0.30510200 |
| S | -3.26175800 | -0.97494000 | -0.64342300 |
| H | -3.43245300 | 0.60198600 | 1.11541900 |
| H | 2.60846700 | 0.90779700 | -1.44945200 |
| **MP2/6-31++G(d,p)** | **TS1-dith-mp2.tif** | | |

**Transition state ST2**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.37876200 | 0.04565400 | 0.08100400 |
| C | -0.76583900 | 1.30706400 | -0.37910100 |
| C | -2.61917600 | -0.18481800 | -0.58116200 |
| C | 0.52151200 | 1.56267600 | 0.40677800 |
| H | -0.54028900 | 1.28158000 | -1.46184600 |
| H | -1.47029300 | 2.12328200 | -0.19390200 |
| N | 1.43302200 | 0.42532400 | 0.28420800 |
| H | 1.01932500 | 2.45998200 | 0.03014300 |
| H | 0.27435100 | 1.71684200 | 1.46546200 |
| C | 0.84091000 | -0.86178200 | 0.64864700 |
| C | -0.45324500 | -1.08932700 | -0.13131300 |
| H | 1.57110200 | -1.64251600 | 0.42900400 |
| H | 0.63085900 | -0.86332600 | 1.72606200 |
| H | -0.21959100 | -1.22659100 | -1.20301000 |
| H | -0.93614200 | -2.00016900 | 0.23333200 |
| C | 2.72233500 | 0.57291500 | -0.07612100 |
| S | 3.89521400 | -0.59237800 | -0.21318000 |
| S | -4.05791500 | -0.30221300 | 0.15463000 |
| H | -2.55211900 | -0.28849100 | -1.67688600 |
| H | 2.96721300 | 1.61562800 | -0.29442600 |
| **B3LYP/6-31++G(d,p)** | **TS2-dith.tif** | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **X** | **Y** | **Z** |
| N | -1.32024400 | 0.07860100 | 0.15105200 |
| C | -0.69503400 | 1.27666300 | -0.43339300 |
| C | -2.47907200 | -0.27051200 | -0.60825100 |
| C | 0.51789300 | 1.65912700 | 0.40455600 |
| H | -0.37647500 | 1.10440600 | -1.47564100 |
| H | -1.42790100 | 2.08569600 | -0.42103400 |
| N | 1.43784400 | 0.53104800 | 0.46524000 |
| H | 1.03426500 | 2.51461900 | -0.03179000 |
| H | 0.19632200 | 1.91358800 | 1.41809400 |
| C | 0.83947800 | -0.68714500 | 0.99265400 |
| C | -0.36969000 | -1.05111900 | 0.14525400 |
| H | 1.59146800 | -1.47346600 | 0.96730300 |
| H | 0.52795200 | -0.50588600 | 2.02452600 |
| H | -0.03599800 | -1.29806700 | -0.87604100 |
| H | -0.87483000 | -1.92105400 | 0.56821300 |
| C | 2.62960200 | 0.54533400 | -0.17576500 |
| S | 3.68007500 | -0.70221300 | -0.38999900 |
| S | -3.97312300 | -0.33245000 | 0.00165600 |
| H | -2.29488900 | -0.50481000 | -1.66574800 |
| H | 2.86660500 | 1.53795600 | -0.55876700 |
| **MP2/6-31++G(d,p)** | **TS2-dith-mp2.tif** | | |

1. **Atomic Partial charges**

The atomic charges were calculated at the B3LYP/6–31G(d,p) using Mulliken approximation**,** NBO analysis**,** and Atomic Polar Tensors APT approaches

* 1. **1,4-diformyl piperazine**
     1. **Mulliken approximation**

|  |  |  |
| --- | --- | --- |
| **Atoms** | **Mulliken charges** | |
| **Cis** | **Trans** |
| **N1** | –0.407806 | –0.407865 |
| **C2** | –0.047832 | –0.057225 |
| **C3** | 0.408835 | 0.408656 |
| **C4** | –0.047832 | –0.049682 |
| **H5** | 0.119434 | 0.124999 |
| **H6** | 0.118095 | 0.119360 |
| **N7** | –0.407805 | –0.407855 |
| **H8** | 0.118094 | 0.153873 |
| **H9** | 0.119432 | 0.116319 |
| **C10** | –0.058325 | –0.057250 |
| **C11** | –0.058325 | –0.049698 |
| **H12** | 0.154752 | 0.119370 |
| **H13** | 0.121539 | 0.125015 |
| **H14** | 0.121542 | 0.116340 |
| **H15** | 0.154752 | 0.153902 |
| **C16** | 0.408837 | 0.408656 |
| **O17(S17)** | –0.473033 | –0.475468 |
| **O18(S18)** | –0.473032 | –0.475476 |
| **H19** | 0.064339 | 0.067010 |
| **H20** | 0.064337 | 0.067018 |

* + 1. **NBO analysis**

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| --- | --- | --- |
| **Atoms** | **NBO charges** | |
| **Cis** | **Trans** |
| **N1** | –0.49397 | –0.49375 |
| **C2** | –0.27150 | –0.27285 |
| **C3** | 0.51693 | 0.51687 |
| **C4** | –0.27150 | –0.28383 |
| **H5** | 0.23507 | 0.23795 |
| **H6** | 0.24850 | 0.24937 |
| **N7** | –0.49397 | –0.49376 |
| **H8** | 0.24850 | 0.27719 |
| **H9** | 0.23507 | 0.23362 |
| **C10** | –0.28476 | –0.27288 |
| **C11** | –0.28476 | –0.28385 |
| **H12** | 0.27765 | 0.24938 |
| **H13** | 0.23620 | 0.23796 |
| **H14** | 0.23620 | 0.23364 |
| **H15** | 0.27765 | 0.27721 |
| **C16** | 0.51693 | 0.51688 |
| **O17(S17)** | –0.60851 | –0.61113 |
| **O18(S18)** | –0.60851 | –0.61116 |
| **H19** | 0.14440 | 0.14657 |
| **H20** | 0.14439 | 0.14657 |

* + 1. **APT**

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| **Atoms** | **APT charges** | |
| **Cis** | **Trans** |
| **N1** | –0.778184 | –0.776368 |
| **C2** | 0.340464 | 0.349431 |
| **C3** | 1.058810 | 1.056933 |
| **C4** | 0.340466 | 0.262175 |
| **H5** | –0.060956 | –0.055495 |
| **H6** | –0.013936 | –0.012953 |
| **N7** | –0.778184 | –0.776380 |
| **H8** | –0.013937 | 0.047126 |
| **H9** | –0.060956 | –0.050225 |
| **C10** | 0.274292 | 0.349349 |
| **C11** | 0.274293 | 0.262057 |
| **H12** | 0.046812 | –0.012939 |
| **H13** | –0.046053 | –0.055449 |
| **H14** | –0.046051 | –0.050147 |
| **H15** | 0.046813 | 0.047180 |
| **C16** | 1.058806 | 1.056960 |
| **O17(S17)** | –0.773208 | –0.775741 |
| **O18(S18)** | –0.773211 | –0.775735 |
| **H19** | –0.048039 | –0.044902 |
| **H20** | –0.048039 | –0.044877 |

* 1. **1,4-dithionl piperazine**
     1. **Mulliken approximation**

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| **Atoms** | **Mulliken charges** | |
| **Cis** | **Trans** |
| **N1** | –0.346500 | –0.346531 |
| **C2** | –0.056623 | –0.066114 |
| **C3** | –0.011082 | –0.010232 |
| **C4** | –0.056617 | –0.054415 |
| **H5** | 0.135188 | 0.141495 |
| **H6** | 0.128154 | 0.130021 |
| **N7** | –0.346503 | –0.346531 |
| **H8** | 0.128152 | 0.166812 |
| **H9** | 0.135186 | 0.130020 |
| **C10** | –0.063474 | –0.066113 |
| **C11** | –0.063476 | –0.054414 |
| **H12** | 0.168454 | 0.130020 |
| **H13** | 0.135573 | 0.141492 |
| **H14** | 0.135580 | 0.130025 |
| **H15** | 0.168455 | 0.166813 |
| **C16** | –0.011077 | –0.010225 |
| **O17(S17)** | –0.217207 | –0.221735 |
| **O18(S18)** | –0.217206 | –0.221735 |
| **H19** | 0.127513 | 0.130675 |
| **H20** | 0.127510 | 0.130673 |

* + 1. **NBO analysis**

|  |  |  |
| --- | --- | --- |
| **Atoms** | **NBO charges** | |
| **Cis** | **Trans** |
| **N1** | –0.42233 | –0.42187 |
| **C2** | –0.27123 | -0.27261 |
| **C3** | –0.12427 | –0.12176 |
| **C4** | –0.27123 | -0.28789 |
| **H5** | 0.24506 | 0.24854 |
| **H6** | 0.25484 | 0.25618 |
| **N7** | –0.42233 | –0.42187 |
| **H8** | 0.25483 | 0.28373 |
| **H9** | 0.24506 | 0.24375 |
| **C10** | –0.28879 | –0.27261 |
| **C11** | –0.28879 | –0.28790 |
| **H12** | 0.28458 | 0.25617 |
| **H13** | 0.24678 | 0.24853 |
| **H14** | 0.24679 | 0.24376 |
| **H15** | 0.28458 | 0.28373 |
| **C16** | –0.12426 | –0.12176 |
| **O17(S17)** | –0.14876 | –0.15463 |
| **O18(S18)** | –0.14876 | –0.15464 |
| **H19** | 0.22411 | 0.22658 |
| **H20** | 0.22411 | 0.22658 |

* + 1. **APT**

|  |  |  |
| --- | --- | --- |
| **Atoms** | **APT charges** | |
| **II-Cis** | **II-Trans** |
| **N1** | –0.816026 | –0.812415 |
| **C2** | 0.349709 | 0.384978 |
| **C3** | 0.853619 | 0.858898 |
| **C4** | 0.349719 | 0.179979 |
| **H5** | –0.058092 | –0.051955 |
| **H6** | –0.009330 | –0.009109 |
| **N7** | –0.816029 | –0.812418 |
| **H8** | –0.009335 | 0.069097 |
| **H9** | –0.058099 | –0.031764 |
| **C10** | 0.222754 | 0.384990 |
| **C11** | 0.222753 | 0.179980 |
| **H12** | 0.063475 | –0.009111 |
| **H13** | –0.028336 | –0.051961 |
| **H14** | –0.028328 | –0.031762 |
| **H15** | 0.063477 | 0.069101 |
| **C16** | 0.853611 | 0.858894 |
| **O17(S17)** | –0.586620 | –0.600549 |
| **O18(S18)** | –0.586630 | –0.600556 |
| **H19** | 0.008856 | 0.012840 |
| **H20** | 0.008854 | 0.012840 |