Supplementary Information:

Microscopic Mechanism of Light-Induced Tetrazole-Quinone 1,3-Dipolar Cycloaddition: A MS-CASPT2 Theoretical Investigation

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1. ALL CASSCF Active Orbitals

The all active space in the CASSCF calculations included 14 electrons in 12 orbitals.

Figure 1: CASSCF(14,12) and MS-CASPT2 methods calculated all active orbitals from ground state minimum energy structure S0-MIN to S1 excited state.

Table 1: Computed vertical excitation energies to the first excited singlet state of the FPT and the experimental value under ultraviolet light

|             | MS-CASPT2 | Exp.    |
|-------------|-----------|---------|
| kcal/mol    | 114.7     | 71.5-112.6 |
| eV          | 4.98      | 3.10-4.88    |

Figure 2: CASSCF computed two-dimensional S1 and S0 potential energy surfaces spanned by the N2-N3 and N4-C5 bond cleavage coordinates (left). Also
shown are the estimated minimum-energy reaction paths (yellow arrows) and the color filled contour maps of $S_1$ and $S_0$ states (right).

**Figure 3:** CASSCF computed minimum energy paths in $S_1$ state along the cleavage of N2-N3 bond and N4-C5 bond respectively based on the stepwise mechanism.

**Figure 4:** CASSCF computed minimum energy paths in $S_1$ state along the cleavage of N2-N3 bond and N4-C5 bond based on the concerted mechanism, where N2-N3 bond equals to N4-C5 bond all the time.

**Table 2:** The energy comparison table of FPNI and NPQ in the ground state [3+2] cycloaddition to generate PFQ precursor is calculated by MS-CASPT2//CASSCF and M06-2X respectively (in kcal/mol).

|               | NPQ+FPNI (R) | S0-TS (TS) | FP2HQ (P) |
|---------------|--------------|------------|-----------|
| M06-2X        | 0            | 5.7        | -48.4     |
| MS-CASPT2//CASSCF | 0            | 2.5        | -49.3     |
# Cartesian Coordinates of All CASSCF Optimized Structures

## S0-MIN

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| C       | 1.17013440  | 0.77689186  | 0.04053993  |
| N       | 0.11189320  | -0.00412458 | 0.01361579  |
| N       | -0.87801712 | -1.48708531 | -0.11933591 |
| C       | 2.85744868  | -1.05464656 | -0.07883282 |
| C       | 4.17338861  | -1.48708531 | -0.11933591 |
| C       | 5.21229189  | 1.22637499  | 0.03151678  |
| C       | 2.57015257  | 0.30550414  | -0.00313485 |
| H       | 2.04967193  | -1.7716936  | -0.10586832 |
| H       | 4.38817623  | -2.5456256  | -0.17813870 |
| H       | 5.73308894  | 1.51205099  | 0.01814793  |
| H       | 3.38898846  | 2.28146668  | 0.09023470  |
| C       | -4.90030723 | -0.23094797 | 0.06896343  |
| C       | -3.93581046 | -1.21885876 | 0.0045561   |
| C       | -2.60074555 | -0.8572737  | 0.00550127  |
| C       | -2.24925717 | 0.48854273  | 0.07126278  |
| H       | -4.23403202 | -2.25378059 | -0.04569880 |
| H       | -1.83273542 | -1.61375197 | -0.04420622 |
| C       | -3.23347689 | 1.47345243  | 0.13588405  |
| C       | -4.56643620 | 1.10718118  | 0.13449730  |
| H       | -2.95354492 | 2.51352255  | 0.18653301  |
| H       | -5.34764560 | 1.85142137  | 0.18381104  |
| H       | 6.23919517  | -0.90524219 | -0.11632015 |
| F       | -6.18130479 | -0.57864432 | 0.06784691  |
| N       | 0.81068086  | 2.08123705  | 0.11405994  |
| N       | -0.47294874 | 2.10421051  | 0.13252035  |

## S1-MIN

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| C       | 1.16153382  | 0.73204484  | 0.03817613  |
| N       | 0.10653402  | -0.09548353 | 0.0084541  |
| N       | -0.90902871 | 0.80164348  | 0.06963797  |
| C       | 2.85859366  | -1.06533335 | -0.07916909 |
| C       | 4.17970262  | -1.47794034 | -0.11861448 |
| C       | 5.20469128  | -0.54088849 | -0.08306232 |
| C       | 4.90359371  | 0.81314941  | -0.00777121 |
| C       | 3.58460475  | 1.23265306  | 0.03200207  |
| C       | 2.54949082  | 0.29496733  | -0.00344532 |
| H       | 2.05965869  | -1.79156296 | -0.10665945 |
| H       | 4.41127708  | -2.53287775 | -0.17723661 |
| H       | 5.69963025  | 1.54482393  | 0.02004836  |
| H       | 3.34565976  | 2.28379691  | 0.09051900  |
| C       | -4.88712789 | -0.20190703 | 0.07037293  |
| C       | -3.93554504 | -1.21567961 | 0.00432138  |
| C       | -2.60246065 | -0.89992773 | 0.00299317  |
| C       | -2.20256969 | 0.46826629  | 0.06950622  |
| H       | -4.26392156 | -2.24372859 | -0.04527572 |
H  -1.84756639 -1.66641962 -0.04742014
C  -3.19945543  1.48694718  0.13642741
C  -4.52871460  1.13467674  0.13578271
H  -2.89798193  2.51897822  0.18659742
H  -5.30168925  1.88768990  0.18573192
H   6.23631221 -0.86540451 -0.11398400
F  -6.17170159 -0.52877001  0.07046340
N   0.80432669  2.06282677  0.11291494
N  -0.49725665  2.14625947  0.13476791

S1-M1
C   1.19020113  1.29162526  0.06716792
N   0.04828191  0.64498430  0.04743153
N  -1.04377267  1.35821630  0.09868695
C   2.43732857 -0.86723830 -0.06433077
C   3.61830870 -1.58428783 -0.11800320
C   4.84123460 -0.92294624 -0.09841943
C   4.87124018  0.45975767 -0.02477111
C   3.68805185  1.18438130  0.02933267
C   2.45751523  0.52924251  0.01013773
H   1.49206951 -1.38538668 -0.07979783
H   3.58629527 -2.66389724 -0.17538010
H   5.81741747  0.98334016 -0.00896725
H   3.72420663  2.26029914  0.08650990
C  -4.67404364 -0.67501620  0.04364303
C  -3.52045692 -1.43482226 -0.01123692
C  -2.29348858 -0.79542068  0.00493155
C  -2.23094833  0.59548623  0.07568212
H  -3.59456202 -2.51108713 -0.06564705
H  -1.38459442 -1.37316824 -0.03726314
C  -3.40894632  1.33326372  0.12970289
C  -4.64208028  0.70228548  0.11409663
H  -3.34116403  2.41019961  0.18416838
H  -5.56607680  1.25982807  0.15541213
H   5.76401698 -1.48604478 -0.14049030
F  -5.84818573 -1.29242481  0.02790414
N   1.36067098  2.71490860  0.14165433
N   0.51207072  3.54675203  0.19431070

S1S0
C   1.20594624  1.04403521 -0.25635408
N   0.06301967  0.51481188 -0.19295022
N  -1.02421252  1.31809103 -0.24082646
C   2.62219550 -1.01556252 -0.02159057
C   3.86926906 -1.61183066  0.02784341
C   5.01793305 -0.83427140 -0.07108748
C   4.91480270  0.53934310 -0.22835597
C   3.66389881  1.13802184 -0.28635513
C   2.50785963  0.36876540 -0.18425993
H   1.72679902 -1.61364005  0.06268403
H   3.94935529 -2.68422654  0.14411182
H   5.80697447  1.14510292 -0.30544213
H   3.57676343  2.20812974 -0.40914573
C  -4.72323682 -0.53839850  0.08915926
C  -3.60386520 -1.34703644  0.12481064
C  -2.35283323  -0.76591625   0.01479847
C  -2.22723855   0.61922840  -0.12441060
H  -3.72049905  -2.41496296   0.23785333
H  -1.46749285  -1.38098914   0.03557233
C  -3.38136896   1.40619445  -0.15059395
C  -4.63534380   0.83371659  -0.04558127
H  -3.27266770   2.47552030  -0.25464113
H  -5.53607702   1.42933297  -0.06571819
H   5.99165285  -1.30364026  -0.02488715
F  -5.92263464  -1.09620349   0.18776968
N   0.93092326   2.78207151   1.22474315
N  -0.11933267   3.06714285   1.29932385
FPNI
C   1.16704365  -0.05858416  -0.00366873
N   0.09527825   0.15932339  -0.53108256
N  -1.00349818   0.61568362  -0.93490678
C   2.44265439  -1.97969041  -0.96692365
C   3.64103803  -2.55372017  -1.35844352
C   4.82468859  -1.83074823  -1.23796621
C   4.81661166  -0.54917834  -0.69717212
C   3.61578077   0.01778154  -0.29793084
C   2.42200913  -0.68645952  -0.44091301
H   1.51808707  -2.53607421  -1.06772015
H   3.64701723  -3.55817677  -1.76027691
H   5.74181884   0.00791643  -0.57558574
H   3.59468125   1.01381108   0.12279187
C  -4.46869438  -1.71197167  -0.67432262
C  -3.29392750  -2.24929284  -0.18223681
C  -2.12477915  -1.50021376  -0.25064807
C  -2.13904591  -0.23497236  -0.82577863
H  -3.29648555  -3.23804001   0.24834367
H  -1.20412120  -1.91234190   0.15454470
C  -3.33884470   0.27282787  -1.32125780
C  -4.51459120  -0.45715873  -1.24148460
C  -3.33034379  -1.25441638  -1.76759013
H  -5.45423494  -0.06410601  -1.60870553
H   5.75605464  -2.27099986   1.56283298
F  -5.59214258  -2.42392422  -0.60005549
S1-TS1
C   1.16771143   0.79697151   0.04147885
N   0.11130649   0.01307517   0.01442576
N  -0.95634922   0.85265560   0.07286021
C   2.81846566  -1.04572798  -0.07761567
C   4.12559361  -1.49679618  -0.11887716
C   5.17927057  -0.59048274  -0.08530919
C   4.91839956   0.77072069  -0.01017825
C   3.61150137   1.22922354   0.03147236
C   2.54948710   0.32380646  -0.00193956
H   1.99804079  -1.74711035  -0.10352771
H   4.32518246  -2.55816018  -0.17740642
H   5.73514099   1.47914493   0.01615403
H   3.40778991   2.28756983   0.08900995
C  -4.89451923  -0.26936211   0.06695801

S.6
| Atom | X       | Y       | Z       | E      |
|------|---------|---------|---------|--------|
| C    | -3.92141611 | -1.26365362 | 0.00162792 |        |
| C    | -2.59475027  | -0.92652893 | 0.00148548 |        |
| C    | -2.20850672  | 0.45528208  | 0.06886576 |        |
| H    | -4.23222729  | -2.29761766 | -0.04850694 |        |
| H    | -1.82699117  | -1.68098449 | -0.04847850 |        |
| C    | -3.55981765  | 1.07678625  | 0.13317125 |        |
| H    | -3.24091397  | 1.45090666  | 0.15066633 |        |
| C    | -4.55981765  | 1.07678625  | 0.13317125 |        |
| H    | -2.95659728  | 2.49004989  | 0.18582966 |        |
| H    | -5.34818357  | 1.81417363  | 0.18253344 |        |
| C    | 6.20056802   | -0.94581003 | -0.11770148 |        |
| F    | 6.617457295  | -0.62036937 | 0.06574755  |        |
| N    | 0.89992900   | 2.16903211  | 0.11725724  |        |
| N    | 0.09992900   | 2.16903211  | 0.11725724  |        |
| S1-TS2 | C     | 1.16945776  | 1.07151436 | 0.05589231 |        |
| N    | 0.05224211   | 0.47716687  | 0.03972154  |        |
| N    | -1.05409582  | 1.26693788  | 0.09608115  |        |
| C    | 2.57187950   | -0.98107035 | -0.07091878 |        |
| C    | 3.80485851   | -1.60428404 | -0.12024481 |        |
| C    | 4.97130698   | -0.84626392 | -0.09598161 |        |
| C    | 4.89495011   | 0.53468347  | -0.02228297 |        |
| C    | 3.65792634   | 1.16515821  | 0.02747584  |        |
| C    | 2.48658904   | 0.41306746  | 0.00359575  |        |
| H    | 1.66507547   | -1.56645553 | -0.08957203 |        |
| H    | 3.85990301   | -2.68306459 | -0.17776382 |        |
| H    | 5.79850946   | 1.12872509  | -0.00312930 |        |
| H    | 3.60656111   | 2.24043344  | 0.08475143  |        |
| C    | -4.74012832  | -0.59230336 | 0.04786519  |        |
| C    | -3.63757527  | -1.40018522 | -0.00934692 |        |
| C    | -2.36891564  | -0.82281883 | 0.00396139  |        |
| C    | -2.22666163  | 0.57799503  | 0.07562950  |        |
| H    | -3.76377280  | -2.47174040 | -0.06391640 |        |
| H    | -1.49165511  | -1.44606613 | -0.04052461 |        |
| C    | -3.40548863  | 1.37790906  | 0.13344076  |        |
| C    | -4.64123004  | 0.80549868  | 0.11994287  |        |
| H    | -3.28827330  | 2.45048667  | 0.18819712  |        |
| H    | -5.54461798  | 1.39630765  | 0.16308241  |        |
| H    | 5.93567541   | -1.33525561 | -0.13463804 |        |
| F    | 5.95133912   | -1.13243918 | 0.03574606  |        |
| N    | 1.23861078   | 2.86775708  | 0.14932667  |        |
| N    | 0.26079805   | 3.39113620  | 0.19007932  |        |
| TS3 | C    | 1.16709415  | 0.67816638  | 0.03513065 |        |
| N    | 0.9983602    | -0.01549409 | 0.01277225  |        |
| N    | -0.94794648  | 0.82683975  | 0.07115749  |        |
| C    | 2.87731131   | -1.11424366 | -0.08220234 |        |
| C    | 4.20157603   | -1.51008044 | -0.12072216 |        |
| C    | 5.21402742   | -0.55609901 | -0.08393792 |        |
| C    | 4.89961287   | 0.79225193  | -0.00865714 |        |
| C    | 3.57250566   | 1.19667923  | 0.03038952  |        |
| C    | 2.55911191   | 0.24352661  | -0.00636903 |        |
| H    | 2.08500987   | -1.84822956 | -0.11033319 |        |
| H    | 4.44825681   | -2.56137286 | -0.17941801 |        |
### 3. Cartesian Coordinates of All DFT Optimized Structures

**NPQ**

| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 2.67051900 | 0.69798700 |
| C       | 1.46899400 | 1.39787100 |
| C       | 0.26295100 | 0.70037500 |
| C       | 0.26295100 | -0.70037500 |
| C       | 1.46899400 | -1.39787100 |
| C       | 2.67051900 | -0.69798700 |
| H       | -1.02238600 | 1.45929600 |
| C       | -1.02238600 | -1.45929600 |
| H       | 3.61137300 | 1.23941200 |
| H       | 1.44099400 | 2.48286800 |
| C       | -1.02238600 | 1.45929600 |
| C       | -1.02238600 | -1.45929600 |
| H       | 3.61137300 | -1.23941200 |
| H       | 1.44099400 | -2.48286800 |
| C       | -2.28339700 | -0.66856000 |
| C       | -2.28339700 | 0.66856000 |
| H       | -3.19853400 | -1.25338300 |
| H       | -3.19853400 | 1.25338300 |
| O       | -1.05424000 | -2.67414000 |
| O       | -1.05424000 | 2.67414000 |

**FPT**

| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 1.44274800 | 0.49685900 | 0.00016200 |
| N       | 0.37795600 | -0.29484400 | 0.00014000 |
| N       | -0.61205300 | 0.58211800 | 0.00015400 |
| C       | 3.11751900 | -1.34057400 | 0.00027300 |
| C       | 4.43887600 | -1.77097500 | 0.00039100 |
| C       | 5.47757900 | -0.84195500 | -0.00022500 |
| C       | 5.19165700 | 0.52163600 | 0.00007100 |
| C       | 3.87230200 | 0.95898400 | 0.00018900 |
| C       | 2.83177900 | 0.02712400 | 0.00024000 |
| H       | 2.30001300 | -2.05489900 | -0.00041400 |
| H       | 4.65911500 | -2.83393400 | -0.00061000 |
| H       | 5.99924400 | 1.24702500 | 0.00021700 |
| H       | 3.63397900 | 2.01775900 | 0.00042400 |
| C       | -4.63331900 | -0.49178900 | -0.00008400 |
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FPNI

C    1.39090200  0.71860700  -0.00020400  
N    0.30806500  1.15069100  -0.00010300  
N   -0.81775600  1.71483100  0.00006000  
C    2.91873400  -1.19145300  0.00036400  
C    4.21146700  -1.69624000  0.00050000  
C    5.30590800  -0.83343500  -0.00049800  
C    5.10239200  0.54534300  -0.00021000  
C    3.81657600  1.06863900  -0.00041700  
C    2.71565100  0.19768300  -0.00008900  
H    2.06317200  -1.85875800  0.00060700  
H    4.36434700  -2.77066000  0.00085100  
H    5.95194900  1.22059900  -0.00040700  
H    3.65309500  2.14092200  -0.00080900  
C   -4.22864900  -0.69962800  -0.00004100  
C   -4.33964900  0.68445900  -0.00046400  
C   -3.18488100  1.45178600  0.00047500  
C   -1.92072200  0.84501600  -0.00021000  
H   -5.32393200  1.13966100  0.00084200  
H   -3.23478300  2.53545400  0.00088500  
H   -1.83929900  -0.55368800  -0.00046600  
C   -2.99518500  -1.32815300  -0.00049800  
H   -0.87046800  -1.04458600  -0.00090900  
H   -2.94987800  -2.41183200  -0.00093900  
H    6.31429000  -1.23399700  0.00031600  
F   -5.34660400  -1.44770800  -0.00069000  

FPNI + NPQ (Reactants)

C    1.31915200  0.53400000  -1.27888500  
N    0.23784700  0.19280700  -1.54693900  
N   -0.88408100  -0.30056600  -1.84784100  
C    2.74982100  1.97950500  0.06723900  
C    4.01715000  2.39755100  0.44873100  
C    5.15009400  1.82427200  -0.12608600  
C    5.01592900  0.82641600  -1.08939900  
C    3.75712000  0.39972100  -1.48797300  
C    2.61966600  0.98139700  -0.91086100  
H    1.86009700  2.40605200  0.51968800  
H    4.12105100  3.17088000  1.20290900  
H    5.89738400  0.37262600  -1.53003300  
H    3.64281200  -0.38841000  -2.22928800
C  -4.29993200  1.51376900  -0.27363800
C  -3.08568200  2.15220800  -0.07868600
C  -1.92971400  1.57894800  -0.59758700
C  -1.99595200  0.37657200  -1.31347400
H  -3.05574400  3.08269900   0.47785400
H  -0.97237400  2.06619500  -0.43499100
C  -3.23885400  -0.24424000  -1.50034800
C  -4.39317500  0.32137100  -0.97851000
H  -3.27155300  -1.18395100  -2.04023100
H  -5.36179100  -0.14897700  -1.10616500
C  0.13232400   0.53022500   2.93279000
C  1.11124000   0.53022500   2.93279000
C  0.73621700  -1.14268800   1.30895200
C  -0.62194000  -1.79444000  -2.24503300
H  0.42066700  -1.28471200   3.65883800
H  2.17004000  -0.00035000   2.40750800
C  1.79347300  -1.86671300   0.54323300
C  -1.03579200  -2.40605700   0.05085100
H  -2.64285100  -0.89616200   1.55148000
H  -1.98115800  -0.00035000   3.22309600
C  0.04360100  -3.01236400  -0.77446900
C  1.30471000  -2.77864200  -0.53651000
H  -0.29439800  -3.68026700  -1.56125900
H  2.13260500  -3.04761400  -1.11408800
C  -2.19737300  -2.73497000  -0.09853800
O  2.97956700  -0.00000000   0.76598300
H  6.13782000  -2.81431000   0.18166400
F  -5.41615800  -2.06419900  -0.23560800

S0-TS (Transition state)

C  1.90787100  -0.50995900   0.34678300
N  0.95039500  -1.22649800   0.52774400
N  -0.10777000  -1.38956100   1.19476200
C  4.08018800   0.45890100  -0.32348500
C  5.40685900   0.29027800  -0.70618300
C  5.94280900  -0.98754900  -0.84134500
C  5.15347300  -2.11058400  -0.59238000
C  3.83033400  -1.95614700  -0.20504800
C  3.28971900  -0.66755500  -0.07219200
H  3.64841000   1.45054900  -0.22614600
H  6.02156500  -1.16239400  -0.90387500
H  5.57246000  -3.10626200  -0.69665800
H  3.20576700  -2.82031000   0.00036300
C  -3.71677800  -1.84623700  -0.83916000
C  -2.57704700  -1.60863600  -1.59658300
C  -1.35910000  -1.46957800  -0.94768700
C  -1.29075400  -1.58700500   0.44704400
H  -2.66108200  -1.52230300  -2.67424100
H  -0.45904800  -1.25782700  -1.51702700
H  -2.45110600   1.83168000   1.18782000
C  -3.67494300  -1.95952800   0.54234200
H  -2.37691500  -1.89479800   2.26767200
H  -4.59132100  -2.14287800   1.09187600
C  -2.00360300  2.47043500  -2.03378100
C  -0.70246200  2.50839200  -1.54478400
C  -0.43368400  2.04173900  -0.25875400
C  -1.47513300  1.56094000   0.54407600
C  -2.77998200  1.54265800  -0.05784200
C  -3.04106700  1.98832700  -1.23287700
H   0.11956600  2.89165800  -2.14120600
C   0.96750000  2.07596200   0.25739100
C  -1.19696600  1.02402900   1.91105800
H  -3.56586800  1.16435900   0.70404300
H  -4.05517300  1.95934600  -1.62013000
C   0.21434800  0.80388300   2.25536400
C   1.24998100  1.27547400   1.48039500
H   0.39231600  0.37500300   3.23589000
H   2.24793600  1.38958400   1.89732700
O  -2.10504600  0.74402000   2.67640300
F  -6.97873800 -1.11177200  -1.14160700
FP2HQ (Pre-oxidation product)
C  -0.35031900  4.38207700   1.53685000
C  -1.00199000  3.60224400   0.59039500
C  -0.29274200  2.61252400  -0.0957100
C   1.07483500  2.43744500   0.14777000
C   1.73340800  3.25021500   1.07123900
C   1.01516900  4.20475500   1.77894400
C  -0.90150800  5.13961500   2.08500800
C  -2.05524400  3.73948500   0.36754700
C  -0.96973300  1.79438800  -1.13172400
C   1.85933300  1.46739400  -0.66397300
C   2.80081400  3.11726500   1.21510100
C   1.51802900  4.82462200   2.51449200
C   1.12343900  0.27532800  -1.28335900
C  -0.41689300  0.38519300  -1.34521500
C   3.05630000  1.58894300  -0.80834200
C  -1.93763000  2.19564900  -1.73920800
C   1.28850500  0.92069800  -0.34074600
N   0.18482100  1.25063900   0.22046100
N  -0.83535200  0.44624600  -0.20595400
C   2.57601400 -2.63171700   0.91386500
C   3.74176900 -3.34292200   1.15359700
C   4.89367400 -3.07550400   0.41235000
C   4.86783900 -2.09119600  -0.56897800
C   3.70032400 -1.37330900  -0.81497300
C   2.54334300 -1.63743900  -0.07535200
H   1.67569600  2.83585100   1.48384200
H   3.75534900 -4.10937700   1.92260600
H   5.76031900 -1.87221600  -1.14664100
H   3.70067400 -0.58918200  -1.56353700
C  -3.17732800  0.53864600  -0.91456500
C  -4.47046200 -1.02221700  -0.72481500
C  -4.72197400 -1.90203800   0.31111900
C  -3.71365500  2.31437000   1.17113600
|   |               |               |               |               |
|---|---------------|---------------|---------------|---------------|
| C | -2.42747400   | -1.83029600   | 0.98908200    |               |
| C | -2.14860600   | -0.93982200   | -0.05732400   |               |
| H | -2.99250700   | 0.16050600    | -1.72108500   |               |
| H | -5.28071500   | -0.71969700   | -1.37878700   |               |
| H | -3.94598000   | -3.00556700   | 1.97384800    |               |
| H | -1.62450200   | -2.14051000   | 1.64606100    |               |
| H | 5.80620700    | -3.63135600   | 0.60454100    |               |
| F | -5.96952800   | -2.36707500   | 0.49349300    |               |
| H | -0.81432800   | -0.00885300   | -2.29024200   |               |
| H | 1.56894200    | 0.08791300    | -2.26385500   |               |