

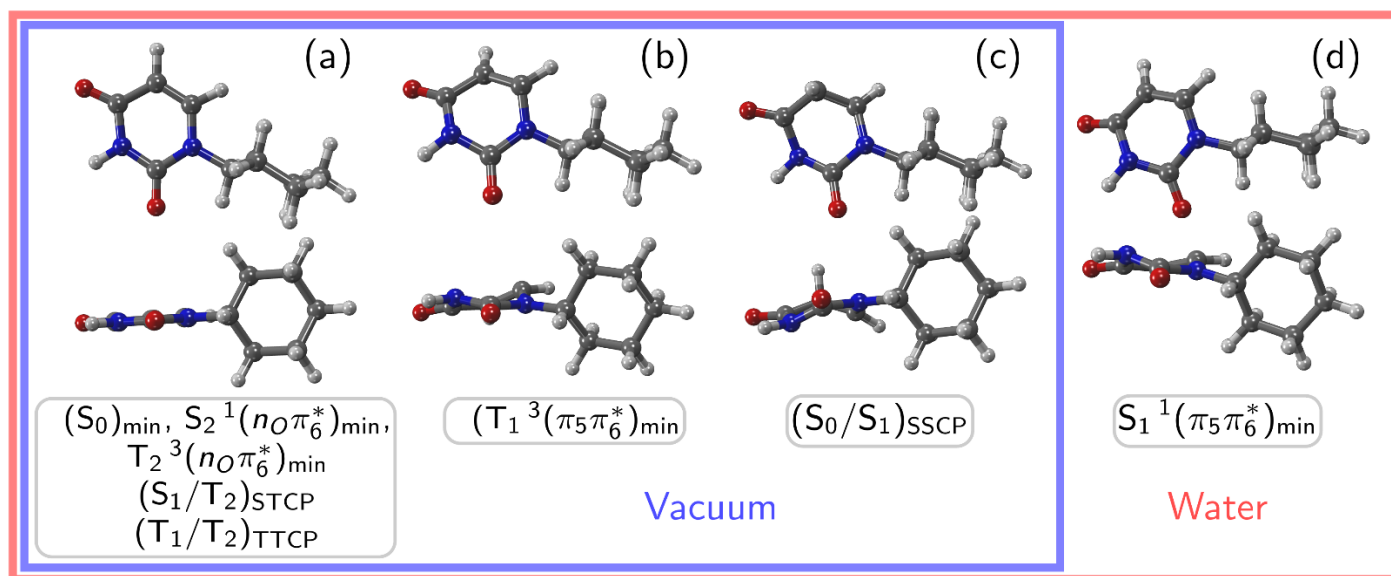
# Photophysical Deactivation Mechanisms of the Pyrimidine Analogue 1-Cyclohexyluracil

Danillo Valverde\*, Adalberto V. S. de Araújo and Antonio Carlos Borin\*

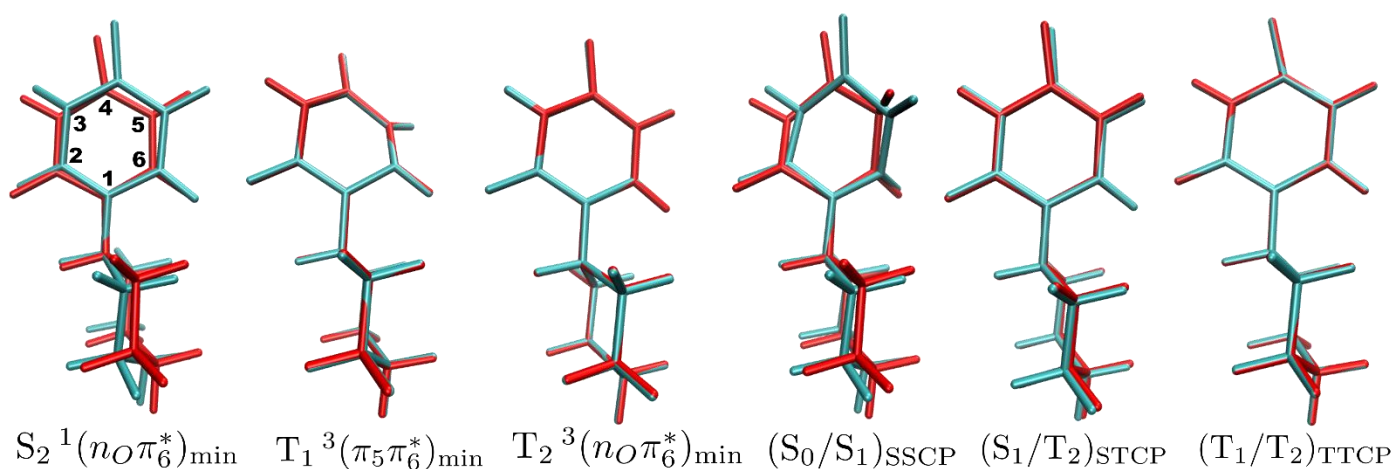
Department of Fundamental Chemistry, Institute of Chemistry, University of São Paulo, Avenida

Professor Lineu Prestes, 748, São Paulo, SP, CEP 05508-000, Brazil

\*Email: dpvalverde@usp.br, ancborin@iq.usp.br



**Figure S1:** Critical point structures of 1-cyclohexyluracil in vacuum (blue line) and water (red line) optimized at the MS-CASPT2(12,9)/cc-pVDZ level of theory. Multiple labels below the geometry indicate that the geometries are similar.



**Figure S2:** Superposition of the optimized structures obtained in gas phase (red) and water (cyan).

**Table S1:** The two low-lying singlet excited states for uracil, 1-cyclohexyluracil (1CHU), 1-trifluoromethyluracil (1CF3U), and 1-methoxyuracil (1OMEU) at the Franck-Condon region. Both optimization of the ground state as the vertical excitation energies calculation were obtained at the MS(3)-CASPT2(12,9)/cc-pVDZ level.

| Nature         | Uracil       | 1CHU         | 1CF3U        | 1OMEU        |
|----------------|--------------|--------------|--------------|--------------|
| $^1(n\pi^*)$   | 4.87 (0.000) | 4.84 (0.001) | 4.79 (0.001) | 4.85 (0.001) |
| $^1(\pi\pi^*)$ | 4.98 (0.285) | 4.71 (0.360) | 5.11 (0.256) | 4.71 (0.303) |

**Table S2:** Influence of the atomic basis sets and active spaces on the nature and energetic order of the electronic states in vacuum and in water (oscillator strength in parenthesis). PCM method is used to take into account the effects of water.

| cc-pVDZ         |             |                  |                 | cc-pVTZ     |                  |             |
|-----------------|-------------|------------------|-----------------|-------------|------------------|-------------|
| MS-CASPT2(12,9) |             | MS-CASPT2(14,10) | MS-CASPT2(12,9) |             | MS-CASPT2(14,10) |             |
| State           | 4S+3T       | 5S+4T            | 6S+5T           | 4S+3T       | 5S+4T            | 6S+5T       |
| Vacuum          |             |                  |                 |             |                  |             |
| T <sub>1</sub>  | 3.73        | 3.57             | 3.65            | 3.66        | 3.57             | 3.57        |
| S <sub>1</sub>  | 4.67(0.31)  | 4.39(0.27)       | 4.63(0.25)      | 4.45(0.30)  | 4.39(0.27)       | 4.41(0.24)  |
| T <sub>2</sub>  | 4.73        | 4.63             | 4.68            | 4.68        | 4.63             | 4.53        |
| S <sub>2</sub>  | 4.83(0.00)  | 4.65(0.00)       | 4.77(0.00)      | 4.75(0.00)  | 4.75(0.00)       | 4.69(0.00)  |
| T <sub>3</sub>  | 5.46        | 5.01             | 5.09            | 5.40        | 5.01             | 4.97        |
| S <sub>3</sub>  | 5.92(0.03)  | 5.89(0.02)       | 5.92(0.02)      | 5.75(0.00)  | 5.89(0.02)       | 5.74(0.02)  |
| T <sub>4</sub>  | —           | 5.97             | 6.07            | —           | 5.97             | 5.97        |
| S <sub>4</sub>  | —           | 6.71(0.00)       | 6.13(0.00)      | —           | 6.71(0.00)       | 5.98(0.00)  |
| Water           |             |                  |                 |             |                  |             |
| T <sub>1</sub>  | 3.81        | 3.71             | 3.70            | 3.76        | 3.64             | 3.63        |
| S <sub>1</sub>  | 4.63(0.316) | 4.59(0.269)      | 4.59(0.252)     | 4.41(0.315) | 4.36(0.268)      | 4.37(0.248) |
| T <sub>2</sub>  | 4.90        | 4.86             | 4.87            | 4.90        | 4.85             | 4.85        |
| S <sub>2</sub>  | 5.04(0.001) | 5.02(0.000)      | 4.99(0.001)     | 5.00(0.000) | 4.97(0.000)      | 4.95(0.000) |
| T <sub>3</sub>  | 5.55        | 5.08             | 5.09            | 5.53        | 4.99             | 4.99        |
| S <sub>3</sub>  | 6.04(0.036) | 6.07(0.021)      | 6.03(0.021)     | 5.89(0.038) | 5.95(0.021)      | 5.87(0.020) |
| T <sub>4</sub>  | —           | 6.15             | 6.12            | —           | 6.01             | 6.05        |
| S <sub>4</sub>  | —           | 6.97(0.000)      | 6.27(0.000)     | —           | 6.83(0.000)      | 6.15(0.000) |

## Molecular Geometries

On the following pages, all geometries employed for calculations in this work are given in XYZ file format

|    |                      |             |             |    |                      |             |             |
|----|----------------------|-------------|-------------|----|----------------------|-------------|-------------|
| 28 | (S0)min in gas phase |             |             | 28 | (T1)min in gas phase |             |             |
| N  | -0.00934476          | 0.05434883  | -0.01056622 | N  | -0.01352336          | 0.05381711  | -0.00951249 |
| C  | -0.11079013          | 0.39557728  | 1.32602837  | C  | -0.26875499          | 0.36479988  | 1.32633742  |
| C  | -1.27836859          | 0.34795616  | 2.02973617  | H  | 0.58826003           | 0.72078508  | 1.90092934  |
| C  | -2.50255628          | -0.09130989 | 1.36867902  | C  | -1.60509640          | 1.00659923  | 1.48998815  |
| N  | -2.29914085          | -0.40295119 | 0.00939356  | H  | -1.75720940          | 1.95161392  | 2.01922854  |
| C  | -1.13360831          | -0.36756331 | -0.73965604 | C  | -2.71954245          | 0.43958555  | 0.75929056  |
| O  | -3.61468918          | -0.19763015 | 1.87252594  | O  | -3.90468259          | 0.71292603  | 0.89972130  |
| O  | -1.09092114          | -0.67733738 | -1.92341761 | N  | -2.29538580          | -0.51529751 | -0.18850282 |
| H  | 0.82527811           | 0.71077571  | 1.79306723  | H  | -3.03213082          | -0.87070749 | -0.79875754 |
| H  | -1.31976795          | 0.62117564  | 3.08405855  | C  | -1.03190820          | -0.50877550 | -0.79259562 |
| H  | -3.12480832          | -0.71188398 | -0.50332050 | O  | -0.84191576          | -0.97856481 | -1.90733579 |
| C  | 1.28508153           | 0.12604982  | -0.71422185 | C  | 1.35956208           | 0.01904525  | -0.54791407 |
| C  | 1.82154850           | 1.56094842  | -0.76402071 | C  | 2.02135874           | 1.39901215  | -0.47355780 |
| C  | 3.13697046           | 1.60704059  | -1.55419823 | C  | 2.20419737           | -1.05484823 | 0.15029417  |
| C  | 4.17164731           | 0.64332675  | -0.95975638 | H  | 1.24101173           | -0.26357048 | -1.60607478 |
| C  | 3.62103932           | -0.78730880 | -0.90710015 | C  | 3.42609114           | 1.34109185  | -1.08999946 |
| C  | 2.30793188           | -0.84473668 | -0.11378346 | H  | 2.10227115           | 1.71860240  | 0.58243799  |
| H  | 1.05128289           | -0.19843354 | -1.74041999 | H  | 1.38849765           | 2.13949042  | -0.99392652 |
| H  | 2.00314263           | 1.93047463  | 0.26419466  | C  | 3.61114072           | -1.10022000 | -0.46184243 |
| H  | 1.06262532           | 2.22073256  | -1.22030287 | H  | 2.27710492           | -0.82329851 | 1.22982840  |
| H  | 2.50963285           | -0.57381043 | 0.94104096  | H  | 1.70073781           | -2.03300611 | 0.05680488  |
| H  | 1.88905621           | -1.86650462 | -0.11555525 | C  | 4.28647797           | 0.27566759  | -0.39858071 |
| H  | 3.52955793           | 2.63858549  | -1.57027123 | H  | 3.90622106           | 2.33280657  | -1.02235982 |
| H  | 2.93630299           | 1.32407720  | -2.60525740 | H  | 3.34044440           | 1.09917788  | -2.16679239 |
| H  | 4.36084771           | -1.47317877 | -0.45906901 | H  | 4.22251567           | -1.85771896 | 0.05869466  |
| H  | 3.43545214           | -1.14506824 | -1.93793800 | H  | 3.53516928           | -1.42079426 | -1.51864929 |
| H  | 5.10508404           | 0.67289449  | -1.54856431 | H  | 5.28766842           | 0.23266635  | -0.86181264 |
| H  | 4.42969907           | 0.97269856  | 0.06590564  | H  | 4.43591126           | 0.56013962  | 0.66141805  |
| 28 | (S2)min in gas phase |             |             | 28 | (T2)min in gas phase |             |             |
| N  | -0.01020960          | 0.05423878  | -0.01034813 | N  | -0.01697960          | 0.05337731  | -0.00864093 |
| C  | -0.11187014          | 0.40230849  | 1.35172835  | C  | -0.06599301          | 0.41254085  | 1.35642821  |
| C  | -1.35760195          | 0.30740425  | 2.01276046  | C  | -1.30448797          | 0.59264967  | 2.00175722  |
| C  | -2.44458342          | -0.11634702 | 1.28610142  | C  | -2.45302690          | 0.37219453  | 1.27077305  |
| N  | -2.30380941          | -0.43192025 | -0.06706811 | N  | -2.36328218          | -0.02957768 | -0.06295841 |
| C  | -1.09091659          | -0.37668646 | -0.76339219 | C  | -1.15831307          | -0.14280281 | -0.77095980 |
| O  | -3.71510671          | -0.27843070 | 1.72563300  | O  | -3.71943993          | 0.49204267  | 1.70673798  |
| O  | -1.03865225          | -0.69186995 | -1.94769547 | O  | -1.16708927          | -0.41239305 | -1.96373228 |
| H  | 0.80338609           | 0.72600878  | 1.84186837  | H  | 0.89284185           | 0.57551984  | 1.84243966  |
| H  | -1.45710363          | 0.56231669  | 3.06749585  | H  | -1.36600123          | 0.87127382  | 3.05258159  |
| H  | -3.09527025          | -0.76142500 | -0.61183623 | H  | -3.20254830          | -0.14211903 | -0.62421618 |
| C  | 1.29253261           | 0.14125873  | -0.68843892 | C  | 1.28922657           | -0.03856957 | -0.68370790 |
| C  | 1.81829458           | 1.58176327  | -0.72075285 | C  | 2.01931588           | 1.31081537  | -0.67070790 |
| C  | 3.14631480           | 1.64427927  | -1.48790624 | C  | 3.33867976           | 1.21879499  | -1.44745622 |
| C  | 4.18032302           | 0.68894039  | -0.87900899 | C  | 4.23460612           | 0.11476357  | -0.87389674 |
| C  | 3.64255575           | -0.74704763 | -0.84216955 | C  | 3.50248744           | -1.23362567 | -0.86228381 |
| C  | 2.31662792           | -0.82009979 | -0.07244450 | C  | 2.17125374           | -1.15083293 | -0.09769882 |
| H  | 1.09091141           | -0.17962857 | -1.72238667 | H  | 1.04611391           | -0.29722497 | -1.72563436 |
| H  | 1.97586064           | 1.94739860  | 0.31149466  | H  | 2.23874208           | 1.60929691  | 0.37173400  |
| H  | 1.06106424           | 2.23637078  | -1.18706878 | H  | 1.35741351           | 2.08344919  | -1.09771910 |
| H  | 2.49399834           | -0.55166670 | 0.98610164  | H  | 2.37669420           | -0.94902848 | 0.97047243  |
| H  | 1.90799104           | -1.84586271 | -0.08511642 | H  | 1.63658414           | -2.11555322 | -0.14587899 |
| H  | 3.52982350           | 2.67953361  | -1.49424540 | H  | 3.85954296           | 2.19190771  | -1.42549973 |
| H  | 2.96842957           | 1.36230993  | -2.54346403 | H  | 3.12519313           | 0.99691143  | -2.51040045 |
| H  | 4.38206919           | -1.42758035 | -0.38513092 | H  | 4.14724633           | -2.01273061 | -0.41929204 |
| H  | 3.47980644           | -1.10072855 | -1.87841181 | H  | 3.30252890           | -1.54623365 | -1.90508326 |
| H  | 5.12446501           | 0.73066810  | -1.44993589 | H  | 5.16923737           | 0.03711342  | -1.45721931 |
| H  | 4.41519162           | 1.01628006  | 0.15265415  | H  | 4.53046382           | 0.38051530  | 0.15984874  |

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## (S0/S1)SSCP in gas phase

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.01201458  | 0.04371155  | -0.00969558 |
| C | -0.37041422 | 0.32386265  | 1.25802064  |
| C | -1.64121155 | -0.24997603 | 1.72546145  |
| C | -2.78148682 | 0.03036963  | 0.82869809  |
| N | -2.30583075 | 0.33982338  | -0.49810590 |
| C | -1.05891553 | -0.01702294 | -0.99000370 |
| O | -3.98150502 | -0.09782129 | 1.01214739  |
| O | -0.81673896 | -0.23133577 | -2.15939959 |
| H | 0.28429386  | 0.97266528  | 1.85419648  |
| H | -1.55350591 | -1.35747948 | 1.76457863  |
| H | -3.02883444 | 0.35363473  | -1.21625218 |
| C | 1.39835275  | 0.13657624  | -0.52016186 |
| C | 2.07317929  | 1.45930370  | -0.14192476 |
| C | 3.48795425  | 1.50422893  | -0.74004927 |
| C | 4.32676413  | 0.30880086  | -0.26823437 |
| C | 3.64021280  | -1.01559899 | -0.61938200 |
| C | 2.21515713  | -1.07320014 | -0.05024274 |
| H | 1.29143902  | 0.09104299  | -1.61439743 |
| H | 2.15084959  | 1.55559131  | 0.95588948  |
| H | 1.46571044  | 2.30615314  | -0.50446448 |
| H | 2.24587830  | -1.07751900 | 1.05722208  |
| H | 1.70070920  | -1.99955944 | -0.36375801 |
| H | 3.97760347  | 2.45698094  | -0.46856297 |
| H | 3.41109836  | 1.48613726  | -1.84408964 |
| H | 4.22039751  | -1.87824773 | -0.24702808 |
| H | 3.58406218  | -1.11600269 | -1.71926262 |
| H | 5.33569751  | 0.34802721  | -0.71460005 |
| H | 4.45869373  | 0.37306293  | 0.82830229  |

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## (S1/T2)STCP in gas phase

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.01020960 | 0.05423878  | -0.01034813 |
| C | -0.11187014 | 0.40230849  | 1.35172835  |
| C | -1.35760195 | 0.30740425  | 2.01276046  |
| C | -2.44458342 | -0.11634702 | 1.28610142  |
| N | -2.30380941 | -0.43192025 | -0.06706811 |
| C | -1.09091659 | -0.37668646 | -0.76339219 |
| O | -3.71510671 | -0.27843070 | 1.72563300  |
| O | -1.03865225 | -0.69186995 | -1.94769547 |
| H | 0.80338609  | 0.72600878  | 1.84186837  |
| H | -1.45710363 | 0.56231669  | 3.06749585  |
| H | -3.09527025 | -0.76142500 | -0.61183623 |
| C | 1.29253261  | 0.14125873  | -0.68843892 |
| C | 1.81829458  | 1.58176327  | -0.72075285 |
| C | 3.14631480  | 1.64427927  | -1.48790624 |
| C | 4.18032302  | 0.68894039  | -0.87900899 |
| C | 3.64255575  | -0.74704763 | -0.84216955 |
| C | 2.31662792  | -0.82009979 | -0.07244450 |
| H | 1.09091141  | -0.17962857 | -1.72238667 |
| H | 1.97586064  | 1.94739860  | 0.31149466  |
| H | 1.06106424  | 2.23637078  | -1.18706878 |
| H | 2.49399834  | -0.55166670 | 0.98610164  |
| H | 1.90799104  | -1.84586271 | -0.08511642 |
| H | 3.52982350  | 2.67953361  | -1.49424540 |
| H | 2.96842957  | 1.36230993  | -2.54346403 |
| H | 4.38206919  | -1.42758035 | -0.38513092 |
| H | 3.47980644  | -1.10072855 | -1.87841181 |
| H | 5.12446501  | 0.73066810  | -1.44993589 |
| H | 4.41519162  | 1.01628006  | 0.15265415  |

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## (T1/T2)TTCP in gas phase

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.00993243 | 0.05292876  | -0.00973904 |
| C | -0.11007561 | 0.40832948  | 1.37397931  |
| C | -1.29093878 | 0.35033662  | 2.05877512  |
| C | -2.39266987 | -0.06851628 | 1.34015963  |
| N | -2.32194932 | -0.39160027 | -0.02214432 |
| C | -1.09595538 | -0.36287891 | -0.72904015 |
| O | -3.72017206 | -0.27606005 | 1.67237027  |
| O | -1.10379889 | -0.69194456 | -1.90907342 |
| H | 0.81735765  | 0.72928300  | 1.84480615  |
| H | -1.34692778 | 0.61653764  | 3.11292163  |
| H | -3.09703585 | -0.74232170 | -0.57669999 |
| C | 1.28475673  | 0.12949251  | -0.69415766 |
| C | 1.82393482  | 1.56497075  | -0.74210013 |
| C | 3.14354346  | 1.61683950  | -1.52452420 |
| C | 4.17925608  | 0.65717523  | -0.92540822 |
| C | 3.63151705  | -0.77453460 | -0.87309784 |
| C | 2.31350127  | -0.83393337 | -0.08888116 |
| H | 1.07403985  | -0.19433333 | -1.72621290 |
| H | 1.99692565  | 1.93620503  | 0.28647320  |
| H | 1.06589888  | 2.22350440  | -1.20194631 |
| H | 2.50642833  | -0.56252901 | 0.96696669  |
| H | 1.89816526  | -1.85725208 | -0.09060253 |
| H | 3.53514966  | 2.64909999  | -1.54026504 |
| H | 2.95144803  | 1.33192230  | -2.57705562 |
| H | 4.37275350  | -1.45696898 | -0.42147863 |
| H | 3.45433533  | -1.13295414 | -1.90557843 |
| H | 5.11611513  | 0.68909002  | -1.50963970 |
| H | 4.43133953  | 0.98829416  | 0.10121145  |

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## (S0)min in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.01271902 | 0.03845108  | -0.01874283 |
| C | -0.09555727 | 0.37794962  | 1.31488917  |
| C | -1.26399006 | 0.34823425  | 2.03029241  |
| C | -2.49444991 | -0.04315007 | 1.36576687  |
| O | -3.62191393 | -0.09338130 | 1.86995565  |
| N | -2.30703821 | -0.38996647 | 0.01958340  |
| C | -1.14610111 | -0.35811269 | -0.73417359 |
| O | -1.12695662 | -0.65544554 | -1.92726409 |
| C | 1.28480844  | 0.10381870  | -0.72510463 |
| C | 1.82394425  | 1.53813339  | -0.77227296 |
| C | 2.30324292  | -0.86710977 | -0.11663572 |
| C | 3.14668699  | 1.58346789  | -1.55017349 |
| C | 3.62372684  | -0.81061184 | -0.89763927 |
| C | 4.17556182  | 0.61971495  | -0.94579642 |
| H | 0.84798694  | 0.68527479  | 1.77633829  |
| H | -1.28720032 | 0.62905784  | 3.08607673  |
| H | -3.15151163 | -0.66832765 | -0.50066886 |
| H | 1.06242215  | -0.22096966 | -1.75413580 |
| H | 1.99620562  | 1.90841375  | 0.25705424  |
| H | 1.06946266  | 2.19793109  | -1.23599323 |
| H | 2.49541992  | -0.59625848 | 0.93976737  |
| H | 1.88381860  | -1.88870990 | -0.12199909 |
| H | 3.53999797  | 2.61489772  | -1.56336174 |
| H | 2.95594008  | 1.29994893  | -2.60304917 |
| H | 4.35928885  | -1.49670783 | -0.44273678 |
| H | 3.44777329  | -1.16854930 | -1.93022598 |
| H | 5.11456016  | 0.64868907  | -1.52593347 |
| H | 4.42420459  | 0.94942142  | 0.08209097  |

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(S1)min in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.02292489  | -0.09508096 | 0.07762557  |
| C | 0.00179932  | 0.11701833  | 1.41447522  |
| C | -1.32017270 | 0.58604224  | 1.93481336  |
| C | -2.50996178 | 0.15219104  | 1.30593988  |
| O | -3.67140628 | 0.38054640  | 1.57235012  |
| N | -2.24304816 | -0.69842492 | 0.12501104  |
| C | -1.14371272 | -0.53129138 | -0.66364766 |
| O | -1.05649475 | -0.75798039 | -1.87737707 |
| C | 1.28216564  | 0.05099218  | -0.68418476 |
| C | 1.78476799  | 1.49847238  | -0.63573123 |
| C | 2.34503442  | -0.93719364 | -0.19027811 |
| C | 3.07680887  | 1.64013838  | -1.45267272 |
| C | 3.63443970  | -0.78421532 | -1.00934573 |
| C | 4.14978815  | 0.65970521  | -0.96262621 |
| H | 0.96801908  | 0.34046044  | 1.88442839  |
| H | -1.33643177 | 1.32487949  | 2.75445589  |
| H | -3.09525795 | -0.95435163 | -0.39547170 |
| H | 1.03025798  | -0.19772940 | -1.72751077 |
| H | 1.98553773  | 1.79117617  | 0.41322742  |
| H | 0.99831849  | 2.17227542  | -1.01926304 |
| H | 2.56906074  | -0.74517501 | 0.87706352  |
| H | 1.95024566  | -1.96605463 | -0.26239076 |
| H | 3.44459703  | 2.67955452  | -1.39736680 |
| H | 2.85464092  | 1.43525136  | -2.51755629 |
| H | 4.40229492  | -1.48404099 | -0.63603500 |
| H | 3.42957072  | -1.06446084 | -2.06044150 |
| H | 5.06604976  | 0.75926988  | -1.57062796 |
| H | 4.42778209  | 0.91413068  | 0.07904091  |

28

(S2)min in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.90587983  | 0.82405983  | -0.05063834 |
| C | 0.15075296  | 2.01713605  | -0.07348924 |
| C | 0.81554156  | 3.26122017  | -0.00150712 |
| C | 2.18918084  | 3.25883693  | 0.01452958  |
| O | 2.99886517  | 4.34925817  | 0.05881147  |
| N | 2.90157548  | 2.06098714  | -0.09585745 |
| C | 2.28551375  | 0.81002028  | -0.00364436 |
| O | 2.97238246  | -0.21100536 | 0.08183834  |
| C | 0.19896396  | -0.47077702 | -0.03010239 |
| C | -0.62254189 | -0.63720138 | 1.25347510  |
| C | -0.66221916 | -0.65554812 | -1.28483040 |
| C | -1.31342699 | -2.00807236 | 1.26830067  |
| C | -1.35286619 | -2.02637129 | -1.25819959 |
| C | -2.18306376 | -2.20125705 | 0.01964520  |
| H | -0.93621585 | 1.91099028  | -0.04549742 |
| H | 0.25702741  | 4.20006571  | 0.03459379  |
| H | 3.90441024  | 2.05473960  | 0.13168860  |
| H | 0.99610755  | -1.23128640 | -0.03704352 |
| H | -1.39210833 | 0.15690946  | 1.31221048  |
| H | 0.03894815  | -0.51803904 | 2.12974791  |
| H | -1.43349404 | 0.13772956  | -1.33098708 |
| H | -0.02847173 | -0.54919493 | -2.18297433 |
| H | -1.91932756 | -2.11391416 | 2.18504975  |
| H | -0.54150457 | -2.80077468 | 1.30130015  |
| H | -1.98702507 | -2.14537460 | -2.15395628 |
| H | -0.58213864 | -2.81962351 | -1.30377544 |
| H | -2.65836471 | -3.19773065 | 0.03428549  |
| H | -3.00238088 | -1.45578260 | 0.02702642  |

28

(T1)min in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.01673874 | 0.03365518  | -0.01962854 |
| C | -0.26003368 | 0.34756095  | 1.32043927  |
| C | -1.59158337 | 1.01026532  | 1.48732021  |
| C | -2.70140557 | 0.45329029  | 0.75680889  |
| O | -3.88760848 | 0.73518345  | 0.92346319  |
| N | -2.30570998 | -0.49514395 | -0.20176627 |
| C | -1.03683888 | -0.51594344 | -0.79447556 |
| O | -0.85135728 | -1.00045522 | -1.90758374 |
| C | 1.35798774  | 0.00654044  | -0.56111734 |
| C | 2.00667230  | 1.39255931  | -0.48319569 |
| C | 2.20658857  | -1.05868970 | 0.14565870  |
| C | 3.41684819  | 1.34654169  | -1.08817965 |
| C | 3.61886163  | -1.09221902 | -0.45492462 |
| C | 4.28125325  | 0.28985131  | -0.38828394 |
| H | 0.60520064  | 0.71219544  | 1.88434992  |
| H | -1.72623407 | 1.94786313  | 2.05267589  |
| H | -3.05513166 | -0.86233044 | -0.80587036 |
| H | 1.25086769  | -0.27857130 | -1.61982923 |
| H | 2.07627437  | 1.71408158  | 0.57302125  |
| H | 1.37136346  | 2.12670098  | -1.00960035 |
| H | 2.26865490  | -0.82487683 | 1.22538594  |
| H | 1.71274833  | -2.04152639 | 0.04963751  |
| H | 3.88745514  | 2.34267266  | -1.01807465 |
| H | 3.34205976  | 1.10242157  | -2.16528482 |
| H | 4.23281657  | -1.84338769 | 0.07178927  |
| H | 3.55437061  | -1.41500952 | -1.51181860 |
| H | 5.28650280  | 0.25525428  | -0.84340072 |
| H | 4.41964191  | 0.57711630  | 0.67246618  |

28

(T2)min in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.01935842 | 0.07215409  | -0.02111147 |
| C | -0.05444682 | 0.40959240  | 1.35251920  |
| C | -1.29003152 | 0.56169678  | 2.00746630  |
| C | -2.44204858 | 0.34831417  | 1.27494374  |
| O | -3.70770156 | 0.45271850  | 1.73810768  |
| N | -2.36339064 | -0.04904757 | -0.06398393 |
| C | -1.16381048 | -0.13581256 | -0.76848758 |
| O | -1.16882758 | -0.39965447 | -1.97340280 |
| C | 1.28360207  | -0.02397465 | -0.70008936 |
| C | 2.02019695  | 1.32191793  | -0.69374413 |
| C | 2.15426517  | -1.13436572 | -0.09388328 |
| C | 3.34671847  | 1.21545676  | -1.45632750 |
| C | 3.49258097  | -1.23153133 | -0.84428161 |
| C | 4.23144394  | 0.11310066  | -0.86251627 |
| H | 0.90954684  | 0.54548651  | 1.84673940  |
| H | -1.33999376 | 0.84363191  | 3.06284529  |
| H | -3.21493972 | -0.09868060 | -0.63729325 |
| H | 1.04954477  | -0.29223556 | -1.74166048 |
| H | 2.23076125  | 1.63012247  | 0.34769566  |
| H | 1.36638921  | 2.09328295  | -1.13527304 |
| H | 2.35011126  | -0.92249746 | 0.97414144  |
| H | 1.61533051  | -2.09693074 | -0.13742821 |
| H | 3.87214888  | 2.18620874  | -1.43922757 |
| H | 3.14267558  | 0.98360389  | -2.51899867 |
| H | 4.12905596  | -2.00911831 | -0.38687772 |
| H | 3.30141672  | -1.55395942 | -1.88573934 |
| H | 5.17141159  | 0.02487864  | -1.43567247 |
| H | 4.51835922  | 0.38811687  | 0.17132665  |

28

(S0/S1)SSCP in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.02863900  | -0.06971900 | 0.04708200  |
| C | -0.18768100 | 0.64391800  | 1.22591100  |
| C | -1.15785600 | -0.04566700 | 2.08775100  |
| C | -2.45841700 | -0.24349300 | 1.45507300  |
| O | -3.52405400 | -0.60159600 | 1.98270700  |
| N | -2.34552100 | -0.13173600 | 0.05568800  |
| C | -1.15471000 | -0.39561000 | -0.64968100 |
| O | -1.17144800 | -0.81705300 | -1.79874900 |
| C | 1.30562600  | 0.00516400  | -0.69573000 |
| C | 1.78437100  | 1.45157200  | -0.85935300 |
| C | 2.35648500  | -0.86595800 | 0.00312400  |
| C | 3.10401700  | 1.47049900  | -1.64645900 |
| C | 3.68701700  | -0.82421900 | -0.76235800 |
| C | 4.17424000  | 0.61616800  | -0.95363900 |
| H | 0.07736900  | 1.70799000  | 1.28878800  |
| H | -0.82108200 | -0.88781200 | 2.73077600  |
| H | -3.19222900 | -0.37907300 | -0.47910100 |
| H | 1.09795600  | -0.41633800 | -1.69075000 |
| H | 1.95521600  | 1.91802000  | 0.12742800  |
| H | 1.01037000  | 2.04567400  | -1.37469400 |
| H | 2.49909500  | -0.49615000 | 1.03769900  |
| H | 1.97527000  | -1.90041200 | 0.07842100  |
| H | 3.45225700  | 2.51246800  | -1.76574000 |
| H | 2.92026100  | 1.07512600  | -2.66383500 |
| H | 4.43789400  | -1.43321500 | -0.22875800 |
| H | 3.53775400  | -1.29250400 | -1.75301600 |
| H | 5.11213100  | 0.62976200  | -1.53579300 |
| H | 4.40353000  | 1.05904500  | 0.03389000  |

28

(S1/T2)STCP in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.01037100  | 0.01818200  | 0.02352700  |
| C | -0.07304100 | 0.37489500  | 1.39722600  |
| C | -1.28931000 | 0.36776300  | 2.03948200  |
| C | -2.48778000 | -0.01716100 | 1.35962100  |
| O | -3.69539200 | 0.01813100  | 1.80204500  |
| N | -2.32040000 | -0.41258200 | -0.00850200 |
| C | -1.12632400 | -0.38436600 | -0.69044900 |
| O | -1.07234200 | -0.69495300 | -1.88601600 |
| C | 1.29259200  | 0.08811400  | -0.71081700 |
| C | 1.82129300  | 1.52650200  | -0.75135700 |
| C | 2.32702600  | -0.88214700 | -0.12887000 |
| C | 3.13107000  | 1.58898600  | -1.54973900 |
| C | 3.63442000  | -0.80850900 | -0.93020200 |
| C | 4.17587700  | 0.62598400  | -0.97206900 |
| H | 0.86104200  | 0.67255600  | 1.86414000  |
| H | -1.37934900 | 0.67871800  | 3.06648300  |
| H | -3.14214700 | -0.69347900 | -0.55065600 |
| H | 1.05603800  | -0.22743000 | -1.73956500 |
| H | 2.00754900  | 1.88714500  | 0.27895500  |
| H | 1.05509500  | 2.18595800  | -1.19595700 |
| H | 2.53429000  | -0.62100800 | 0.92712700  |
| H | 1.91435500  | -1.90646500 | -0.13827400 |
| H | 3.51726100  | 2.62315200  | -1.55829800 |
| H | 2.92536300  | 1.31520900  | -2.60237700 |
| H | 4.38172700  | -1.49427800 | -0.49435000 |
| H | 3.44432900  | -1.15684900 | -1.96356500 |
| H | 5.10524100  | 0.66741700  | -1.56678100 |
| H | 4.43876100  | 0.94661900  | 0.05514500  |

28

(T1/T2)TTCP in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.01002379 | 0.05306445  | -0.00999308 |
| C | -0.10946650 | 0.40815692  | 1.37336616  |
| C | -1.29177014 | 0.34999493  | 2.05791822  |
| C | -2.39395346 | -0.06879184 | 1.33992868  |
| O | -3.71994569 | -0.27454216 | 1.67610641  |
| N | -2.32158066 | -0.39174541 | -0.02219480 |
| C | -1.09631994 | -0.36257995 | -0.72961480 |
| O | -1.10328653 | -0.69223788 | -1.90968907 |
| C | 1.28481540  | 0.12958215  | -0.69441466 |
| C | 1.82402520  | 1.56505125  | -0.74227397 |
| C | 2.31344434  | -0.83385846 | -0.08896515 |
| C | 3.14376343  | 1.61689506  | -1.52448109 |
| C | 3.63159013  | -0.77448461 | -0.87296517 |
| C | 4.17936152  | 0.65721593  | -0.92519098 |
| H | 0.81795504  | 0.72919831  | 1.84409836  |
| H | -1.34794406 | 0.61537660  | 3.11235702  |
| H | -3.09727744 | -0.74286662 | -0.57601310 |
| H | 1.07426297  | -0.19424420 | -1.72650330 |
| H | 1.99685294  | 1.93628665  | 0.28632637  |
| H | 1.06607586  | 2.22359570  | -1.20224743 |
| H | 2.50620216  | -0.56245320 | 0.96691338  |
| H | 1.89809163  | -1.85717028 | -0.09075090 |
| H | 3.53538934  | 2.64914899  | -1.54016150 |
| H | 2.95183646  | 1.33197697  | -2.57704300 |
| H | 4.37274093  | -1.45692954 | -0.42122136 |
| H | 3.45457235  | -1.13290521 | -1.90547352 |
| H | 5.11631722  | 0.68911290  | -1.50926841 |
| H | 4.43128153  | 0.98833466  | 0.10146887  |

28

(S1)TS in water

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.00697013 | 0.01452692  | 0.03256046  |
| C | -0.04355062 | 0.35906307  | 1.35496265  |
| C | -1.35344868 | 0.32165925  | 2.07479543  |
| C | -2.41787765 | -0.11268341 | 1.35981860  |
| O | -3.69069451 | -0.25931313 | 1.75102205  |
| N | -2.27705073 | -0.46290956 | 0.05449327  |
| C | -1.10525298 | -0.40095732 | -0.67142668 |
| O | -1.10064906 | -0.70524193 | -1.84875413 |
| C | 1.28621795  | 0.08707629  | -0.69941705 |
| C | 1.81814869  | 1.52350773  | -0.75452582 |
| C | 2.31942814  | -0.87986170 | -0.10931592 |
| C | 3.12260411  | 1.56924103  | -1.56381430 |
| C | 3.62737139  | -0.81931125 | -0.91114457 |
| C | 4.16994382  | 0.61323354  | -0.97829242 |
| H | 0.88264633  | 0.64083092  | 1.82406798  |
| H | -1.43036682 | 0.61798529  | 3.10724776  |
| H | -3.09720592 | -0.77659628 | -0.44626711 |
| H | 1.04256217  | -0.23844138 | -1.72280347 |
| H | 2.01760323  | 1.89495311  | 0.26832430  |
| H | 1.05371054  | 2.18360201  | -1.20030715 |
| H | 2.51903009  | -0.60776202 | 0.94560765  |
| H | 1.90230877  | -1.90270749 | -0.10914749 |
| H | 3.51035265  | 2.60296317  | -1.59167265 |
| H | 2.90726089  | 1.27938764  | -2.61016867 |
| H | 4.37111006  | -1.50148386 | -0.46338128 |
| H | 3.43421978  | -1.18428003 | -1.93772420 |
| H | 5.09584246  | 0.64464075  | -1.57886287 |
| H | 4.43828100  | 0.95023061  | 0.04163363  |