# Contents



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# 1 Computed Structures and Energies

## 1.1 Methods and keywords

The structures of monomers, 1:1 and 1:2 complexes of DTBN and TEMPO were obtained from manual starting structures computed at the unrestricted open-shell B3LYP-D3BJ/def2-TZVP level[1–4] using ORCA 4.2.1[5] and with the help of the CREST[6, 7] program at GFN2-xTB level[8, 9], as described in the main document.

Reoptimizations were then performed using different functionals (open-shell B3LYP[1–3], B2PLYP[10] and TPSS[11]) with def2-TZVP and QZVP[4] basis sets, always including Grimme's three-body term dispersion correction D3[12] and Becke-Johnson (BJ) damping[13–16]. These calculations were carried out with the ORCA[5] software package.

Relaxed potential energy surface scans around the C-C-N-C, C-C-N-O, C-C···C-C dihedral angles of monomer and 1:1 structures, and C-N-O···O of 1:1 structures were obtained at UB3LYP/def2-TZVP level of theory using Gaussian16 Rev A.03[17].

Further single point calculations were performed at the B3LYP geometries with the DPLNO-CCSD(T)[18–21] method using aug-cc-pVTZ[22], and matching auxiliary basis sets, in the unrestricted open-shell[21] variant, with the ORCA software package.[5] Local energy decomposition (LED) was also carried out.[23, 24] For this purpose, two fragments were defined in the input file. The atoms which define DTBN were assigned to fragment (1), and the atoms of solvents were assigned to fragment (2) (see Tables S2 - S16).

When the basic variable that commands the type of wavefunction to be computed (HFTyp in the %scf block) is not specified, the program checks the multiplicity given in the input file, and performs the calculation based on it.[5]. For open-shell systems with multiplicity = 2 (DTBN and DTBN complexes), UKS/UHF were employed. UHF (Unrestricted Hartree-Fock) is replaced by UKS (Unrestricted Kohn-Sham) in DFT computations.[5] By program default, quasi-restricted orbitals (QRO[25]) were used to avoid spin contamination[26].

**Table S1:** Methods and keywords applied for open-shell quantum chemical calculations of DTBN and TEMPO monomers and solvates using ORCA[5] and Gaussian 16[17] software packages.

| Method | Program | Basis set | Keywords |
|---|---|---|---|
| B3LYP-D3(BJ) | Gaussian 16 Rev.A.03 | def2-TZVP | `# opt ub3lyp def2tzvp empiricaldispersion=gd3bj int=ultrafine freq` (multiplicity = 2) |
| B3LYP-D3(BJ) | ORCA 4.2.1 | def2-TZVP | `B3LYP D3BJ ABC def2-TZVP GRID5 NOFINALGRID VERYTIGHTSCF TIGHTOPT FREQ` (multiplicity = 2) |
| B3LYP-D3(BJ) | ORCA 4.2.1 | def2-QZVP | `B3LYP D3BJ ABC def2-QZVP GRID5 NOFINALGRID VERYTIGHTSCF TIGHTOPT FREQ` (multiplicity = 2) |
| B2PLYP-D3(BJ) | ORCA 4.2.1 | def2-TZVP | `B2PLYP D3 def2-TZVP GRID5 NOFINALGRID VERYTIGHTSCF TIGHTOPT NumFreq` (multiplicity = 2) |
| TPSS-D3(BJ) | ORCA 4.2.1 | def2-TZVP | `TPSS D3BJ def2-TZVP ABC GRID5 NOFINALGRID VERYTIGHTSCF TIGHTOPT NumFreq` (multiplicity = 2) |
| DLPNO-CCSD(T) | ORCA 4.2.1 | aug-cc-pVTZ | `DLPNO-CCSD(T) TightPNO aug-cc-pVTZ aug-cc-pVTZ/C TightSCF LED` (multiplicity = 2) |

## 1.2 Cartesian coordinates

Selected cartesian coordinates (in Å) of DTBN and TEMPO solvates (shown in figure 2 of the main document) are given in the Tables S2, S3 S4, S5,S6 S7, S8, S9, S10, S11, S12, S13, S14, S15, S16

**Table S2:** Cartesian coordinates of 1:1 DTBN t···HOH computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | -0.53247525809028 | 1.19645606619857 | -0.90457129344892 |
| C | (1) | -1.17576202268707 | -0.89664198471922 | -0.09311010966260 |
| C | (1) | -2.14486224728637 | -0.95704593113227 | -1.28101551191418 |
| C | (1) | -0.67869075038164 | -2.31331963542261 | 0.19066164407326 |
| C | (1) | -1.89745784853815 | -0.33776187519741 | 1.14242503548568 |
| H | (1) | -2.56049068822159 | 0.02407800133320 | -1.49374393424113 |
| H | (1) | -1.63413827427472 | -1.31871961188057 | -2.17519464178305 |
| H | (1) | -2.95812770812340 | -1.64515616064096 | -1.04601893406426 |
| H | (1) | 0.01749153744213 | -2.36323913495688 | 1.02454997971430 |
| H | (1) | -1.54608863195043 | -2.91847819578340 | 0.45760681080145 |
| H | (1) | -0.21865647612903 | -2.76610407036673 | -0.68622529386096 |
| H | (1) | -1.25102690652534 | -0.34054933635187 | 2.01919896766279 |
| H | (1) | -2.22476053303254 | 0.68453307139368 | 0.96336092293387 |
| H | (1) | -2.77269103522197 | -0.95218008536047 | 1.36111117554009 |
| C | (1) | 1.37088305639188 | 0.03214083148208 | -0.07534184370153 |
| C | (1) | 2.07111756309778 | -1.19077403402748 | -0.68659498819283 |
| C | (1) | 2.04252078139191 | 1.28953979874648 | -0.63668825793842 |
| C | (1) | 1.50119442455090 | 0.04744226052165 | 1.45470409506753 |
| H | (1) | 1.80626620944141 | -2.12462258153796 | -0.20120163746219 |
| H | (1) | 1.84509968738603 | -1.27153322608974 | -1.75085778466513 |
| H | (1) | 3.14933029608854 | -1.06279759239848 | -0.58116961429901 |
| H | (1) | 1.92489458243808 | 1.35166631280124 | -1.71777863864890 |
| H | (1) | 1.63831197691474 | 2.19451173370708 | -0.19161884447584 |
| H | (1) | 3.10668388679081 | 1.23377898623048 | -0.40322773776527 |
| H | (1) | 1.08220000746342 | -0.84450401224032 | 1.91707207236703 |
| H | (1) | 2.55974065798183 | 0.08892176189567 | 1.71918283851288 |
| H | (1) | 1.01011721260973 | 0.92723050619767 | 1.87006370720683 |
| N | (1) | -0.08573669278700 | 0.07504896249126 | -0.47702022110060 |
| O | (2) | -0.50386228985968 | 2.98602277913587 | 1.25602216630103 |
| H | (2) | -0.69957187065074 | 3.89874240123692 | 1.02339561483983 |
| H | (2) | -0.57898264622925 | 2.48387399473456 | 0.42349425671825 |

**Table S3:** Cartesian coordinates of 1:1 DTBN o···HOH computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | 0.41567117298258 | -1.42020424987360 | -0.63144026970744 |
| C | (1) | 1.27099120622909 | 0.69388754340038 | -0.09251935584857 |
| C | (1) | 1.65663664841111 | 1.15570184219707 | -1.50603247152449 |
| C | (1) | 0.99857434254054 | 1.89837954590040 | 0.80977205700574 |
| C | (1) | 2.42868025200800 | -0.10281212938397 | 0.52509783097452 |
| H | (1) | 0.89690272300582 | 1.80545642800899 | -1.93964362125725 |
| H | (1) | 2.59647771386852 | 1.70970362994228 | -1.46897239308447 |
| H | (1) | 1.79037257770667 | 0.29006815513801 | -2.15441302234975 |
| H | (1) | 0.79899922873605 | 1.59012887567704 | 1.83486176531354 |
| H | (1) | 1.89762259612261 | 2.51618209506579 | 0.81762665677259 |
| H | (1) | 0.18080834109913 | 2.52499751650549 | 0.46367392483009 |
| H | (1) | 3.27124760982164 | 0.57028302003468 | 0.69103842759261 |
| H | (1) | 2.13010101893747 | -0.53356572998329 | 1.48141093359179 |
| H | (1) | 2.74583307380200 | -0.90952356449016 | -0.13012373554562 |
| C | (1) | -1.36582361803467 | 0.08348713703955 | -0.13046518624085 |
| C | (1) | -2.15217014194207 | -1.16778352027193 | -0.53249948111866 |
| C | (1) | -1.75018493384255 | 0.44298628105332 | 1.31351444894082 |
| C | (1) | -1.72065649262555 | 1.21156759076890 | -1.10942857230714 |
| H | (1) | -1.97068598956774 | -1.98849599656516 | 0.15828827110536 |
| H | (1) | -3.21416166595455 | -0.91884771756881 | -0.50498264740159 |
| H | (1) | -1.89364828044040 | -1.49785717893917 | -1.53630796097325 |
| H | (1) | -1.37511355892891 | -0.31640782367521 | 2.00008113607944 |
| H | (1) | -1.37956220113729 | 1.41646765046688 | 1.62150272755114 |
| H | (1) | -2.83874122757579 | 0.46606342461191 | 1.39098322428124 |
| H | (1) | -1.22149403857735 | 2.14970725759504 | -0.87865028789385 |
| H | (1) | -1.46785879722272 | 0.92645745427706 | -2.13131093356351 |
| H | (1) | -2.79595338138628 | 1.39261739086114 | -1.06443686423816 |
| N | (1) | 0.10387169989351 | -0.24995961449702 | -0.21418401506929 |
| O | (2) | 0.08467343846170 | -2.61644659870416 | 1.90097009519162 |
| H | (2) | 0.26682561131019 | -2.39345277334389 | 0.97044375818955 |
| H | (2) | 0.37441507229918 | -3.52708594124760 | 2.01045556070383 |

**Table S4:** Cartesian coordinates of 1:1 DTBN p···HOH computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | -0.61928012751018 | -1.21575037302829 | -0.50869349528988 |
| C | (1) | -0.64221298547621 | 1.08342186823928 | -0.02318433829677 |
| C | (1) | 0.23426778262754 | 2.33587993072099 | -0.06306947111475 |
| C | (1) | -1.69805829851507 | 1.21233868563791 | -1.13032097224564 |
| C | (1) | -1.32931536087169 | 0.96902587604286 | 1.34668671548680 |
| H | (1) | 1.01918670307701 | 2.33745942063871 | 0.68958508877685 |
| H | (1) | 0.68139660303907 | 2.48572736003073 | -1.04472453988908 |
| H | (1) | -0.40869059217051 | 3.19278485812956 | 0.14109802363973 |
| H | (1) | -2.42552418100982 | 0.40673364825497 | -1.09432236618861 |
| H | (1) | -2.22718530663620 | 2.15804113494468 | -1.00407460266028 |
| H | (1) | -1.22223761197151 | 1.21309764228756 | -2.11249574651523 |
| H | (1) | -1.93686206802855 | 0.06785872075287 | 1.40354139965014 |
| H | (1) | -0.60173770785933 | 0.95893597376815 | 2.15814019436752 |
| H | (1) | -1.98602351505550 | 1.82839905653595 | 1.49316668965403 |
| C | (1) | 1.56953873175181 | -0.47798763715863 | 0.01862820477315 |
| C | (1) | 2.49657771000485 | 0.36521548125527 | -0.87012532508654 |
| C | (1) | 1.85900750838940 | -0.24119963284883 | 1.50781379592764 |
| C | (1) | 1.82777489365808 | -1.95405615790104 | -0.29795405856419 |
| H | (1) | 2.18877519620636 | 0.29755013795681 | -1.91439148895706 |
| H | (1) | 2.52988604323567 | 1.41159664213980 | -0.58364939872693 |
| H | (1) | 3.51106343638897 | -0.02881231668547 | -0.79188916594863 |
| H | (1) | 1.73870104569326 | 0.79983529369778 | 1.79945199665153 |
| H | (1) | 1.20155909345652 | -0.85281490730181 | 2.12624713091842 |
| H | (1) | 2.89071057647449 | -0.52713250604280 | 1.72110280400814 |
| H | (1) | 1.61915320923403 | -2.17743925855902 | -1.34311227677135 |
| H | (1) | 2.87951740740857 | -2.16401717845909 | -0.09783997790832 |
| H | (1) | 1.21422915687414 | -2.60961996340360 | 0.31479507799697 |
| N | (1) | 0.11841493202290 | -0.19303276492788 | -0.28830079422812 |
| O | (2) | -3.31549089177392 | -1.66883391687779 | 0.18042092361442 |
| H | (2) | -3.54371245506324 | -2.57621185361810 | -0.04241049727808 |
| H | (2) | -2.38697092760094 | -1.55963726422153 | -0.09489652979590 |

**Table S5:** Cartesian coordinates of 1:1 DTBN t···$HOCH_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | 0.59295641625733 | 0.45259467377100 | -1.17254945084802 |
| C | (1) | -1.25939812028856 | 1.21531154036220 | 0.02804962794556 |
| C | (1) | -2.60406851470312 | 0.79056922962370 | 0.61613940686717 |
| C | (1) | -0.43294652440404 | 1.95508110163992 | 1.09119408244934 |
| C | (1) | -1.52848379625993 | 2.14486123994194 | -1.16243322093635 |
| H | (1) | -2.50695704866786 | 0.12955561266402 | 1.47430421089260 |
| H | (1) | -3.11209578886269 | 1.69253818748304 | 0.96005124790766 |
| H | (1) | -3.24175942616305 | 0.31695726186284 | -0.12866916900224 |
| H | (1) | 0.54276699175699 | 2.22957477261738 | 0.69468958219976 |
| H | (1) | -0.95682526682350 | 2.86504270761079 | 1.38909131525734 |
| H | (1) | -0.28177303151046 | 1.34271295061698 | 1.97927949926411 |
| H | (1) | -2.12348683682872 | 2.99525822081235 | -0.82627805760658 |
| H | (1) | -0.59817287314189 | 2.50943781805941 | -1.58917164704831 |
| H | (1) | -2.08526702595404 | 1.62064070126930 | -1.94116025213401 |
| C | (1) | -0.43058056546684 | -1.36455355022494 | -0.02716525539332 |
| C | (1) | -1.77711019145183 | -2.03888012252051 | -0.32891023814053 |
| C | (1) | 0.65550553016724 | -2.11034643349442 | -0.80885946676909 |
| C | (1) | -0.09078852842463 | -1.43024828133611 | 1.46901474406204 |
| H | (1) | -2.07530178936691 | -1.85656689169052 | -1.36239516441855 |
| H | (1) | -1.66442889390115 | -3.11583628122560 | -0.19663506934326 |
| H | (1) | -2.57713542278169 | -1.71313118754613 | 0.32799741616268 |
| H | (1) | 0.49017762581796 | -2.03975128957571 | -1.88307196454424 |
| H | (1) | 1.64628919272562 | -1.72490149170221 | -0.58609029763791 |
| H | (1) | 0.61887571711050 | -3.16078450598833 | -0.51711604819005 |
| H | (1) | 0.87423026424142 | -0.96056040154368 | 1.66006401030649 |
| H | (1) | -0.84682042307877 | -0.95195093385455 | 2.08915732804772 |
| H | (1) | -0.02955957530095 | -2.47728361590685 | 1.77261404828706 |
| N | (1) | -0.42853607664913 | 0.07074548874193 | -0.50084739665895 |
| O | (2) | 2.80156650507555 | 0.46383189913251 | 0.53689475621957 |
| H | (2) | 2.10706294691201 | 0.51556203075016 | -0.14394188612298 |
| C | (2) | 4.05443527099546 | 0.31815434862798 | -0.10507974902617 |
| H | (2) | 4.81685875604908 | 0.25397190630645 | 0.67211903167673 |
| H | (2) | 4.10514045288768 | -0.59466411328237 | -0.71191899119248 |
| H | (2) | 4.29019005003292 | 1.17408740799802 | -0.74849698253280 |

**Table S6:** Cartesian coordinates of 1:1 DTBN o···$HOCH_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | 0.65472430631493 | -0.28446656600048 | -1.20770983029700 |
| C | (1) | -0.51417298928488 | 1.44461250082922 | -0.14710283968077 |
| C | (1) | -1.16122223505076 | 2.04877708883339 | -1.40234581121459 |
| C | (1) | -1.35987002918191 | 1.74955441900046 | 1.08976003423531 |
| C | (1) | 0.87467803278187 | 2.06137749281800 | 0.07082889883454 |
| H | (1) | -1.18731380548181 | 3.13671423819627 | -1.31759304853558 |
| H | (1) | -0.57791453150657 | 1.78293458310764 | -2.28337474358878 |
| H | (1) | -2.18293225396096 | 1.69412706310076 | -1.53761587666924 |
| H | (1) | -0.87641306924180 | 1.39926735518558 | 2.00020966552707 |
| H | (1) | -1.45874019972258 | 2.83348368439677 | 1.16302044567430 |
| H | (1) | -2.36451076851158 | 1.33774505079756 | 1.04175242818383 |
| H | (1) | 1.49482015441443 | 1.95616423383947 | -0.81511417068881 |
| H | (1) | 0.76087259259568 | 3.12194192852306 | 0.29987434763648 |
| H | (1) | 1.37923814959483 | 1.57575210290419 | 0.90695947261307 |
| C | (1) | -1.20844755577555 | -1.16971082191402 | -0.01266147016959 |
| C | (1) | -0.64618049301599 | -2.44460734592659 | -0.64859927151904 |
| C | (1) | -1.20800036342548 | -1.35948765234288 | 1.51231854894331 |
| C | (1) | -2.62570120291515 | -0.94153911320446 | -0.55687867789138 |
| H | (1) | 0.34503272894612 | -2.67758452828301 | -0.26453175820384 |
| H | (1) | -1.31701194145429 | -3.26748077844761 | -0.39703226970350 |
| H | (1) | -0.58420074133728 | -2.35906830933071 | -1.73111456154069 |
| H | (1) | -0.18381330351119 | -1.37376719795344 | 1.88633622741415 |
| H | (1) | -1.76827843003358 | -0.59061627009472 | 2.03642304396828 |
| H | (1) | -1.67023825074323 | -2.31997955444737 | 1.74661508454504 |
| H | (1) | -3.10851388621109 | -0.06467584331658 | -0.13175366558151 |
| H | (1) | -2.60640539531534 | -0.83504319941508 | -1.64213088191287 |
| H | (1) | -3.24279147418390 | -1.80769229238972 | -0.31174842453996 |
| N | (1) | -0.30474422627388 | -0.02507915180961 | -0.39956548043520 |
| O | (2) | 2.39943276317495 | -1.20047041616519 | 0.79382770711224 |
| H | (2) | 1.93274796834127 | -0.92597314895169 | -0.01434782236912 |
| C | (2) | 3.75289743566033 | -0.79908123385943 | 0.69696859680887 |
| H | (2) | 3.85489294268292 | 0.28928352342407 | 0.60246997336727 |
| H | (2) | 4.25515415785049 | -1.11097924543364 | 1.61345204568265 |
| H | (2) | 4.26341591378098 | -1.26940259567022 | -0.15183591600495 |

**Table S7:** Cartesian coordinates of 1:1 DTBN p···$HOCH_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | -0.69173486555471 | -0.74391979025288 | -0.48403700654533 |
| C | (1) | 0.23808521088093 | 1.36626417606461 | -0.02932249939500 |
| C | (1) | 1.55025679129497 | 2.14773874453083 | -0.10693941589599 |
| C | (1) | -0.69580814692248 | 1.90382330538131 | -1.12302052624978 |
| C | (1) | -0.40632321106480 | 1.56114241582467 | 1.35242610686462 |
| H | (1) | 2.28161802558865 | 1.83778039038848 | 0.63567008286769 |
| H | (1) | 1.99956110806031 | 2.08576512058199 | -1.09706614055631 |
| H | (1) | 1.32014317120704 | 3.19606046282780 | 0.08643779482942 |
| H | (1) | -1.68956654625616 | 1.47040656021717 | -1.05803052453317 |
| H | (1) | -0.78534046193181 | 2.98511560367464 | -1.00922784254257 |
| H | (1) | -0.28518211649336 | 1.69467561390505 | -2.11222284848535 |
| H | (1) | -1.33027879692198 | 0.99168459669882 | 1.43604209704263 |
| H | (1) | 0.26932989511768 | 1.26153839569291 | 2.15326558631497 |
| H | (1) | -0.64736789932821 | 2.61650782424119 | 1.49172615531562 |
| C | (1) | 1.61266582935118 | -0.96617841313443 | 0.01945523712767 |
| C | (1) | 2.78994989786445 | -0.59211012911873 | -0.89381190617824 |
| C | (1) | 1.99809330949948 | -0.84881154248693 | 1.50100945550635 |
| C | (1) | 1.23506577916179 | -2.42187902475155 | -0.27055118165566 |
| H | (1) | 2.46442665499820 | -0.54121089903042 | -1.93362398348894 |
| H | (1) | 3.25615969709751 | 0.35133333937379 | -0.62797379989973 |
| H | (1) | 3.55330222945296 | -1.36799434424357 | -0.81756064852906 |
| H | (1) | 2.32188750236511 | 0.15329224159197 | 1.77361749923535 |
| H | (1) | 1.15742913054391 | -1.12672193595817 | 2.13721823434768 |
| H | (1) | 2.82384658891337 | -1.53140439744358 | 1.71017005676143 |
| H | (1) | 0.93780942802977 | -2.55475885399078 | -1.30958531612200 |
| H | (1) | 2.10981714667952 | -3.04343068081874 | -0.07382288264848 |
| H | (1) | 0.41488576867396 | -2.75756260297765 | 0.35897831571351 |
| N | (1) | 0.40318451755457 | -0.11273439528594 | -0.28038333749636 |
| O | (2) | -3.30816099601599 | -0.06971379393214 | 0.25640481492098 |
| H | (2) | -2.41177081064704 | -0.32309458666400 | -0.02619504954427 |
| C | (2) | -4.19514801247697 | -1.12936121685343 | -0.04520537399833 |
| H | (2) | -3.92874399591930 | -2.05436859442760 | 0.48115162783215 |
| H | (2) | -5.19217499586156 | -0.82783909693414 | 0.27903331747997 |
| H | (2) | -4.23429582694099 | -1.34324849269052 | -1.12044509839548 |

**Table S8:** Cartesian coordinates of 1:1 DTBN t···$HOC(CH_3)_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | 0.09533782814065 | -0.26727294601942 | -1.15326414182886 |
| C | (1) | 1.64179570573856 | -1.35173612276303 | 0.29360903326476 |
| C | (1) | 3.06558325282587 | -1.83912262412881 | -0.01385764110002 |
| C | (1) | 1.49580477809231 | -0.93305575403756 | 1.76396861172739 |
| C | (1) | 0.67731405113892 | -2.50910726488072 | 0.01338746725314 |
| H | (1) | 3.21511957378967 | -2.80418572603763 | 0.47206720331616 |
| H | (1) | 3.20098449936055 | -1.97957814730698 | -1.08728472477612 |
| H | (1) | 3.83753544322510 | -1.16948593222876 | 0.35135171509304 |
| H | (1) | 0.47841254795251 | -0.59863725118865 | 1.96684929987452 |
| H | (1) | 1.70630582236684 | -1.79487407763610 | 2.40047388132152 |
| H | (1) | 2.19089939813664 | -0.14221389728199 | 2.04106443297798 |
| H | (1) | -0.34488564609934 | -2.26052837658191 | 0.28447803645372 |
| H | (1) | 0.69741678536213 | -2.79442957347752 | -1.03772973217350 |
| H | (1) | 0.99524416069698 | -3.36306727900703 | 0.61312116869577 |
| C | (1) | 1.86699566005448 | 1.17300328377707 | -0.67030437980650 |
| C | (1) | 3.32587755866194 | 1.23115504784148 | -0.22077677569851 |
| C | (1) | 1.79665339801955 | 1.62155654742644 | -2.13575971867866 |
| C | (1) | 1.01437106526076 | 2.10575997249473 | 0.20298463363363 |
| H | (1) | 3.65305513438753 | 2.26871132754138 | -0.30030768616798 |
| H | (1) | 3.46621911086553 | 0.92796694414396 | 0.81423519216737 |
| H | (1) | 3.97317618979250 | 0.63233606874809 | -0.85927700694177 |
| H | (1) | 2.21244871382628 | 2.62621767538435 | -2.22514414617004 |
| H | (1) | 2.37701765751383 | 0.95033223371007 | -2.77127625675837 |
| H | (1) | 0.76939706659280 | 1.63047312473915 | -2.49000887260068 |
| H | (1) | 1.36448780170101 | 3.13296763421554 | 0.08666754767957 |
| H | (1) | -0.03020792860552 | 2.05722438158103 | -0.09672356689412 |
| H | (1) | 1.08101334640533 | 1.83914798875469 | 1.25711802665357 |
| N | (1) | 1.25594213847933 | -0.20647940239933 | -0.61442828843673 |
| O | (2) | -1.82648884606674 | -0.12911451915880 | 0.88886052299399 |
| H | (2) | -1.24112741848644 | -0.19593779041408 | 0.11266795770185 |
| C | (2) | -3.15103393134671 | 0.16413081742132 | 0.42737279255126 |
| C | (2) | -4.01242821693803 | 0.25618068275089 | 1.68108114183619 |
| H | (2) | -5.04986995945547 | 0.47910219574339 | 1.42511469333086 |
| H | (2) | -3.98334567047379 | -0.68779147360342 | 2.22769777221029 |
| H | (2) | -3.63833901327243 | 1.04347836989296 | 2.33763052688579 |
| C | (2) | -3.14530663696555 | 1.49640689006972 | -0.32727320073201 |
| H | (2) | -2.49180616803891 | 1.43561659993603 | -1.20064227040735 |
| H | (2) | -4.14784635397941 | 1.76143978122319 | -0.67070769828784 |
| H | (2) | -2.77945440884687 | 2.29372030981071 | 0.32205364201966 |
| C | (2) | -3.63467759735426 | -0.96615457944922 | -0.48461455290495 |
| H | (2) | -2.98488210766122 | -1.05486643929531 | -1.35827933535699 |
| H | (2) | -3.61677971165594 | -1.91550774213174 | 0.05323791281019 |
| H | (2) | -4.65333907314095 | -0.78420095817815 | -0.83485321673127 |

**Table S9:** Cartesian coordinates of 1:1 DTBN o···HOC$(CH_3)_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | 0.39877071573462 | -0.65971193037477 | -1.03983675660335 |
| C | (1) | 1.73577097509368 | -1.24404445065739 | 0.79280577227533 |
| C | (1) | 2.75593806808957 | -2.11400414547978 | 0.04327452915641 |
| C | (1) | 2.35983875697780 | -0.65865875864647 | 2.06014553814647 |
| C | (1) | 0.53237517774646 | -2.09932133971434 | 1.21300998293076 |
| H | (1) | 2.31860409319208 | -2.47961793518184 | -0.88541162207030 |
| H | (1) | 3.66384051341123 | -1.55850319851701 | -0.19090019754925 |
| H | (1) | 3.03218151240008 | -2.97238315066144 | 0.65841948152244 |
| H | (1) | 1.62771279311372 | -0.10440321068028 | 2.64523814931538 |
| H | (1) | 2.71107737490951 | -1.49145790461566 | 2.67095020155546 |
| H | (1) | 3.21633184423867 | -0.01822999240331 | 1.86622888081273 |
| H | (1) | -0.24748817926489 | -1.47452243774725 | 1.64933813105215 |
| H | (1) | 0.10987547855622 | -2.62943787577106 | 0.36398356161190 |
| H | (1) | 0.85800388930781 | -2.82681896755823 | 1.95799874361676 |
| C | (1) | 1.72505497025621 | 1.20336906945413 | -0.36730746091913 |
| C | (1) | 1.00612018227583 | 1.78962664020260 | -1.58597674912153 |
| C | (1) | 1.37876925842081 | 2.07339712137842 | 0.85130800375220 |
| C | (1) | 3.23368078708767 | 1.19882712578583 | -0.65101392747202 |
| H | (1) | -0.06710243431050 | 1.85509489193929 | -1.41942889658374 |
| H | (1) | 1.39362114528186 | 2.79617866305690 | -1.75066422751995 |
| H | (1) | 1.18015632574803 | 1.19453634387837 | -2.47961459407710 |
| H | (1) | 0.32529734050715 | 1.95668867087755 | 1.10732251816771 |
| H | (1) | 1.98482348582567 | 1.84371929605967 | 1.72281438271902 |
| H | (1) | 1.55375368587568 | 3.12000014167114 | 0.59573477535505 |
| H | (1) | 3.45552697838645 | 0.59863845878710 | -1.53415963954752 |
| H | (1) | 3.56072475334755 | 2.22179017726727 | -0.84516558044130 |
| H | (1) | 3.82191912146735 | 0.81964733450781 | 0.18130843521605 |
| N | (1) | 1.22063007045290 | -0.20508551372928 | -0.16837861770335 |
| O | (2) | -1.86099682228902 | 0.50056703931006 | 0.21112167949016 |
| H | (2) | -1.18238650194394 | 0.05159335039160 | -0.32248057497947 |
| C | (2) | -3.14832660555503 | 0.08817186415333 | -0.26512842373109 |
| C | (2) | -3.26420550524192 | -1.43480240875942 | -0.16445533105164 |
| H | (2) | -2.50390815966042 | -1.91539768837243 | -0.78432811275385 |
| H | (2) | -3.11672043815665 | -1.75554588482996 | 0.86809295738675 |
| H | (2) | -4.24503821750929 | -1.77993670030623 | -0.49920834357994 |
| C | (2) | -4.16232368327669 | 0.77123747373408 | 0.64447825239885 |
| H | (2) | -4.00954856258480 | 0.46033054870506 | 1.67926837582719 |
| H | (2) | -4.04506467132493 | 1.85488266900448 | 0.59171431967302 |
| H | (2) | -5.18216285693261 | 0.51634910325039 | 0.35061746809229 |
| C | (2) | -3.32454160965509 | 0.54487728416532 | -1.71578053837874 |
| H | (2) | -2.56671176869190 | 0.08533653144558 | -2.35449284232163 |
| H | (2) | -4.30826514315361 | 0.26769246094647 | -2.10160305721310 |
| H | (2) | -3.21797813815329 | 1.62889123403369 | -1.78309864645611 |

**Table S10:** Cartesian coordinates of 1:1 DTBN p···$HOC(CH_3)_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| O | (1) | 0.01333058138695 | 0.03474422447572 | 1.01463699623354 |
| C | (1) | 1.58204840212531 | -1.33219827167279 | -0.08174972377413 |
| C | (1) | 3.08976748633624 | -1.49503874902610 | -0.27787421075831 |
| C | (1) | 1.10896856551371 | -2.42892962744831 | 0.88195142742796 |
| C | (1) | 0.85650914665206 | -1.47926042716126 | -1.42852157333683 |
| H | (1) | 3.62695474062893 | -1.45591292071990 | 0.66883927103175 |
| H | (1) | 3.26195617330969 | -2.47895279915435 | -0.71563462879121 |
| H | (1) | 3.51637349141401 | -0.76226994261945 | -0.95872293933124 |
| H | (1) | 1.41584453506274 | -3.39940381180152 | 0.48959332193341 |
| H | (1) | 1.56023672237468 | -2.29567318052873 | 1.86639338355866 |
| H | (1) | 0.02865515103362 | -2.42784882141231 | 0.99401599350215 |
| H | (1) | 1.03737231378417 | -2.48005527608674 | -1.82530107180655 |
| H | (1) | -0.21772341330619 | -1.35433553026798 | -1.30546432211354 |
| H | (1) | 1.21764631231541 | -0.75738101290892 | -2.16018607356698 |
| C | (1) | 1.90479083594032 | 1.31604783981448 | 0.37731401705917 |
| C | (1) | 2.05899904668953 | 1.67019813299583 | -1.10846696844147 |
| C | (1) | 1.03573887079415 | 2.38679892987861 | 1.04332035137456 |
| C | (1) | 3.26648037508605 | 1.30183435006447 | 1.08913313033181 |
| H | (1) | 1.08626183677050 | 1.69579313000527 | -1.60022223255903 |
| H | (1) | 2.50824992063705 | 2.66143464095301 | -1.19260028996265 |
| H | (1) | 2.69935160566017 | 0.97244574303039 | -1.64360129120858 |
| H | (1) | 0.05836234010576 | 2.46245548070977 | 0.57335949346993 |
| H | (1) | 0.88459825769821 | 2.17473676039393 | 2.10027810225193 |
| H | (1) | 1.54734213932119 | 3.34547867628134 | 0.94694843466181 |
| H | (1) | 3.16099747496996 | 0.91899877494400 | 2.10501037465755 |
| H | (1) | 4.01432670731410 | 0.71086534380799 | 0.56976110740841 |
| H | (1) | 3.64158787949573 | 2.32456431460812 | 1.15141617756639 |
| N | (1) | 1.20033898631217 | -0.01013544740140 | 0.53792231547482 |
| O | (2) | -2.34795709123579 | -1.09597294065493 | -0.04487217286288 |
| H | (2) | -1.55146018734285 | -0.75867281161624 | 0.40134931344398 |
| C | (2) | -3.17038967508917 | 0.02194104370515 | -0.39817381846649 |
| C | (2) | -2.43164321834285 | 0.90672160077945 | -1.40810519691785 |
| H | (2) | -3.04992220695029 | 1.75076453072050 | -1.72251921688036 |
| H | (2) | -1.51579683117240 | 1.30149600095166 | -0.96389543568871 |
| H | (2) | -2.16327063388953 | 0.32537802173444 | -2.29199399702028 |
| C | (2) | -4.42553690939176 | -0.57444517964715 | -1.02425986932878 |
| H | (2) | -5.11977325832756 | 0.21034087017851 | -1.33064333581247 |
| H | (2) | -4.16250077351284 | -1.16905572802261 | -1.90076294668478 |
| H | (2) | -4.92840345057801 | -1.22602447478616 | -0.30807624700394 |
| C | (2) | -3.51585231100999 | 0.82305247399523 | 0.85953989646855 |
| H | (2) | -4.02520417013327 | 0.18367957753493 | 1.58233485733546 |
| H | (2) | -2.60637528663952 | 1.20969119697456 | 1.32475684538968 |
| H | (2) | -4.16629048181046 | 1.66864529439948 | 0.62363275173555 |

**Table S11:** Cartesian coordinates of 1:1 TEMPO p···$HOCH_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| C | (1) | 2.63417702252661 | -0.53637455452458 | 0.00335068213640 |
| C | (1) | 2.63941524995298 | 0.80020812981734 | -0.72323995183042 |
| C | (1) | 1.69579587861952 | 1.75535067349238 | -0.00763318754117 |
| H | (1) | 3.31579977586428 | -1.24716131627998 | -0.46923393690497 |
| H | (1) | 2.34713919924590 | 0.67594217955717 | -1.76879194511927 |
| H | (1) | 2.05386986853127 | 1.89956078083835 | 1.01655892092492 |
| C | (1) | 0.24292437242723 | 1.26179938673632 | 0.04505467985633 |
| C | (1) | -0.44640171797841 | 1.41318699152796 | -1.32047747326180 |
| H | (1) | -0.52655025034288 | 2.47394988988299 | -1.56480833615659 |
| H | (1) | -1.45240444938479 | 0.99740555038801 | -1.28730383586998 |
| H | (1) | 0.11229205137596 | 0.92617952313286 | -2.11835461752705 |
| C | (1) | -0.52243193188837 | 2.06807056990863 | 1.09747701426414 |
| H | (1) | -1.58464166456804 | 1.83739078533594 | 1.09529474127600 |
| H | (1) | -0.40326486482424 | 3.13081592592589 | 0.87935070701300 |
| H | (1) | -0.12346847366705 | 1.87354813472080 | 2.09391419143063 |
| C | (1) | 1.24806459660804 | -1.19105281582991 | 0.07223451858271 |
| C | (1) | 0.85294765527942 | -1.80977111487524 | -1.27796886750677 |
| H | (1) | -0.17957574128110 | -2.15528798239722 | -1.23800428142133 |
| H | (1) | 1.49802947674712 | -2.66397837174012 | -1.49053980524766 |
| H | (1) | 0.94899674378340 | -1.10151328518465 | -2.09934640530115 |
| C | (1) | 1.25372930394826 | -2.27937664100149 | 1.14767678981752 |
| H | (1) | 1.43781113547920 | -1.84600546729595 | 2.13158422028526 |
| H | (1) | 2.05007240994173 | -2.99269699357371 | 0.92834944858909 |
| H | (1) | 0.30405026944399 | -2.80797553794661 | 1.17759604842677 |
| H | (1) | 3.65049105580423 | 1.21334589129470 | -0.73325653590211 |
| H | (1) | 2.99806775973527 | -0.38060199400246 | 1.02359357360353 |
| H | (1) | 1.69459213235675 | 2.73878746604695 | -0.48234630733765 |
| N | (1) | 0.21604342811710 | -0.17770549250928 | 0.45955148889221 |
| O | (1) | -0.91379021226543 | -0.65731381170775 | 0.81691959997269 |
| O | (2) | -3.45023426453146 | 0.29836622009037 | 0.11975244457892 |
| H | (2) | -2.58990169595232 | -0.02704277510781 | 0.43898452380280 |
| C | (2) | -4.30753755892246 | -0.80988901286854 | -0.07378877014037 |
| H | (2) | -3.91562161224167 | -1.51177157237403 | -0.82067274795168 |
| H | (2) | -4.48574217467319 | -1.36169624911689 | 0.85727511394804 |
| H | (2) | -5.26450277326690 | -0.42864311036042 | -0.43269170238096 |

**Table S12:** Cartesian coordinates of 1:1 TEMPO o···$HOCH_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| C | (1) | -1.65244393081233 | -0.86186207120621 | 1.25215890579359 |
| C | (1) | -2.34515508078859 | 0.49291272226027 | 1.27876206908258 |
| C | (1) | -1.29751251397819 | 1.58849706020882 | 1.14443577468403 |
| H | (1) | -0.96577271677916 | -0.91997222618797 | 2.10190491641384 |
| H | (1) | -2.88912380933260 | 0.61268891543732 | 2.21833440935602 |
| H | (1) | -1.75447756136057 | 2.57977219993681 | 1.18486189978117 |
| C | (1) | -0.48087545662921 | 1.50113624748008 | -0.15165283193423 |
| C | (1) | 0.78401238836536 | 2.35120864482099 | -0.01355001442136 |
| H | (1) | 1.34402522897513 | 2.37770459018672 | -0.94548524758456 |
| H | (1) | 1.43480525440669 | 1.95406829627272 | 0.76591640425218 |
| H | (1) | 0.49804482406746 | 3.36996570576816 | 0.25394555994691 |
| C | (1) | -1.29500815209955 | 1.98339625342727 | -1.36271061134124 |
| H | (1) | -0.73913858644442 | 1.79235725738937 | -2.28020525177323 |
| H | (1) | -1.47054964366299 | 3.05731994585446 | -1.27960751759098 |
| H | (1) | -2.26233297831737 | 1.48782622843192 | -1.43326964117135 |
| C | (1) | -0.85772163083392 | -1.12046208247165 | -0.03497342249933 |
| C | (1) | 0.12070785507213 | -2.27425937745490 | 0.19692244050098 |
| H | (1) | 0.86927173927380 | -1.99788641189387 | 0.93979218905508 |
| H | (1) | 0.63282135691602 | -2.54531894144132 | -0.72371143693525 |
| H | (1) | -0.43329077032622 | -3.14190546458984 | 0.55930601090921 |
| C | (1) | -1.78573105322120 | -1.46241407131589 | -1.21093120310380 |
| H | (1) | -2.25249597162858 | -2.43345822734707 | -1.03666852245940 |
| H | (1) | -1.20749266107756 | -1.51547134751757 | -2.13296490193663 |
| H | (1) | -2.57770395609669 | -0.72601953222625 | -1.34057678231343 |
| H | (1) | -3.08932549290116 | 0.56566563202452 | 0.48168149249330 |
| H | (1) | -2.37096719266269 | -1.67612183892023 | 1.36977496036060 |
| H | (1) | -0.61046276188341 | 1.52186378573738 | 1.99323550188119 |
| N | (1) | -0.05315184418359 | 0.08825813516639 | -0.39238946096369 |
| O | (1) | 0.86471227074692 | -0.08329687871178 | -1.26624218804476 |
| O | (1) | 3.07938023259275 | -0.33745365871799 | 0.47444746058024 |
| H | (1) | 2.42113963362840 | -0.23086849129969 | -0.23280130430193 |
| C | (1) | 3.96542074895435 | -1.37847207006700 | 0.11143598927542 |
| H | (1) | 4.50564605444922 | -1.15742127846793 | -0.81700093233547 |
| H | (1) | 4.69605645210596 | -1.48360212671264 | 0.91451384816839 |
| H | (1) | 3.44821972546582 | -2.33874552385343 | -0.01007856182409 |

**Table S13:** Cartesian coordinates of 1:1 TEMPO p···$HOC(CH_3)_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| C | (1) | 2.55394716973031 | 0.81002868435446 | -1.27662339113347 |
| C | (1) | 3.51045233592148 | -0.30242633769390 | -0.87260362192540 |
| C | (1) | 2.71072913419454 | -1.56133608421356 | -0.57080314311702 |
| H | (1) | 3.09431684722054 | 1.72882576885446 | -1.51535742690907 |
| H | (1) | 4.10800302312373 | -0.00602144851305 | -0.00707380484661 |
| H | (1) | 2.17695684879012 | -1.86382682079334 | -1.47721249869476 |
| C | (1) | 1.69085564252694 | -1.38521432733957 | 0.56331821197542 |
| C | (1) | 2.38418984337387 | -1.34368111489161 | 1.93483371509137 |
| H | (1) | 1.66244609590013 | -1.13231544271424 | 2.72250020403502 |
| H | (1) | 3.17550565964076 | -0.59665132871480 | 1.97140304633284 |
| H | (1) | 2.83168142135219 | -2.31827631857792 | 2.13791109213039 |
| C | (1) | 0.69489683727243 | -2.54718466940524 | 0.52886433501928 |
| H | (1) | 0.02163364596923 | -2.53174882995544 | 1.38219779065470 |
| H | (1) | 1.25098528790138 | -3.48602963015775 | 0.54852909163834 |
| H | (1) | 0.10109910141212 | -2.51660549714708 | -0.38557319149011 |
| C | (1) | 1.51135086897616 | 1.14397773025400 | -0.20131365678382 |
| C | (1) | 2.13033134438729 | 1.95305189805521 | 0.94924747038986 |
| H | (1) | 3.02768741491311 | 1.48370072199850 | 1.34881108473032 |
| H | (1) | 1.40841443538641 | 2.06058584416340 | 1.75806030734271 |
| H | (1) | 2.40039625808122 | 2.94779813183144 | 0.59064780312834 |
| C | (1) | 0.37265226257127 | 1.94853871737980 | -0.83142112116976 |
| H | (1) | 0.78865518389579 | 2.83432457212440 | -1.31441600362532 |
| H | (1) | -0.35035323526362 | 2.26156987759528 | -0.08212514354911 |
| H | (1) | -0.14725868782282 | 1.35471642002288 | -1.58423538813658 |
| H | (1) | 4.21742306316079 | -0.49584664808866 | -1.68244696771030 |
| H | (1) | 2.02943158047597 | 0.50641899462004 | -2.18784960459377 |
| H | (1) | 3.36805138459433 | -2.39040760593269 | -0.30036681276187 |
| N | (1) | 0.92318566731775 | -0.11654031980932 | 0.35175931114913 |
| O | (1) | -0.15369720120709 | 0.02782665622452 | 1.02519899101249 |
| C | (2) | -2.80400542607372 | 0.12579476888118 | 3.59350999479972 |
| C | (2) | -1.46723946193875 | -0.17351556109332 | 4.27693100166396 |
| H | (2) | -3.38700558604320 | -0.79118383612184 | 3.49359537815793 |
| H | (2) | -3.38854563675860 | 0.84949341305061 | 4.16653813249319 |
| H | (2) | -2.63585314015086 | 0.53630745748125 | 2.59535009408615 |
| C | (2) | -1.68736369043557 | -0.80386200602044 | 5.64698305821012 |
| C | (2) | -0.62990333301711 | 1.10368336350581 | 4.39494510080172 |
| H | (2) | -2.23788867202891 | -0.12752483593178 | 6.30358192252867 |
| H | (2) | -2.25381830609139 | -1.73096414801996 | 5.54615097808649 |
| H | (2) | -0.72841911776720 | -1.03821136637213 | 6.11226213452159 |
| H | (2) | 0.33489483127849 | 0.87841436321831 | 4.85300292120580 |
| H | (2) | -0.45123706597075 | 1.52953002504064 | 3.40531398535491 |
| H | (2) | -1.13673058535655 | 1.85556532690905 | 5.00441523958111 |
| O | (2) | -0.74792852875838 | -1.14880620759088 | 3.51339086732653 |
| H | (2) | -0.60077314668390 | -0.78748903446673 | 2.62087760499861 |

**Table S14:** Cartesian coordinates of 1:1 TEMPO o···$HOC(CH_3)_3$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| C | (1) | 2.66964172499097 | 0.70700222015519 | -1.34860179362496 |
| C | (1) | 3.43159414706997 | -0.54603171565215 | -0.94198211994994 |
| C | (1) | 2.43581651972781 | -1.64410394000685 | -0.59727769463452 |
| H | (1) | 3.35307523526644 | 1.51246332954241 | -1.62662696983565 |
| H | (1) | 4.09338042689371 | -0.34236404478733 | -0.09628130358893 |
| H | (1) | 1.83613691474405 | -1.86527073513441 | -1.48521976534797 |
| C | (1) | 1.48763591164796 | -1.27358110268504 | 0.55101605950477 |
| C | (1) | 2.19789075721168 | -1.34230861700015 | 1.91204672785263 |
| H | (1) | 1.54223810465099 | -0.95178264070404 | 2.68983638772374 |
| H | (1) | 3.12707497392876 | -0.77416337659534 | 1.92412806129439 |
| H | (1) | 2.43453225767664 | -2.38159707933770 | 2.14653088085633 |
| C | (1) | 0.29171213366230 | -2.22841619199647 | 0.55122532321537 |
| H | (1) | -0.35103621338649 | -2.05500398669819 | 1.41129295579506 |
| H | (1) | 0.66000624983665 | -3.25514938543056 | 0.58933681712819 |
| H | (1) | -0.30619802526634 | -2.10188037675293 | -0.35147885989260 |
| C | (1) | 1.73652335874886 | 1.24037742880659 | -0.25338949845388 |
| C | (1) | 2.52338907568114 | 1.95162296626282 | 0.85884614726120 |
| H | (1) | 3.33484357843096 | 1.33820723648129 | 1.24790825881691 |
| H | (1) | 1.85367389583676 | 2.20369010589747 | 1.68059855157632 |
| H | (1) | 2.95494644937570 | 2.87408458386992 | 0.46659977095932 |
| C | (1) | 0.73147158722392 | 2.21497713360659 | -0.87141415304628 |
| H | (1) | 1.27805093007424 | 2.99457214206315 | -1.40503433223198 |
| H | (1) | 0.11351620664856 | 2.68067997500054 | -0.10706171261980 |
| H | (1) | 0.07491465402344 | 1.70188655806199 | -1.57428294432622 |
| H | (1) | 4.07404140685035 | -0.87219569427259 | -1.76291200478598 |
| H | (1) | 2.07042705918039 | 0.48029767558286 | -2.23544340617744 |
| H | (1) | 2.94737404150692 | -2.56934530044521 | -0.32274072496433 |
| N | (1) | 0.96176806752952 | 0.11226407182163 | 0.35087485729038 |
| O | (1) | -0.05214926159804 | 0.43910764033767 | 1.05902407876373 |
| C | (2) | -3.56667597961586 | 1.66553466265405 | 0.14884851547244 |
| C | (2) | -3.41441251616547 | 0.22320004270536 | -0.34178315127621 |
| H | (2) | -3.38547189961334 | 2.36140019174428 | -0.67204661087034 |
| H | (2) | -4.56899337442949 | 1.84648204704253 | 0.54407066630138 |
| H | (2) | -2.84468392662778 | 1.87447163133234 | 0.94155588646441 |
| C | (2) | -4.37623804321457 | -0.06407612262756 | -1.48830910986872 |
| C | (2) | -3.63129901745906 | -0.76067788901703 | 0.81121513967777 |
| H | (2) | -5.41240440310487 | 0.05319746706123 | -1.16557688642236 |
| H | (2) | -4.18931221799461 | 0.62102942452420 | -2.31686142157391 |
| H | (2) | -4.23693987683293 | -1.08425026900080 | -1.84981798347363 |
| H | (2) | -3.49561029771409 | -1.78512006265574 | 0.46035768382069 |
| H | (2) | -2.91005720448428 | -0.57308873345509 | 1.60978269786599 |
| H | (2) | -4.63614355731433 | -0.66591819105114 | 1.22933395688211 |
| O | (2) | -2.10044576538304 | 0.04092943548932 | -0.88309895813327 |
| H | (2) | -1.46037408821404 | 0.20943748526291 | -0.17073801942423 |

**Table S15:** Cartesian coordinates of 1:1 TEMPO p···$HOC_6H_5$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| C | (1) | 3.46154890714554 | 1.38399686121575 | 0.23241679060532 |
| C | (1) | 3.66468311450320 | 0.42873706483711 | -0.93380348612965 |
| C | (1) | 3.22469431343684 | -0.96537682462016 | -0.51299592421986 |
| H | (1) | 4.08818178453849 | 1.05532786192038 | 1.06716198433181 |
| H | (1) | 4.71772751015481 | 0.41470924052284 | -1.22312781149926 |
| H | (1) | 3.38104513662040 | -1.68805871610318 | -1.31655827825415 |
| C | (1) | 1.74949200242294 | -1.04851547247245 | -0.09476177095461 |
| C | (1) | 1.52141715913828 | -2.35546365561711 | 0.66907864483384 |
| H | (1) | 1.90057031712055 | -3.18190410982936 | 0.06545846726251 |
| H | (1) | 0.46805588840261 | -2.53584391751186 | 0.86624293623000 |
| H | (1) | 2.06068315393605 | -2.34591176560903 | 1.61707538147729 |
| C | (1) | 0.82248405757683 | -0.99658293374104 | -1.31905980323258 |
| H | (1) | 1.03619261724247 | -0.14377088617588 | -1.96140678090905 |
| H | (1) | -0.22029041728511 | -0.94357035839002 | -1.01321752432952 |
| H | (1) | 0.95676016503989 | -1.90474957871151 | -1.90894139368571 |
| C | (1) | 2.00675200725940 | 1.46438442674540 | 0.71378646149431 |
| C | (1) | 1.96707577783318 | 2.09731880663985 | 2.10601811026759 |
| H | (1) | 0.94442589086138 | 2.22898561925400 | 2.45086085836055 |
| H | (1) | 2.45601128888136 | 3.07212965964022 | 2.06684635957653 |
| H | (1) | 2.49634682962095 | 1.47307474947593 | 2.82701196251031 |
| C | (1) | 1.14432132145871 | 2.29418258747069 | -0.24993545334047 |
| H | (1) | 1.21154140917540 | 1.93881137215051 | -1.27670827668168 |
| H | (1) | 1.47417504216405 | 3.33411063012008 | -0.22841940188697 |
| H | (1) | 0.10051682402400 | 2.25783952693514 | 0.05872726632150 |
| H | (1) | 3.10858474395082 | 0.76309424359532 | -1.81290147202880 |
| H | (1) | 3.78396995798543 | 2.39572986914369 | -0.02313004739985 |
| H | (1) | 3.84483457350478 | -1.28974169316509 | 0.32837195143164 |
| N | (1) | 1.42278362099325 | 0.08911640880499 | 0.82370478178796 |
| O | (1) | 0.32875227830788 | 0.01314127186080 | 1.48218686805085 |
| O | (2) | -1.84713565689355 | -1.63949269464435 | 1.12451821981432 |
| H | (2) | -1.09404583771603 | -1.04048824345449 | 1.30970911156966 |
| C | (2) | -2.75276496721189 | -1.02917300007474 | 0.32156681239225 |
| C | (2) | -3.81750727112876 | -1.79079778415782 | -0.16189392239587 |
| C | (2) | -2.65255258796697 | 0.31820247787189 | -0.03258898364884 |
| C | (2) | -4.76526131849410 | -1.20853813736724 | -0.99090162122779 |
| H | (2) | -3.88356193040243 | -2.83283973710025 | 0.12283802694458 |
| C | (2) | -3.60732690294106 | 0.88820122114217 | -0.86613354743532 |
| H | (2) | -1.83305186074720 | 0.90803538411937 | 0.35727985689003 |
| C | (2) | -4.66769269845230 | 0.13252608815636 | -1.35227135720368 |
| H | (2) | -5.58812017840053 | -1.80895863173739 | -1.35928545524941 |
| H | (2) | -3.52047439506539 | 1.93454599639471 | -1.13316386757928 |
| H | (2) | -5.40976167059428 | 0.58128677246576 | -1.99938467286046 |

**Table S16:** Cartesian coordinates of 1:1 TEMPO o···$HOC_6H_5$ computed at UB3LYP-D3(BJ)/def2-TZVP level of theory.

| Atom | Fragment | X | Y | Z |
|---|---|---|---|---|
| C | (1) | 3.28710299310683 | 0.95777477307372 | 0.95286718250212 |
| C | (1) | 3.72083457225580 | -0.49018804093411 | 1.12763574550463 |
| C | (1) | 2.48392145018975 | -1.36321713083445 | 1.27915051147688 |
| H | (1) | 2.73816465399053 | 1.26931724007965 | 1.84662858628020 |
| H | (1) | 4.35177814718835 | -0.58393835558068 | 2.01414982849107 |
| H | (1) | 2.75479589551516 | -2.41006439975299 | 1.43240729439091 |
| C | (1) | 1.53314586315855 | -1.29857152174830 | 0.07617773520466 |
| C | (1) | 0.16223759319123 | -1.84271008434305 | 0.48309378230808 |
| H | (1) | -0.29849306127346 | -1.20518073242383 | 1.23792158030646 |
| H | (1) | 0.28814444585756 | -2.84248142969955 | 0.90177512800361 |
| H | (1) | -0.51167979799172 | -1.90447627769953 | -0.36747048623357 |
| C | (1) | 2.07608401727367 | -2.10433733911340 | -1.11394801306810 |
| H | (1) | 1.44447451668436 | -1.94414564249660 | -1.98712213262660 |
| H | (1) | 2.06632268116210 | -3.16732308710784 | -0.86772017139592 |
| H | (1) | 3.09750995713039 | -1.82522399982547 | -1.36892490622462 |
| C | (1) | 2.39570869028500 | 1.18722375689552 | -0.27471661781152 |
| C | (1) | 1.67951200535270 | 2.53283695178869 | -0.14077903164226 |
| H | (1) | 0.99854048465456 | 2.52634515657619 | 0.71090984715581 |
| H | (1) | 1.10762466527580 | 2.76720248491340 | -1.03569642997866 |
| H | (1) | 2.42352440969201 | 3.31579822376928 | 0.01466432333634 |
| C | (1) | 3.21431210001471 | 1.16709099825671 | -1.57508376525193 |
| H | (1) | 3.87202970385179 | 2.03735366818452 | -1.60377157476656 |
| H | (1) | 2.54464446017013 | 1.20896903716003 | -2.43341882999849 |
| H | (1) | 3.83187980307223 | 0.27390738073385 | -1.65973519914666 |
| H | (1) | 4.32903898261967 | -0.81960862834702 | 0.28153260341866 |
| H | (1) | 4.14983200699057 | 1.62179893923822 | 0.86564848445340 |
| H | (1) | 1.93779131501732 | -1.04498218007606 | 2.17222367318302 |
| N | (1) | 1.34758029573348 | 0.12227443585712 | -0.35435426289306 |
| O | (1) | 0.38431566295579 | 0.34245658514278 | -1.16739298209195 |
| O | (2) | -1.65670825335374 | 1.29778427660413 | 0.40347625662245 |
| H | (2) | -0.99675650429008 | 1.01644984446162 | -0.26220576596040 |
| C | (2) | -2.82486500790709 | 0.63531490203343 | 0.21030604621721 |
| C | (2) | -3.02054183349998 | -0.23709707951646 | -0.86231570931525 |
| C | (2) | -3.85602758519501 | 0.84629320117520 | 1.12585343115520 |
| C | (2) | -4.23775834892589 | -0.89105778276590 | -1.00772920738331 |
| H | (2) | -2.21810199744059 | -0.39405586677111 | -1.57234982218798 |
| C | (2) | -5.06715501811880 | 0.18781811129805 | 0.96768327167236 |
| H | (2) | -3.68975476352452 | 1.52719881865403 | 1.95055879724379 |
| C | (2) | -5.26807711590472 | -0.68576629254544 | -0.09718403785194 |
| H | (2) | -4.38012056999096 | -1.56548835479976 | -1.84344084428881 |
| H | (2) | -5.86175090427392 | 0.35919562412121 | 1.68365074710892 |
| H | (2) | -6.21452061069956 | -1.19663018363585 | -0.21600506591821 |

### 1.3 Structures

UB3LYP/def2-TZVP computed structures of DTBN and TEMPO 1:2 solvates are given in Figures S1, S2 and S3, along with their relative energies (in kJ $mol^{-1}$). For DTBN, the asymmetry of the NO environment leads to two isomers of similar energy, which are depicted in a mirror-image representation of the monomeric radical. For TEMPO, this asymmetry is absent and only one of the enantiomeric complexes is shown.

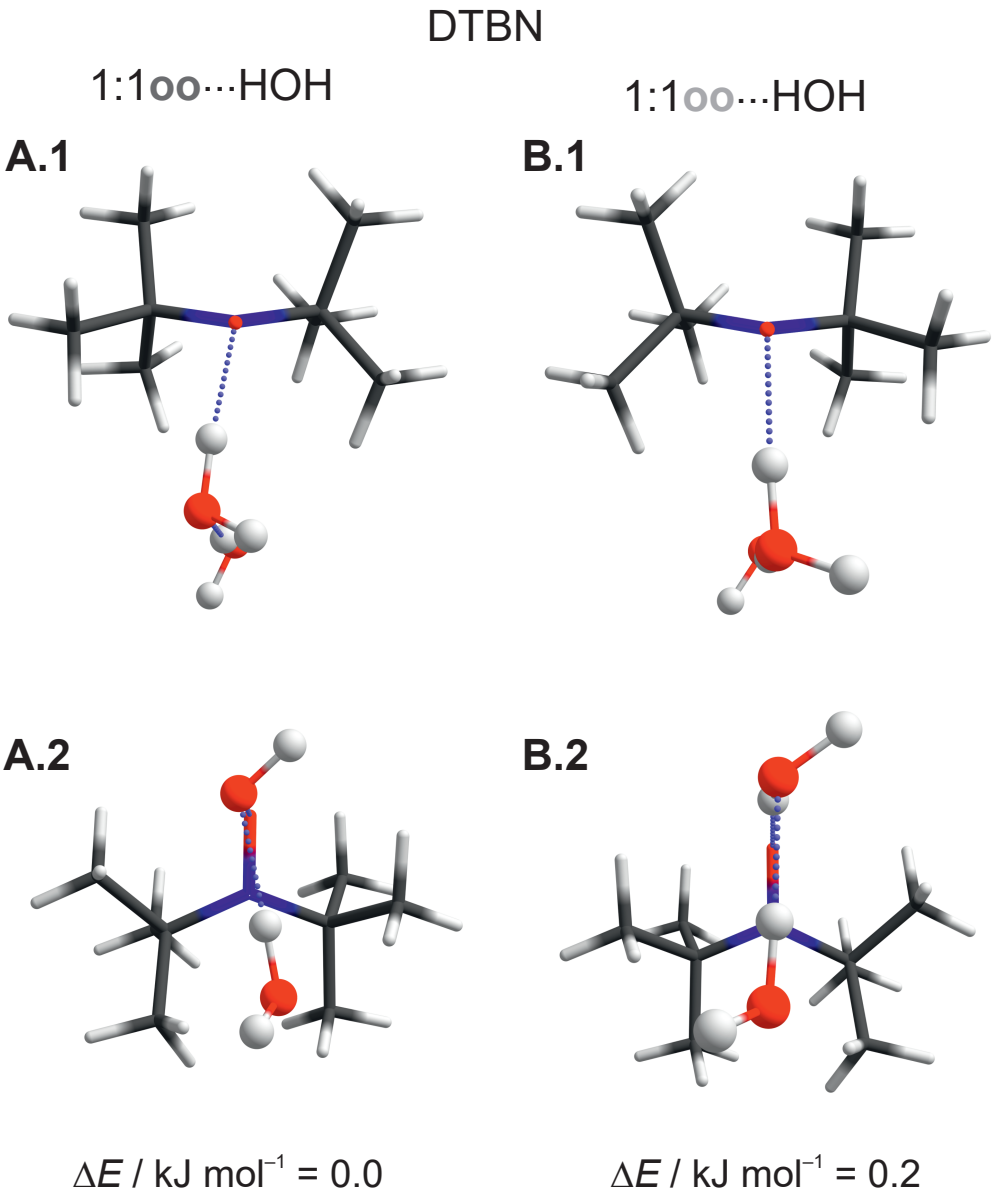


**Figure S1:** Structure of DTBN 1:2 water solvates (A and B) shown from two different perspectives on the top (A.1 and B.1) and on the bottom (A.2 and B.2) of the figure.

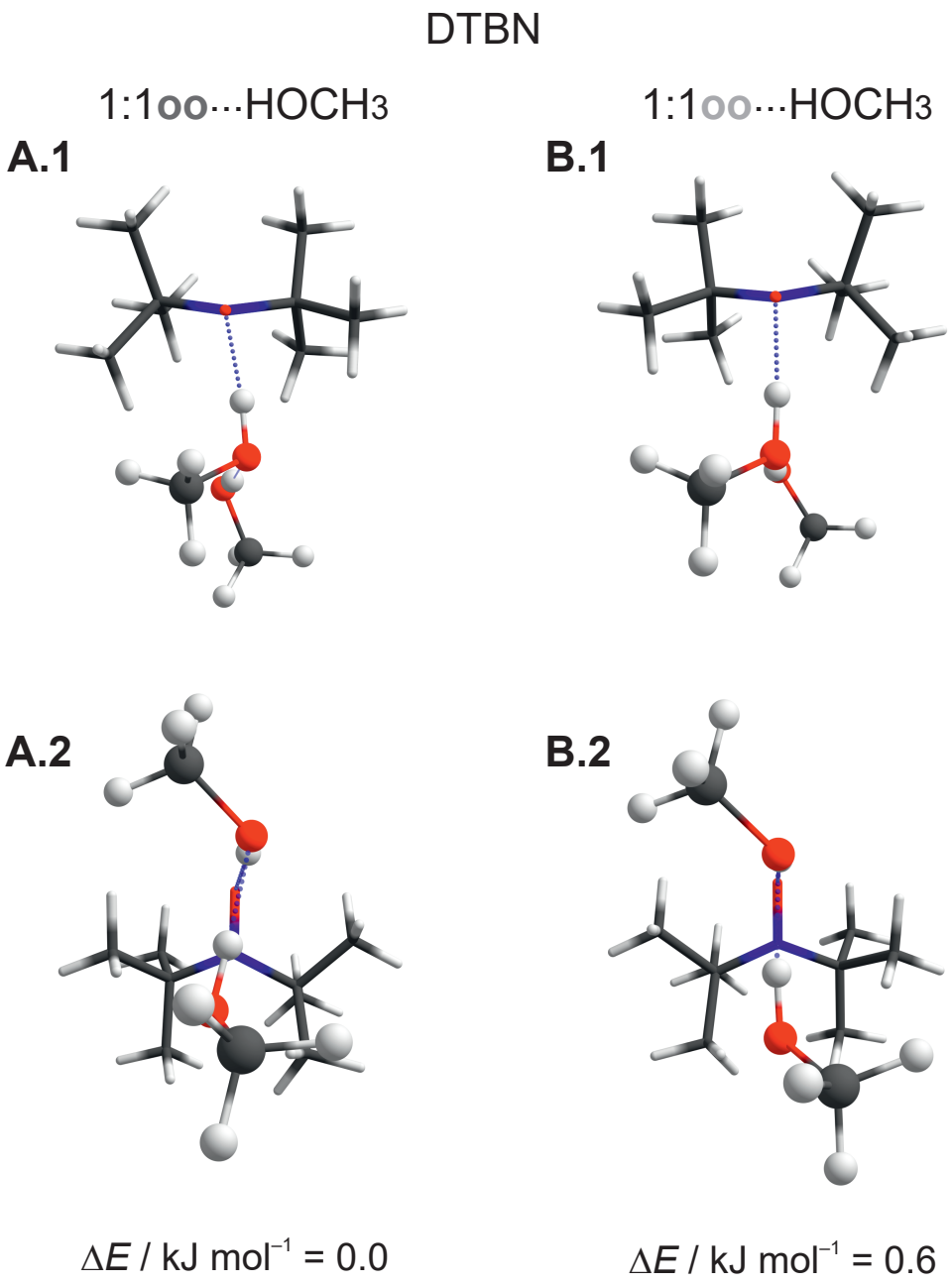


**Figure S2:** Structure of DTBN 1:2 methanol solvates (A and B) shown from two different perspectives on the top (A.1 and B.1) and on the bottom (A.2 and B.2) of the figure.

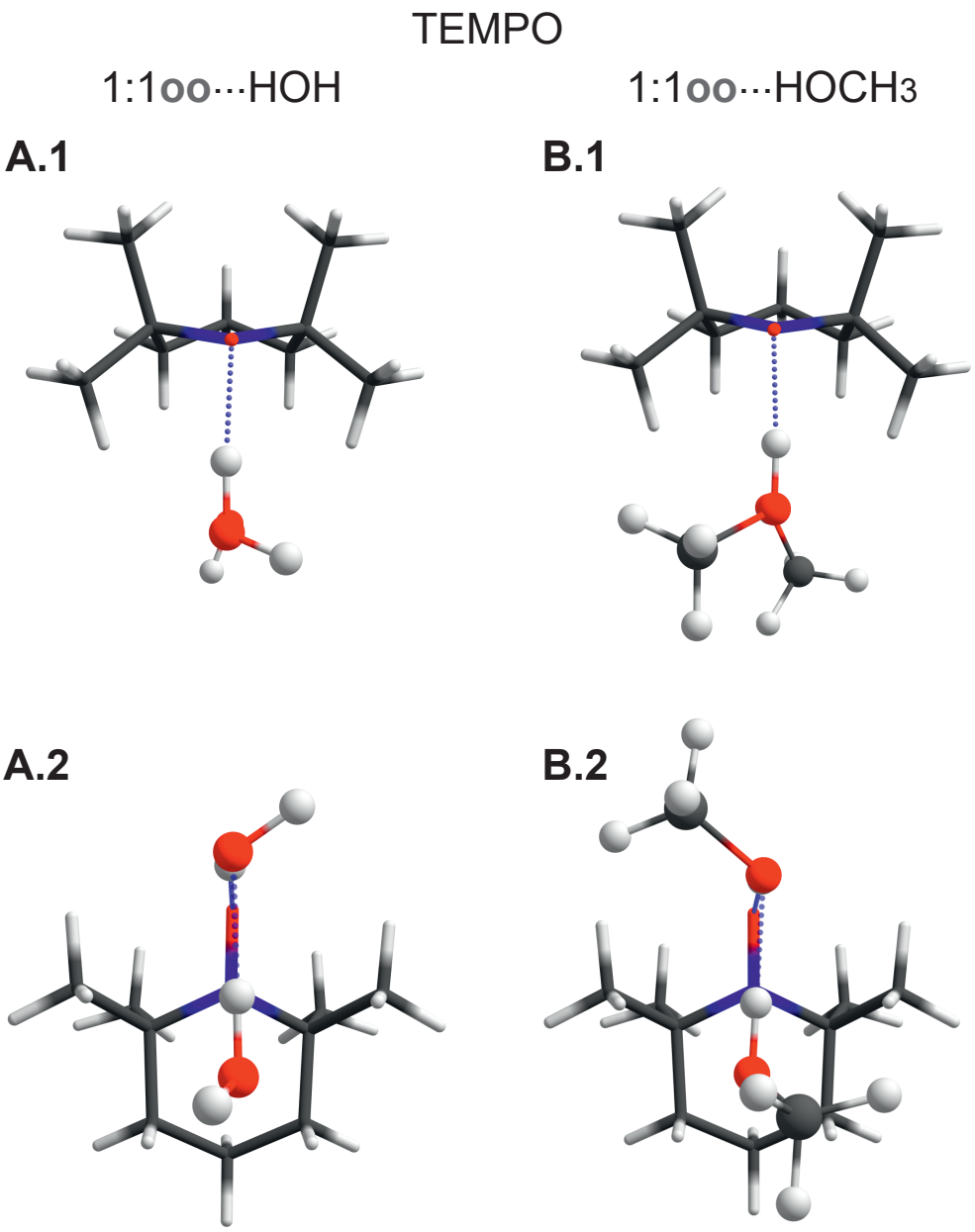


**Figure S3:** Structure of TEMPO 1:2 water and methanol solvates (A and B) from two different perspectives on the top (A.1 and B.1) and on the bottom (A.2 and B.2) of the figure.

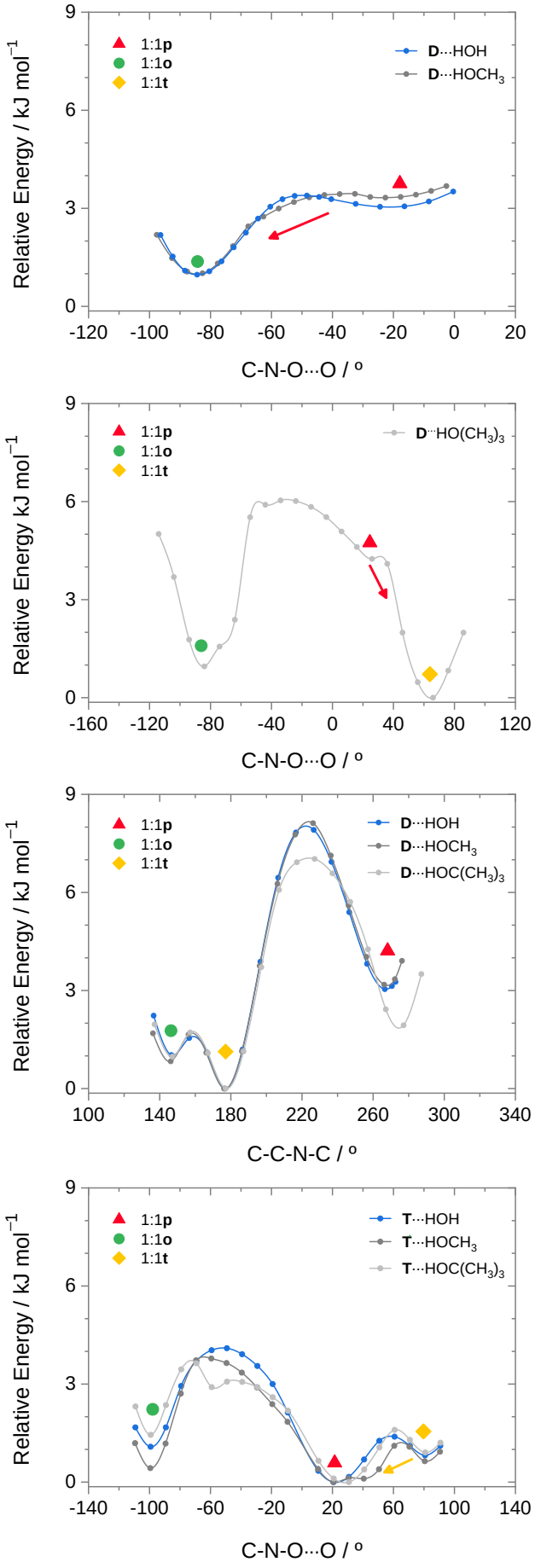


**Figure S4:** Barriers between the different conformations of monosolvates of DTBN and TEMPO, showing that relaxation from p to o/t (red arrows) for DTBN and also from t to p for TEMPO (yellow arrow) is feasible, when there is a driving force. For color definitions, see figures in the main text. C-C-N-C is the torsion of the *t*-butyl groups of the radical, which also provides a path to switch the monohydrate conformations.

## 1.4 Solvation energies

Absolute and relative computed energies are given in Table S17 for checking purposes for the unrestricted open-shell B3LYP calculations.

**Table S17:** Electronic energies $E_{el}$ (in $E_h$), zero-point vibrational energies ZPVE (in $E_h$), and relative zero-point corrected relative energies $\Delta E_0$ (in kJ mol$^{-1}$, conversion factor 2625.49963948 kJ mol$^{-1}$/$E_h$) of the DTBN and TEMPO 1:1 and 1:2 complexes obtained at unrestricted open-shell B3LYP-D3(BJ,ABC)/def2-TZVP level and improved by DLPNO-CCSD(T)/aug-cc-pVTZ electronic energies at the B3LYP-D3(BJ,ABC)/def2-TZVP-optimized structures

| | $E_{el}^{UB3LYP}$ ($E_h$) | ZPVE ($E_h$) | $\Delta E_0^{UB3LYP}$ (kJ mol$^{-1}$) | $E_{el}^{DLPNO}$ ($E_h$) | $\Delta E_0^{DLPNO}$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|
| DTBN | | | | | |
| t···HOH | -521.96286462 | 0.27668926 | 0.0 | -521.21769281 | 0.0 |
| o···HOH | -521.96251528 | 0.27661049 | 0.7 | -521.21748477 | 0.3 |
| p···HOH | -521.96178146 | 0.27665978 | 2.8 | -521.21690572 | 2.0 |
| | | | | | |
| oo···HOH | -598.40683952 | 0.30182280 | 0.0 | -597.57508481 | 0.0 |
| oo···HOH | -598.40668750 | 0.30174471 | 0.2 | -597.57463966 | 1.0 |
| | | | | | |
| t···HOCH$_3$ | -561.24950408 | 0.30564064 | 0.0 | -560.43854376 | 0.0 |
| o···HOCH$_3$ | -561.24916050 | 0.30558674 | 0.8 | -560.43828409 | 0.7 |
| p···HOCH$_3$ | -561.24834478 | 0.30555387 | 2.8 | -560.43746986 | 2.7 |
| | | | | | |
| oo···HOCH$_3$ | -676.98087451 | 0.35931741 | 0.0 | -676.0181413 | 0.0 |
| oo···HOCH$_3$ | -676.98044578 | 0.35912118 | 0.6 | -676.0177608 | 0.5 |
| | | | | | |
| t···HOC(CH$_3$)$_3$ | -679.17608407 | 0.38946091 | 0.0 | -678.1838391 | 0.0 |
| o···HOC(CH$_3$)$_3$ | -679.17572965 | 0.38934704 | 0.6 | -678.1833769 | 0.9 |
| p···HOC(CH$_3$)$_3$ | -679.17531484 | 0.38952238 | 2.2 | -678.1829846 | 2.4 |
| | | | | | |
| TEMPO | | | | | |
| t···HOH | -560.07574018 | 0.28533849 | 0.0 | -559.2703389 | 0.5 |
| o···HOH | -560.07558957 | 0.28532752 | 0.4 | -559.2704849 | 0.1 |
| p···HOH | -560.07594089 | 0.28554610 | 0.0 | -559.2707348 | 0.0 |
| | | | | | |
| t···HOCH$_3$ | -599.36238799 | 0.31424650 | 0.0 | -598.4908260 | 0.7 |
| o···HOCH$_3$ | -599.36242930 | 0.31443855 | 0.4 | -598.4912241 | 0.1 |
| p···HOCH$_3$ | -599.36258800 | 0.31447788 | 0.1 | -598.4913199 | 0.0 |
| | | | | | |
| t···HOC(CH$_3$)$_3$ | -717.28907136 | 0.39819014 | 0.4 | -716.2362657 | 0.7 |
| o···HOC(CH$_3$)$_3$ | -717.28890734 | 0.39815167 | 0.7 | -716.2362761 | 0.5 |
| p···HOC(CH$_3$)$_3$ | -717.28942010 | 0.39839686 | 0.0 | -716.2367251 | 0.0 |
| | | | | | |
| p'···HOC$_6$H$_5$ | -791.08351286 | 0.36760684 | 0.9 | -789.8887915 | 1.4 |
| o···HOC$_6$H$_5$ | -791.08325220 | 0.36743067 | 1.2 | -789.8885185 | 1.7 |
| p···HOC$_6$H$_5$ | -791.08388021 | 0.36761840 | 0.0 | -789.8893473 | 0.0 |

## 1.5 Fragment energies

**Table S18:** Electronic energies $E_{el}$ (in $E_h$) and zero-point vibrational energies (in $E_h$) of DTBN, TEMPO, water, methanol, t-butanol and phenol monomers and selected dimers and trimers obtained at closed-shell and unrestricted open-shell B3LYP-D3(BJ,ABC)/def2-TZVP.

| | $E_{el}^{B3LYP/TZVP}$ ($E_h$) | ZPVE ($E_h$) |
|---|---|---|
| $H_2O$ monomer | -76.42649306 | 0.02115550 |
| $H_2O$ dimer | -152.86285904 | 0.04573284 |
| $H_2O$ trimer | -229.31062345 | 0.07271290 |
| $HOCH_3$ monomer | -115.71252120 | 0.05099693 |
| $HOCH_3$ dimer | -231.43594570 | 0.10426402 |
| $HOCH_3$ trimer | -347.17004218 | 0.15883233 |
| $HOC(CH_3)_3$ monomer | -233.63844773 | 0.13502409 |
| $HOC(CH_3)_3$ dimer | -467.29008951 | 0.27221408 |
| $HOC_6H_5$ monomer | -307.42934517 | 0.10422733 |
| $HOC_6H_5$ dimer | -614.87094233 | 0.21017281 |
| DTBN monomer | -445.52258443 | 0.25255897 |
| TEMPO monomer | -483.63642104 | 0.26144033 |

## 1.6 Dissociation energies

**Table S19:** Dissociation energies of DTBN and TEMPO solvates (in kJ mol$^{-1}$), determined by the difference between the electronic energies of the solvates $E^{AB}$ (in kJ mol$^{-1}$) and the sum of the electronic energies of the 1:0 and 0:1 monomers $E^A + E^B$ (in kJ mol$^{-1}$) obtained at closed- and unrestricted open-shell B3LYP-D3(BJ,ABC)/def2-TZVP. The corresponding ZPVE-corrected results are also included.

| | $E_{el}^A + E_{el}^B$ (kJ mol$^{-1}$) | $E_0^A + E_0^B$ (kJ mol$^{-1}$) | $E_{el}^{AB}$ (kJ mol$^{-1}$) | $E_0^{AB}$ (kJ mol$^{-1}$) | $\Delta E_{el}$ (kJ mol$^{-1}$) | $\Delta E_0$ (kJ mol$^{-1}$) |
|---|---|---|---|---|---|---|
| DTBN | | | | | | |
| t···$H_2O$ | -1370377.115 | -1369658.478 | -1370413.313 | -1369686.865 | 36.2 | 28.4 |
| o···$H_2O$ | -1370377.115 | -1369658.478 | -1370412.396 | -1369686.155 | 35.3 | 27.7 |
| p···$H_2O$ | -1370377.115 | -1369658.478 | -1370410.469 | -1369684.099 | 33.4 | 25.6 |
| t···$HOCH_3$ | -1473522.567 | -1472725.582 | -1473560.371 | -1472757.911 | 37.8 | 32.3 |
| o···$HOCH_3$ | -1473522.567 | -1472725.582 | -1473559.469 | -1472757.151 | 36.9 | 31.6 |
| p···$HOCH_3$ | -1473522.567 | -1472725.582 | -1473557.327 | -1472755.095 | 34.8 | 29.5 |
| t···$HOC(CH_3)_3$ | -1783137.045 | -1782119.446 | -1783176.564 | -1782154.034 | 39.5 | 34.6 |
| o···$HOC(CH_3)_3$ | -1783137.045 | -1782119.446 | -1783175.633 | -1782153.403 | 38.6 | 34.0 |
| p···$HOC(CH_3)_3$ | -1783137.045 | -1782119.446 | -1783174.544 | -1782151.853 | 37.5 | 32.4 |
| TEMPO | | | | | | |
| t···$H_2O$ | -1470444.979 | -1469703.024 | -1470478.654 | -1469729.498 | 33.7 | 26.5 |
| o···$H_2O$ | -1470444.979 | -1469703.024 | -1470478.258 | -1469729.131 | 33.3 | 26.1 |
| p···$H_2O$ | -1470444.979 | -1469703.024 | -1470479.181 | -1469729.480 | 34.2 | 26.5 |
| t···$HOCH_3$ | -1573590.432 | -1572770.128 | -1573625.734 | -1572800.680 | 35.3 | 30.6 |
| o···$HOCH_3$ | -1573590.432 | -1572770.128 | -1573625.842 | -1572800.284 | 35.4 | 30.2 |
| p···$HOCH_3$ | -1573590.432 | -1572770.128 | -1573626.259 | -1572800.597 | 35.8 | 30.5 |
| t···$HOC(CH_3)_3$ | -1883204.909 | -1882163.992 | -1883242.198 | -1882196.750 | 37.3 | 32.8 |
| o···$HOC(CH_3)_3$ | -1883204.909 | -1882163.992 | -1883241.768 | -1882196.421 | 36.9 | 32.4 |
| p···$HOC(CH_3)_3$ | -1883204.909 | -1882163.992 | -1883243.114 | -1882197.123 | 38.2 | 33.1 |
| p···$HOC_6H_5$ | -2076942.884 | -2075982.824 | -2076990.442 | -2076025.260 | 47.6 | 42.4 |
| p'···$HOC_6H_5$ | -2076942.884 | -2075982.824 | -2076989.478 | -2076024.326 | 46.6 | 41.5 |
| o···$HOC_6H_5$ | -2076942.884 | -2075982.824 | -2076988.793 | -2076024.104 | 45.9 | 41.3 |

## 1.7 LED analysis

To further analyze how intermolecular interactions contribute to the different torsional potentials of water around the N-O bond in DTBN complexes, a LED-analysis with DLPNO-CCSD(T)/aug-cc-pVTZ method[27] of London dispersion contributions was carried out for the DFT-optimized 1:1 structures (Tables S20, S21, S22). The energy results are summarized in Table S23, relative to the most stable isomer of each complex, with and without DFT ZPVE added. One can see that the relative ZPVE correction is larger for TEMPO complexes, often reaching the same order of magnitude as the relative London dispersion contributions. Therefore we do not discuss the trends in detail, although we note that for phenol the London dispersion appears to switch between two p-type structures. For DTBN complexes, the ZPVE corrections are less isomer dependent and one can observe that for water and methanol, London dispersion favours t structures relative to p structures. For the bulky *t*-BuOH solvent, the p structure is always less stable than t, but surprisingly more so without London dispersion. No systematic trends spanning all solvent molecules can be identified.

**Table S20:** Selected results (in $E_h$) of the LED analysis carried out at the stationary points of the 1:1 DTBN solvates at unrestricted open-shell DLPNO-CCSD(T)/aug-cc-pVTZ//UB3LYP-D3(BJ,ABC)/def2-TZVP level.

| DTBN | 1:1 t···HOH | 1:1 p···HOH | 1:1 o···HOH |
|---|---|---|---|
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -442.7573065 | -442.7703945 | -442.762830 |
| Intra fragment 2 (REF.) | -76.03750343 | -76.03289252 | -76.03895266 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.062534701 | -0.057779186 | -0.05739387 |
| Exchange (REF.) | -0.014267003 | -0.011123090 | -0.012551217 |
| Dispersion (strong pairs) | -0.005604805 | -0.004861762 | -0.005659446 |
| Dispersion (weak pairs) | -0.000545353 | -0.000462412 | -0.000508010 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -2.244406263 | -2.244074384 | -2.244117794 |
| Non dispersion (weak pairs) | -0.004765617 | -0.004774328 | -0.004785124 |
| DTBN | 1:1 t···$HOCH_3$ | 1:1 p···$HOCH_3$ | 1:1 o···$HOCH_3$ |
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -442.7533988 | -442.7675394 | -442.7601312 |
| Intra fragment 2 (REF.) | -115.0675475 | -115.0626008 | -115.0690439 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.066235627 | -0.06145750 | -0.060183104 |
| Exchange (REF.) | -0.015689296 | -0.012051509 | -0.01361650 |
| Dispersion (strong pairs) | -0.006578470 | -0.005287371 | -0.006549331 |
| Dispersion (weak pairs) | -0.000868431 | -0.000758636 | -0.000818655 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -2.425417711 | -2.425236011 | -2.425182645 |
| Non dispersion (weak pairs) | -0.004952238 | -0.004953941 | -0.004986028 |
| DTBN | 1:1 t···$HOC(CH_3)_3$ | 1:1 p···$HOC(CH_3)_3$ | 1:1 o···$HOC(CH_3)_3$ |
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -442.7528284 | -442.7631036 | -442.7604928 |
| Intra fragment 2 (REF.) | -232.2207066 | -232.2158289 | -232.2230918 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.068353742 | -0.063892714 | -0.060854324 |
| Exchange (REF.) | -0.016522026 | -0.014707930 | -0.014132134 |
| Dispersion (strong pairs) | -0.007835535 | -0.008223963 | -0.007582220 |
| Dispersion (weak pairs) | -0.001630381 | -0.001642262 | -0.001572660 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -2.988801968 | -2.988459727 | -2.988595161 |
| Non dispersion (weak pairs) | -0.005830899 | -0.005834088 | -0.005836789 |

**Table S21:** Selected results (in $E_h$) of the LED analysis carried out at the stationary points of the 1:1 TEMPO solvates at DLPNO-CCSD(T)/aug-cc-pVTZ level

| TEMPO | 1:1 t···HOH | 1:1 p···HOH | 1:1 o···HOH |
|---|---|---|---|
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -480.6546869 | -480.6657798 | -480.6633423 |
| Intra fragment 2 (REF.) | -76.03852119 | -76.03232582 | -76.04081553 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.061153338 | -0.059475289 | -0.052839170 |
| Exchange (REF.) | -0.014098292 | -0.011568815 | -0.011696286 |
| Dispersion (strong pairs) | -0.004869395 | -0.004779702 | -0.004953241 |
| Dispersion (weak pairs) | -0.000562829 | -0.00047226 | -0.000533904 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -2.392591648 | -2.392486622 | -2.392416424 |
| Non dispersion (weak pairs) | -0.005207015 | -0.005261219 | -0.005284910 |
| TEMPO | 1:1 t···$HOCH_3$ | 1:1 p···$HOCH_3$ | 1:1 o···$HOCH_3$ |
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -480.6502307 | -480.6633663 | -480.6602110 |
| Intra fragment 2 (REF.) | -115.068248 | -115.0623423 | -115.0708819 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.065761478 | -0.062525035 | -0.055972490 |
| Exchange (REF.) | -0.015620611 | -0.012352595 | -0.012971215 |
| Dispersion (strong pairs) | -0.005582021 | -0.005518503 | -0.006004878 |
| Dispersion (weak pairs) | -0.000894144 | -0.000800089 | -0.000862026 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -2.573527319 | -2.573427182 | -2.573311708 |
| Non dispersion (weak pairs) | -0.005387701 | -0.005439193 | -0.005479905 |
| TEMPO | 1:1 t···$HOC(CH_3)_3$ | 1:1 p···$HOC(CH_3)_3$ | 1:1 o···$HOC(CH_3)_3$ |
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -480.6497781 | -480.6608265 | -480.6605541 |
| Intra fragment 2 (REF.) | -232.2212308 | -232.2152479 | -232.2246057 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.067506215 | -0.065446805 | -0.057196065 |
| Exchange (REF.) | -0.016619790 | -0.014053707 | -0.013440133 |
| Dispersion (strong pairs) | -0.007413012 | -0.007471197 | -0.006929736 |
| Dispersion (weak pairs) | -0.001573479 | -0.001563031 | -0.001551763 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -3.136619020 | -3.136575602 | -3.13653382 |
| Non dispersion (weak pairs) | -0.006279348 | -0.006328804 | -0.006354168 |

**Table S22:** Selected results (in $E_h$) of the LED analysis carried out at the stationary points of the 1:1 TEMPO solvates at DLPNO-CCSD(T)/aug-cc-pVTZ level

| TEMPO | 1:1 t···$HOC_6H_5$ | 1:1 p···$HOC_6H_5$ | 1:1 o···$HOC_6H_5$ |
|---|---|---|---|
| FINAL SUMMARY DLPNO-CCSD ENERGY DECOMPOSITION (Eh) | | | |
| Intrafragment REF. energy: | | | |
| Intra fragment 1 (REF.) | -480.6550902 | -480.6528033 | -480.6461734 |
| Intra fragment 2 (REF.) | -305.6345063 | -305.6322632 | -305.6424592 |
| Interaction of fragments 2 and 1: | | | |
| Electrostatics (REF.) | -0.078625582 | -0.08038416 | -0.077489731 |
| Exchange (REF.) | -0.014842611 | -0.01620787 | -0.016720264 |
| Dispersion (strong pairs) | -0.007489209 | -0.008828952 | -0.007630852 |
| Dispersion (weak pairs) | -0.001446703 | -0.001573852 | -0.001555936 |
| Sum of non dispersive correlation terms: | | | |
| Non dispersion (strong pairs) | -3.339684621 | -3.339961566 | -3.339423483 |
| Non dispersion (weak pairs) | -0.006856432 | -0.006823132 | -0.006816266 |

**Table S23:** Relative electronic energies ($\Delta E$ in kJ mol$^{-1}$) for different 1:1 complex conformations and relative electronic energies without London Dispersion (LD) terms (strong and weak-pairs) obtained from a LED analysis. The calculations were carried out at DLPNO-CCSD(T)/aug-cc-pVTZ//UB3LYP/def2-TZVP level. For comparison, the effect of DFT ZPVE correction on the relative DLPNO-CCSD(T) energies is also given as $\Delta E_0$.

| DTBN + $H_2O$ | 1:1 t | 1:1 p | 1:1 o |
|---|---|---|---|
| $\Delta E$ | 0.0 | 2.1 | 0.5 |
| $\Delta E_0$ | 0.0 | 2.0 | 0.3 |
| $\Delta E$ (without LD term) | 0.1 | 0.0 | 0.7 |
| DTBN + $HOCH_3$ | | | |
| $\Delta E$ | 0.0 | 2.8 | 0.7 |
| $\Delta E_0$ | 0.0 | 2.7 | 0.7 |
| $\Delta E$ (without LD term) | 0.9 | 0.0 | 1.3 |
| DTBN + $HOC(CH_3)_3$ | | | |
| $\Delta E$ | 0.0 | 2.2 | 1.2 |
| $\Delta E_0$ | 0.0 | 2.4 | 0.9 |
| $\Delta E$ (without LD term) | 0.0 | 3.3 | 0.4 |
| TEMPO + $H_2O$ | 1:1 t | 1:1 p | 1:1 o |
| $\Delta E$ | 1.0 | 0.0 | 0.7 |
| $\Delta E_0$ | 0.5 | 0.0 | 0.1 |
| $\Delta E$ (without LD term) | 1.5 | 0.0 | 1.3 |
| TEMPO + $HOCH_3$ | | | |
| $\Delta E$ | 1.3 | 0.0 | 0.3 |
| $\Delta E_0$ | 0.7 | 0.0 | 0.1 |
| $\Delta E$ (without LD term) | 1.7 | 0.0 | 1.7 |
| TEMPO + $HOC(CH_3)_3$ | | | |
| $\Delta E$ | 1.2 | 0.0 | 1.2 |
| $\Delta E_0$ | 0.7 | 0.0 | 0.5 |
| $\Delta E$ (without LD term) | 1.4 | 0.3 | 0.0 |
| TEMPO + $HOC_6H_5$ | 1:1 p' | 1:1 p | 1:1 o |
| $\Delta E$ | 1.5 | 0.0 | 2.2 |
| $\Delta E_0$ | 1.4 | 0.0 | 1.7 |
| $\Delta E$ (without LD term) | 0.0 | 2.4 | 1.4 |

# 2 Experimental and Computed Spectra

## 2.1 Measurement details

Previous gratin jet measurements[28]:

TEMPO and DTBN hydrate complexes were prepared in supersonic jet expansions through a 0.2 mm × 700 mm slit nozzle at a stagnation pressure of 750 mbar. $CaF_2$ optics, an optical filter (F20: wavenumber range <4000 $cm^{-1}$), an InSb/HgCdTe detector, a 150 W tungsten lamp and a VERTEX 70v FTIR spectrometer (scanning speed 140 kHz, double sided mode, 2 $cm^{-1}$ resolution) were used to probe the gas pulses. A more detailed description of the experimental setup can be found in Ref.[29].

Current filet jet measurements:

The new spectra reported in this work were obtained in supersonic jet expansions through a 0.2 mm × 600 mm slit nozzle from gas mixtures prepared in a 67 L reservoir at a stagnation pressure of 750 mbar and at room temperature. Continuous pumping and large vacuum buffers with a volume of 23 $m^3$ allowed for a sufficiently low background pressure during the experiment. A liquid nitrogen-cooled InSb detector, a 150 W tungsten lamp, $CaF_2$ optics, and an optical filter (2500 to 4100 $cm^{-1}$) were employed in a Bruker IFS 66v/S FTIR spectrometer (scanning speed 80 kHz with gain ranging, 2 $cm^{-1}$ resolution) to probe the gas pulses. A more detailed description of the experimental setup can be found in Ref.[30]

**Table S24:** The spectra shown in Fig. 4 and Fig. 5 of the manuscript are the average of # gas pulses recorded on the dates dd/mm/yyyy using different setups. Further spectra recorded to find the best expansion conditions and to support the identity of absorption features in terms of cluster stoichiometry are not listed.

| Spectrum | # | Setup | dd/mm/yyyy | Figure |
|---|---|---|---|---|
| DTBN + $H_2O$ | 150 | Filet Jet | 22/10/2021 | 4 |
| DTBN + $HOCH_3$ | 100 | Filet Jet | 21/09/2021 | 4 |
| TEMPO + $H_2O$ [28] | 900 | Gratin Jet | 19/01/2021 | 4 |
| TEMPO + $HOCH_3$ | 500 | Filet Jet | 23/04/2021 | 4 |
| DTBN + $HOC(CH_3)_3$ | 300 | Filet Jet | 14/12/2021 | 5 |
| 150 scans (14/12/2021) *plus* 150 scans (15/11/2021) | | | 15/12/2021 | |
| TEMPO + $HOC(CH_3)_3$ | 125 | Filet Jet | 19/05/2021 | 5 |
| TEMPO + $HOC_6H_5$ | 575 | Filet Jet | 11/05/2021 | 5 |

**Table S25:** Relative scaling of spectra shown in Fig. 4 and Fig. 5 of the manuscript.

| Spectrum | Figure | Scaling factor |
|---|---|---|
| DTBN + $H_2O$ | 4 | $\frac{7}{10}$ (21/10/2021) |
| DTBN + $HOCH_3$ | 4 | $\frac{3}{10}$ (21/09/2021) |
| TEMPO + $H_2O$ [28] | | (19/01/2021) |
| TEMPO + $HOCH_3$ | 4 | $\frac{1}{2}$ (23/04/2021) |
| 4 DTBN + $HOC(CH_3)_3$ | 5 | $\frac{7}{10}$ (14/12/2021 + 15/12/2021) |
| TEMPO + $HOC(CH_3)_3$ | 5 | $\frac{3}{5}$ (19/05/2021) |
| TEMPO + $HOC_6H_5$ | 5 | $\frac{3}{5}$ (11/05/2021) |

## 2.2 Comparison to computations

**Table S26:** Experimental wavenumbers of DTBN and TEMPO complexes (in $cm^{-1}$) along with the unscaled computed wavenumbers $\tilde{\nu}$ (in $cm^{-1}$) and absolute infrared intensities $I$ (in km $mol^{-1}$) at unrestricted open-shell B3LYP-D3(BJ,ABC)/def2-TZVP level.

| Structure | Experiment $\tilde{\nu}$ | Computed $\tilde{\nu}$ | $I$ |
|---|---|---|---|
| DTBN + $H_2O$ | | | |
| t···HOH | 3483.5 | 3578 | 382 |
| o···HOH | 3509 | 3600 | 339 |
| p···HOH | - | 3594 | 556 |
| oo···HOH (dark grey) | -/3389 | 3528/3435 | 489/613 |
| oo···HOH (light grey) | -/3389 | 3537/3452 | 484/579 |
| DTBN + $HOCH_3$ | | | |
| t···H$OCH_3$ | 3469.5 | 3575 | 523 |
| o···H$OCH_3$ | 3496 | 3601 | 471 |
| p···H$OCH_3$ | - | 3593 | 750 |
| oo···H$OCH_3$ (dark grey) | 3415/3352 | 3498/3436 | 731/664 |
| oo···H$OCH_3$ (light grey) | 3415/3352 | 3515/3452 | 751/645 |
| DTBN + $HOC(CH_3)_3$ | | | |
| t···H$OC(CH_3)_3$ | 3438.5 | 3569 | 503 |
| o···H$OC(CH_3)_3$ | - | 3601 | 462 |
| p···H$OC(CH_3)_3$ | - | 3604 | 522 |
| TEMPO + $H_2O$ | | | |
| t···HOH | - | 3589 | 405 |
| o···HOH | 3521 | 3620 | 347 |
| p···HOH | 3497 | 3583 | 587 |
| oo···HOH | 3486/3399 | 3535/3459 | 497/483 |
| TEMPO + $HOCH_3$ | | | |
| t···H$OCH_3$ | - | 3583 | 549 |
| o···H$OCH_3$ | 3509 | 3619 | 481 |
| p···H$OCH_3$ | 3490 | 3590 | 710 |
| oo···H$OCH_3$ | 3416/3365 | 3513/3458 | 769/513 |
| TEMPO + $HOC(CH_3)_3$ | | | |
| t···H$OCH(CH_3)_3$ | - | 3582 | 496 |
| o···H$OCH(CH_3)_3$ | - | 3616 | 485 |
| p···H$OCH(CH_3)_3$ | 3463 | 3585 | 618 |
| TEMPO + $HOC_6H_5$ | | | |
| o···H$OC_6H_5$ | 3360 | 3490 | 1059 |
| p···H$OC_6H_5$ | 3348 | 3478 | 1101 |
| p'···H$OC_6H_5$ | 3348? | 3475 | 1314 |

**Table S27:** Computed wavenumbers of DTBN and TEMPO complexes (in $cm^{-1}$) with unrestricted open-shell B3LYP-D3(BJ,ABC), B2PLYP-D3 and TPSS-D3(BJ) functionals using different basis sets.

| Structure | B3LYP def2-QZVP $\tilde{\nu}$ | B2PLYP def2-TZVP $\tilde{\nu}$ | TPSS def2-TZVP $\tilde{\nu}$ | TPSS def2-QZVP $\tilde{\nu}$ |
|---|---|---|---|---|
| DTBN + $H_2O$ | | | | |
| t···HOH | 3592 | 3614 | 3426 | 3435 |
| o···HOH | 3610 | 3640 | 3454 | 3457 |
| p···HOH | 3608 | 3634 | 3449 | 3454 |
| DTBN + $HOCH_3$ | | | | |
| t···H$OCH_3$ | 3594 | 3608 | 3415 | 3424 |
| o···H$OCH_3$ | 3617 | 3638 | 3443 | 3452 |
| p···H$OCH_3$ | 3613 | 3629 | 3445 | 3457 |
| DTBN + $HOC(CH_3)_3$ | | | | |
| t···H$OC(CH_3)_3$ | 3587 | 3584 | 3403 | 3415 |
| o···H$OC(CH_3)_3$ | 3618 | 3621 | 3436 | 3446 |
| p···H$OC(CH_3)_3$ | 3619 | 3619 | 3444 | 3451 |
| TEMPO + $H_2O$ | | | | |
| o···HOH | 3630 | 3655 | 3484 | 3485 |
| p···HOH | 3597 | 3621 | 3438 | 3443 |
| t···H$OH_3$ | 3630 | 3655 | 3484 | 3485 |
| TEMPO + $HOCH_3$ | | | | |
| o···H$OCH_3$ | 3635 | 3650 | 3462 | 3469 |
| p···H$OCH_3$ | 3603 | 3621 | 3439 | 3449 |
| t···H$OCH_3$ | 3635 | 3650 | 3462 | 3469 |
| TEMPO + $HOC(CH_3)_3$ | | | | |
| o···H$OCH(CH_3)_3$ | 3633 | 3635 | 3456 | 3467 |
| p···H$OCH(CH_3)_3$ | 3603 | 3601 | 3426 | 3438 |
| t···H$OCH(CH_3)_3$ | 3633 | 3635 | 3456 | 3467 |
| TEMPO + $HOC_6H_5$ | | | | |
| o···H$OC_6H_5$ | 3508 | 3513 | 3330 | 3348 |
| p···H$OC_6H_5$ | 3494 | 3501 | 3306 | 3314 |
| p'···H$OC_6H_5$ | 3492 | 3497 | 3304 | 3315 |

## 2.3 Closed shell reference data

**Table S28:** Experimental hydrogen-bonded ($OH_b$) stretching wavenumbers of water, methanol, tert-butanol and phenol dimers and trimers along with the harmonic B3LYP-D3(BJ)/def2-TZVP computed values.

| | He-jet [31–35] $\tilde{\nu}$ | B3LYP-D3(BJ,ABC)/def2-TZVP $\tilde{\nu}$ |
|---|---|---|
| $OH_b$ ($H_2O$ dimer) | 3602 | 3666 |
| $OH_b$ ($H_2O$ trimer) | 3533 | 3574/3564 |
| $OH_b$ ($HOCH_3$ dimer) | 3575 | 3647 |
| $OH_b$ ($HOCH_3$ trimer) | 3474/3469 | 3548/3542 |
| $OH_b$ ($HOC(CH_3)_3$ dimer) | 3497 | 3609 |
| $OH_b$ ($HOC_6H_5$ dimer) | 3530 | 3647 |

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