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Heme Models

A Cytochrome P450 TxtE Model System with Mechanistic and Theoretical Evidence for a Heme Peroxynitrite Active Species

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Abstract: The cytochrome P450 homolog, TxtE, efficiently catalyzes the direct and regioselective aromatic nitration of the indolyl moiety of L-tryptophan to 4-nitro-L-tryptophan, using nitric oxide (NO) and dioxygen (O_2) as co-substrates. Pathways for such direct and selective nitration of heteroaromatic motifs present platforms for engineering new nitration biocatalysts for pharmacologically beneficial targets, among a medley of other pivotal industrial applications. Precise mechanistic details concerning this pathway are only weakly understood, albeit a heme iron(III)-peroxynitrite active species has been postulated. To shed light on this unique reaction landscape, we investigated the indole nitration pathway of a series of biomimetic ferric heme superoxide mimics, $[(Por)Fe^{III}(O_2^{-\bullet})]$, in the presence of NO. Therein, our model systems gave rise to three distinct nitroindole products, including 4-nitroindole, the product analogous to that obtained with TxtE. Moreover, ^{15}N and ^{18}O isotope labeling studies, along with meticulously designed control experiments lend credence to a heme peroxynitrite active nitrating agent, drawing close similarities to the tryptophan nitration mechanism of TxtE. All organic and inorganic reaction components have been fully characterized using spectroscopic methods. Theoretical investigation into several mechanistic possibilities deem a unique indolyl radical based reaction pathway as the most energetically favorable, products of which, are in excellent agreement with experimental findings.

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Introduction

Cytochrome P450 enzymes (Cyt P450s) are a superfamily of heme-containing monooxygenases that encompass some of the most exquisite and versatile biocatalysts in Nature.[1–9] These enzymes play crucial roles in many biosynthetic and biodegradative processes in bacteria that provide access to a wide variety of secondary metabolites with altered bioactivities.[7,10] A majority of these metabolites have already been put to use in human therapeutics; for example, known antibiotics,[11–12] immunosuppressants,[13] and anticancer agents[14–15] encompass these as multifaceted pharmacophores, underscoring the urgency of understanding the subtle details surrounding their biosynthetic pathways. Recently, the discovery of a novel Cyt P450 homologue, TxtE, has been reported in the literature,[16–24] which is central to the eccentric biosynthetic pathway of the secondary metabolite thaxtomin, a phytotoxin produced by plant pathogenic *Streptomyces* species that causes common scab of potato.[25–28] Scab is a disease situation that causes lesions in root vegetables which drastically reduces their marketability, where potato scab is by far the most economically impactful. Thaxtomin A, which inhibits cellulose biosynthesis[28] is predominantly produced by *Streptomyces scabies*, and is essentially effected by the condensation of nitrotryptophan and phenylalanine, followed by a hydroxylation step. (Figure 1A).[29–31] The very first step in this particular pathway involves the direct and regioselective nitration of the indolyl moiety of L-tryptophan (L-Trp) to 4-nitro-L-tryptophan (4-NO_2-Trp; Figure 1A) using nitric oxide (NO)[32] and dioxygen (O_2),[17] which is catalyzed by the aforementioned TxtE P450 enzyme. Indeed, the nitro group of thaxtomin A has been deemed indispensable for its observed virulence against the host. However, the precise mechanistic details surrounding how these primarily monooxygenase enzymes facilitate the high-fidelity insertion of $–NO_2$ groups into various biorelevant organic moieties remain enigmatic to-date.[33] This lack of comprehension in turn severely limits the prospects of corresponding biosynthetic pathways being targeted by prolific bactericides with significant agricultural and health benefits.

On the other hand, facile aromatic nitration is of paramount significance in industry, especially regarding the preparation of dyes, pesticides, food additives, and pharmaceuticals.[34–37] In fact, nitro compounds constitute a broad array of cardinal pharmacophores and are common to numerous building blocks that get integrated into complex drug molecules (e.g., anticancer drug nilutamine, antiparkin-

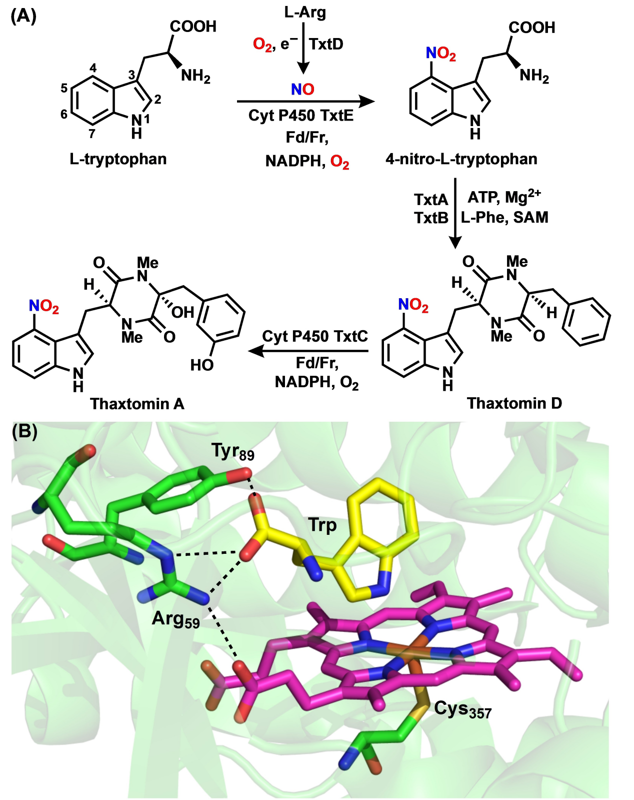
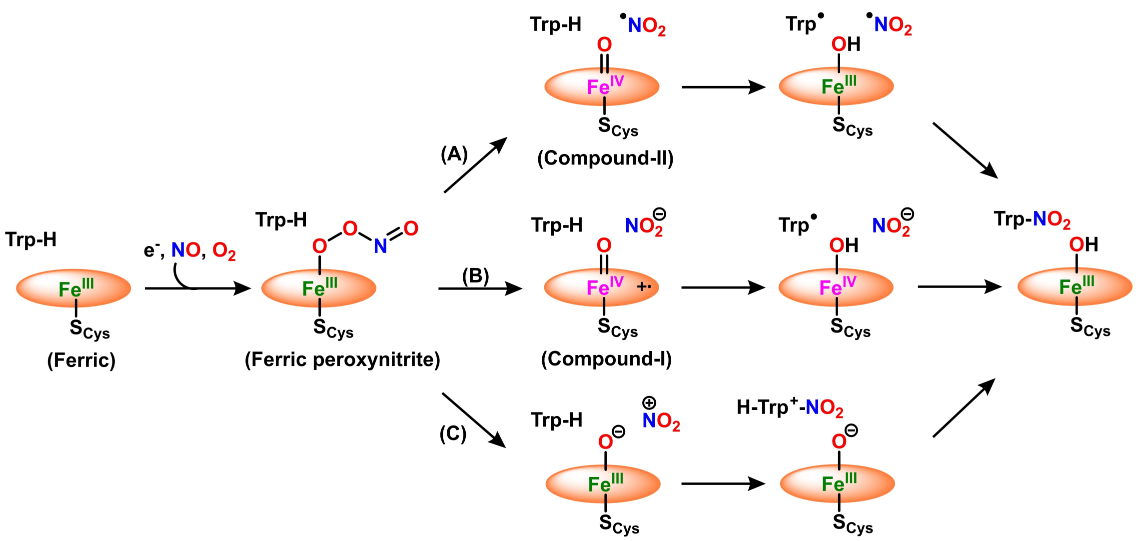


Figure 1. (A) Proposed pathway for thaxtomin A biosynthesis.[17] (B) Substrate (L-tryptophan) bound active site structure of TxtE (PDB: 4TPO)[19] showing the heme cofactor (pink), L-tryptophan (yellow) and other H-bonding (dashed lines) amino acid residues (green).

son agent tolcapone, and antiinfective agent chloramphenicol and the recently approved delamanid[38] and nifurtimox-eflornithine combination).[39] To this end, high-yielding, environmentally benign nitration pathways such as those mediated by enzymatic systems (i.e., using biocatalysis) are of high demand, particularly in light of their exceptional stereo-, regio-, and chemo-selectivities.[22,40] Therefore, the exact mechanistic events of TxtE pose remarkable potential in synthetic biology and directed protein engineering efforts; nonetheless, a comprehensive mechanistic understanding is yet far from complete.

Early insights into the mechanism of nitration by TxtE came from $^{18}O_2$ labeling studies where each of the two oxygen atoms of the nitro group in 4-NO_2-Trp were shown to originate from O_2 and NO.[17] Suitably, several mechanistic proposals have been put forward, all of which invoke a heme ferric peroxynitrite adduct as the active nitrating species (Scheme 1).[16,33,41] Peroxynitrite has been implicated in numerous detrimental pathways that lead to complicated pathological conditions in humans, including neurodegenerative and autoimmune diseases, and various of types of cancers.[74] In light of the ubiquitous nature of heme superoxo (or heme-oxy) species within the physiological space, the momentous significance of heme-based ferric peroxynitrite adducts in pathogenesis has been discussed at length,[74] although a detailed understanding of their reaction mechanisms is largely lacking. Indeed, this deficit in knowledge has been fueled by the extremely transient nature of heme peroxynitrite compounds within both enzymatic systems, as well as in their synthetic analogs.

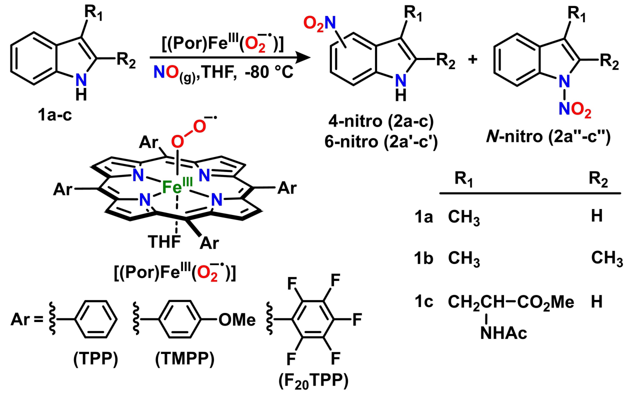
In TxtE, three distinct reaction landscapes[33] via which an active heme peroxynitrite species may facilitate the generation of 4-NO_2-Trp have been described: (1) homolytic O–O bond cleavage to yield $^{\bullet}NO_2$ and an $Fe^{IV}{=}O$ species (i.e., Compound II; Scheme 1, path A), where the latter subsequently engenders the $Trp^{\bullet}$ radical, which then combines with $^{\bullet}NO_2$ to give 4-NO_2-Trp; (2) canonical Cyt P450 type heterolytic O–O bond cleavage yields $P^{+\bullet}Fe^{IV}{=}O$ (Compound I; P = porphyrin supporting ligand) and nitrite (NO_2^-; Scheme 1, path B), wherein Compound I mediates $^{\bullet}$Trp formation, and Compound II converts NO_2^- into $^{\bullet}NO_2$; radical recombination results in 4-NO_2-Trp formation; (3) heterolytic cleavage of the O–O bond (note that the



Scheme 1. Proposed mechanistic possibilities for the nitration of L-tryptophan (Trp-H) to 4-nitro-L-tryptophan mediated by the TxtE enzyme.

electrons now move toward heme) leading to nitronium ion (NO_2^+), which can readily nitrate Trp via electrophilic aromatic substitution (Scheme 1, path C). Recent work from Scrutton, Challis, de Visser and their co-workers further substantiates the involvement of an iron(III)-peroxynitrite intermediate in the TxtE pathway, which splits homolytically to form Compound II and $^{\bullet}NO_2$ radical via a small free energy of activation.[16] The latter activates the substrate on the aromatic ring, while Compound II ultimately picks up the *ipso*-hydrogen forming the 4-NO_2-Trp product. In agreement with these proposals that implicate a heme peroxynitrite active species (which is proposed to form from heme superoxo + NO), the superoxo/oxy intermediate of TxtE has a significantly low 1-electron reduction potential, thwarting its reduction to the peroxo form.[41] How this putative peroxynitrite intermediate of TxtE carries out the high-fidelity Trp nitration circumventing the formation of nitrates is a fascinating unknown,[16] especially since some other heme peroxynitrite intermediates are known to only produce nitrate, but not aromatic nitration.[42] Nitration of Trp within biological systems is however not an unequivocal footprint of peroxynitrite, since: (1) heme peroxidases are known to nitrate L-tryptophan in the presence of NO_2^- and H_2O_2 (i.e., by formation of $^{\bullet}NO_2$ radicals via the single-electron oxidation of NO_2^- to $^{\bullet}NO_2$ by high-valent heme oxidants), although with poor regioselectivity;[43–46] (2) nitric oxide synthase (in conjunction with tRNA synthetase) has been found to carry out the regioselective nitration of L-tryptophan to 4-nitrotryptophan.[47] Furthermore, the $^{\bullet}$Trp radical, upon exposure to free peroxynitrite, has been shown to undergo nitration predominantly generating 6-nitrotryptophan.[48–50] Therefore, it remains to be seen if a ferric peroxynitrite species would definitively be viable as the active catalytic intermediate in TxtE, which choreographs the explicit conversion of Trp to 4-NO_2-Trp.

Small molecule synthetic model systems can be powerful tools in addressing these impactful unknowns,[51–56] and shedding light on pivotal mechanistic events pertaining to the unique nitration reaction landscape driven by TxtE. Markedly, there is *only one* well-defined heme peroxynitrite model system reported in the literature,[57] and whether or not it is able to nitrate a broad scope of substrates outside phenols remains to be studied. In the present investigation, we have employed three structurally similar, yet electronically disparate synthetic heme superoxo complexes (Scheme 2) and have interrogated their competency in nitrating a series of 3-substituted indole substrates (i.e., as Trp mimics) in the presence of NO. Interestingly, we observe a mixture of nitroindole products, including 4-nitroindole, which resembles the 4-NO_2-Trp product of TxtE. Exhaustive mechanistic studies involving (1) ^{18}O- and ^{15}N-isotope labeling, and (2) meticulously designed control experiments, along with (3) in depth computational investigations all unequivocally point to an indole nitration pathway mediated by a short-lived heme peroxynitrite intermediate. To the best of our knowledge, this work marks the first report where metal peroxynitrite intermediates are demonstrated to nitrate indole substrates. Therefore, the present study describes a remarkable synthetic model system



Scheme 2. Generalized reaction depicting the series of electronically divergent heme superoxide intermediates and indole substrates involved in this work.

for the only known Trp nitrating heme enzyme, TxtE. Noteworthily, the nitration of Trp is not only significant with respect to TxtE, but is also central to understanding how Trp might get nitrated under escalated nitrative stress, which is known to lead to some of the most burdensome pathogenic situations known to humans.[58–59] Hence, the detailed spectroscopic, reactivity, and theoretical investigations we describe herein shed light on subtleties that are of prime importance in understanding (1) mechanistic aspects of heme peroxynitrite reactivities with bio-relevant substrates, (2) the development of methodologies that will allow the high-yielding conversion of indoles to nitroindoles, which are multipotent drug candidates, and (3) how heme peroxynitrite mediated biological pathways may be exploited in the design and implementation of novel therapeutic agents. Unfortunately, most of these areas have remained only faintly understood, despite decades of work on both enzymatic systems as well as their synthetic counterparts.

Results and Discussion

Reactivity of [(Por)Fe^{III}($O_2^{-\bullet}$)] Adducts with $NO_{(g)}$. The cryogenic generation and in detail spectroscopic characterization of the aforementioned series of electronically disparate heme superoxo intermediates, ([(Por)Fe^{III}($O_2^{-\bullet}$)], where Por = TPP (5,10,15,20-tetraphenylporphyrin), TMPP (5,10,15,20-tetrakis(4-methoxyphenyl)-porphyrin), or F_{20}TPP (5,10,15,20-tetrakis(pentafluorophenyl)-porphyrin)), have been furnished in our recent reports.[60–62] When $NO_{(g)}$ (1 mL) was bubbled into a 50 μM solution of [(TPP)Fe^{III}-($O_2^{-\bullet}$)] in THF at −80 °C, immediate changes in absorption features (Soret: from 417 to 428 nm ($\varepsilon = 3.0\times10^5$ $M^{-1}cm^{-1}$); Q-band: from 540 to 541 nm ($\varepsilon = 2.5\times10^4$ $M^{-1}cm^{-1}$)) were evidenced (Figure 2A, blue trace). These final electronic absorption features are in line with those of the six-coordinate heme ferric nitrate complexes with an axially ligated NO ligand (i.e., [(NO)(TPP)Fe^{III}(NO_3)]), as also further confirmed by our authentic standards (Figure 2 and Scheme 3). Similar chemistries have also been previously reported,[63–64] and our findings here are in close agreement.

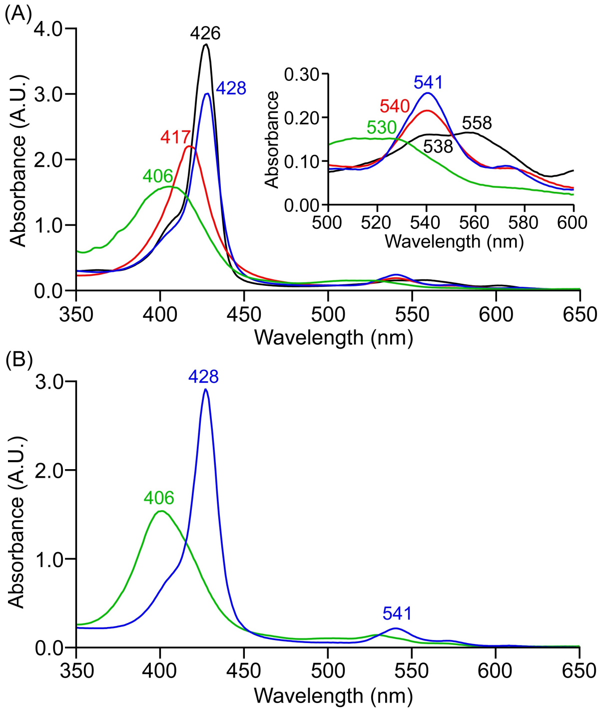
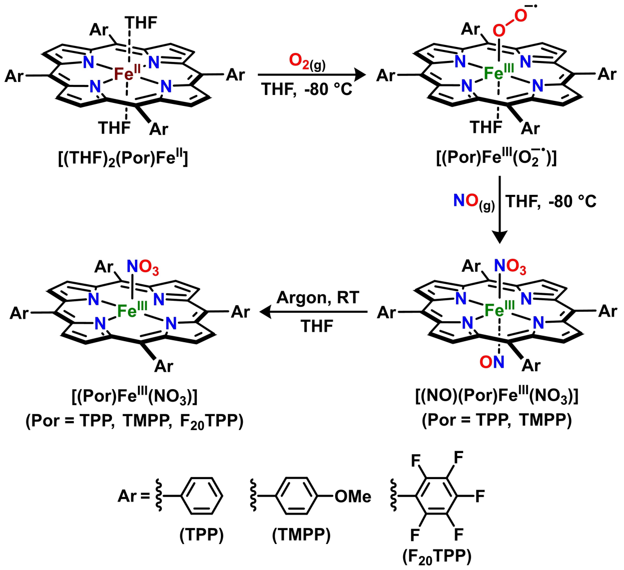


Figure 2. UV–vis spectra (in THF at −80 °C) for 50 μM solutions of (A) $[(THF)_2(TPP)Fe^{II}]$ (black), $[(TPP)Fe^{III}(O_2^{-\bullet})]$ (red), the product after bubbling of 1 mL of $NO_{(g)}$ into $[(TPP)Fe^{III}(O_2^{-\bullet})]$ (blue), and the final product at RT after Ar bubbling (green); inset shows the expanded Q-band region; (B) authentic $[(TPP)Fe^{III}(NO_3)]$ (green) and product after the addition of 1 mL of $NO_{(g)}$ at −80 °C; i.e., $[(NO)(TPP)Fe^{III}(NO_3)]$ (blue).



Scheme 3. Generalized reaction landscape depicting the formation and $NO_{(g)}$ reactivity of $[(Por)Fe^{III}(O_2^{-\bullet})]$ complexes.

This six-coordinate intermediate is only stable at cryogenic temperatures under an $NO_{(g)}$-rich atmosphere, whereas warming it up to room temperature, followed by argon sparging, results in the five-coordinate heme ferric nitrate species, $[(TPP)Fe^{III}(NO_3)]$ (Scheme 3). The final $[(TPP)Fe^{III}(NO_3)]$ adduct was characterized in detail using electronic absorption, EPR, and FT-IR spectroscopies (Figures 2, S1 and S5). Structurally analogous, yet electronically rich ferric superoxide complex, $[(TMPP)Fe^{III}(O_2^{-\bullet})]$, also followed the exact same pattern of reactivity with NO (Figure S2). Contrastingly, the addition of NO into the electron deficient superoxo adduct, $[(F_{20}TPP)Fe^{III}(O_2^{-\bullet})]$, led to the exclusive production of the five-coordinate heme nitrate complex, $[(F_{20}TPP)Fe^{III}(NO_3)]$, even at cryogenic temperatures (Figure S3). In consistence, formation of only five-coordinate heme nitrate complexes were evidenced by Karlin and co-workers when $[(F_8TPP)Fe^{III}(O_2^{-\bullet})]$ superoxo complex, supported by the electron-deficient F_8TPP porphyrin (F_8TPP = 5,10,15,20-tetrakis(2,6-difluorophenyl)-porphyrin), was subjected to reactivity with excess NO.[65,66]

This reactivity between $[(Por)Fe^{III}(O_2^{-\bullet})]$ complexes and NO was further evaluated by ^{2}H NMR spectroscopy using the pyrrole-position deuterated TPP-d_8 porphyrin, where the $[(THF)_2(TPP\text{-}d_8)Fe^{II}]$ and $[(TPP\text{-}d_8)Fe^{III}(O_2^{-\bullet})]$ complexes exhibited single ^{2}H NMR resonances at $\delta_{pyrrole}$ = 86.4 ppm and $\delta_{pyrrole}$ = 8.4 ppm, respectively (Figure 3). The

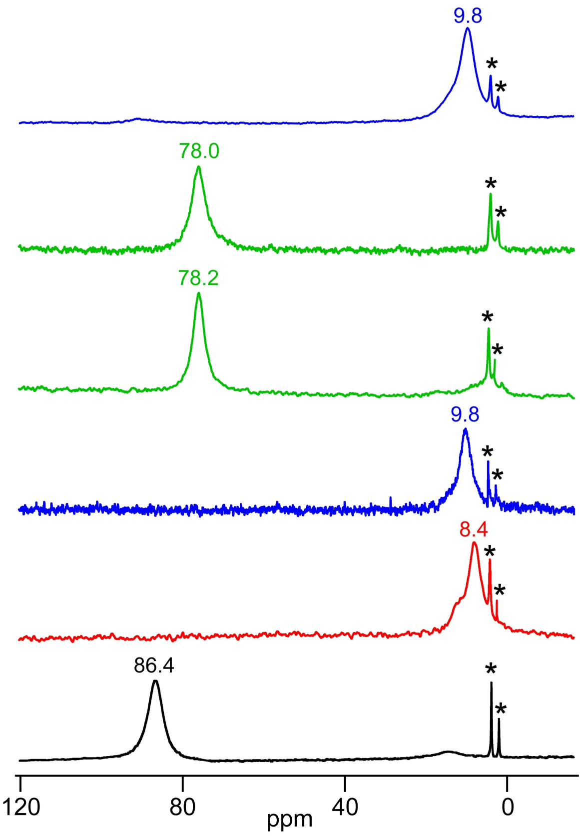
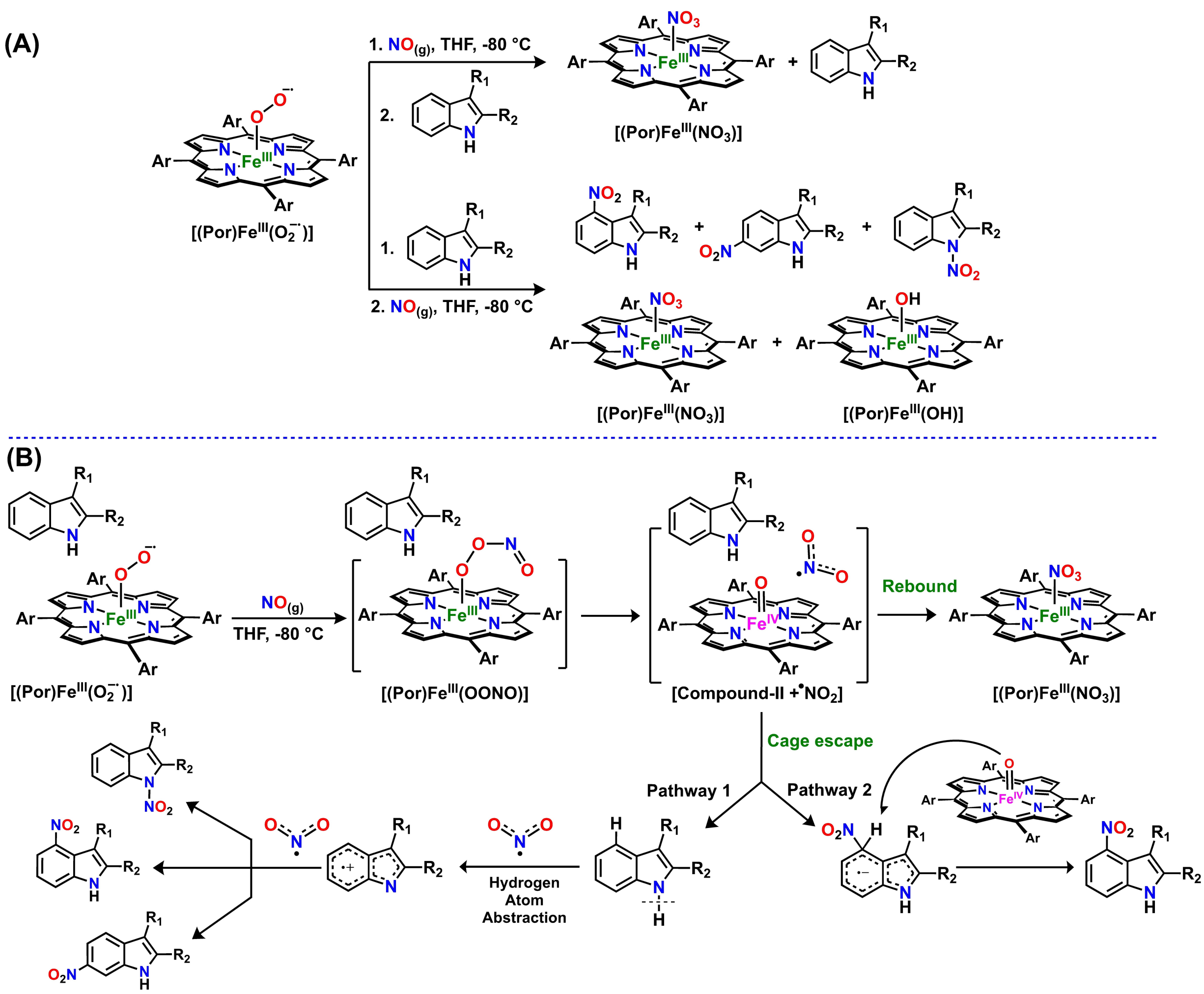


Figure 3. ^{2}H NMR spectra (bottom to top; in THF at −80 °C) of $[(THF)_2(TPP\text{-}d_8)Fe^{II}]$ (black), $[(TPP\text{-}d_8)Fe^{III}(O_2^{-\bullet})]$ (red), the product after bubbling of 1 mL of $NO_{(g)}$ into $[(TPP\text{-}d_8)Fe^{III}(O_2^{-\bullet})]$ (blue), and the final product at RT after Ar bubbling (green; i.e., $[(TPP\text{-}d_8)Fe^{III}(NO_3)]$), authentic $[(TPP\text{-}d_8)Fe^{III}(NO_3)]$ (green) at RT and the product after the addition of 1 mL of $NO_{(g)}$ into $[(TPP\text{-}d_8)Fe^{III}(NO_3)]$ at −80 °C (blue; i.e., $[(NO)(TPP\text{-}d_8)Fe^{III}(NO_3)]$). *peaks at 3.58 and 1.73 ppm correspond to the THF solvent.

reaction product between [(TPP-d_8)Fe^{III}($O_2^{-\bullet}$)] and $NO_{(g)}$ at −80 °C displayed a feature at $\delta_{pyrrole}$ = 9.8 ppm (Figure 3), and was EPR-silent (Figure S5), lending credence to its assignment as the aforementioned six-coordinate [(NO)-(TPP)Fe^{III}(NO_3)] species.[67] Following subsequent argon purging at RT, this [(NO)(TPP-d_8)Fe^{III}(NO_3)] was converted into the five-coordinate [(TPP-d_8)Fe^{III}(NO_3)] adduct, which was accompanied by the shifting of the ^{2}H NMR signal to $\delta_{pyrrole}$ = 78.2 ppm (Figure 3). This final five-coordinate heme ferric nitrate complex is EPR active, with features centered at g = 6.0 and 1.98 (Figure S5), indicating the presence of a high-spin Fe^{III} center. To definitively elucidate the ultimate production of [(TPP)Fe^{III}(NO_3)], we analyzed the final nitrate content using QUANTOFIX nitrate/nitrite test strips, which revealed the presence of near stoichiometric yields of nitrate anions (~85 ± 12.5 %). These observations in concert infer the formation of a heme peroxynitrite type intermediate upon the reaction of heme superoxide with NO,[68] which then isomerizes via homolytic O–O bond cleavage to give nitrate (see below for supporting theoretical findings).

Indole Nitration Using [(Por)Fe^{III}($O_2^{-\bullet}$)] Adducts and $NO_{(g)}$. We then set out to evaluate the competency of these synthetic heme systems to model the indole nitration chemistry of TxtE, especially considering the likelihood of a key heme peroxynitrite intermediate en route to the final nitrate complex. Accordingly, a series of 3-substituted indoles were tested against the aforementioned heme superoxo systems (Scheme 2) for the formation of nitroindole products. Interestingly, when **1b** substrate was introduced to a 50 μM solution of [(TPP)Fe^{III}($O_2^{-\bullet}$)] following the addition of 1 mL $NO_{(g)}$ (i.e., excess NO), there were minimal alterations to the electronic absorption features described above (Figure S6), and **1b** remained unreacted (Scheme 4A). This finding indicates that even if a heme peroxynitrite intermediate were to form following the reaction of [(TPP)Fe^{III}($O_2^{-\bullet}$)] with $NO_{(g)}$, its isomerization outcompetes any possible reactivity with **1b**. This reactivity trend is common to all three [(Por)Fe^{III}($O_2^{-\bullet}$)] systems (Scheme 2), wherein no hint of nitroindole was observed.

Interestingly, when the indole substrate, **1b**, was introduced to [(TPP)Fe^{III}($O_2^{-\bullet}$)] prior to the addition of 1 mL of



Scheme 4. (A) Nitration reactivity of indole substrates in presence of [(Por)Fe^{III}($O_2^{-\bullet}$)] and $NO_{(g)}$. (B) Plausible mechanistic pathways for the nitration of indole substrates by [(Por)Fe^{III}($O_2^{-\bullet}$)] adducts in the presence of $NO_{(g)}$.

$NO_{(g)}$ (i.e., under same conditions as above), the formation of 4-nitro- (**2b**; 10±1 %), 6-nitro- (**2b′**; 8±1 %) and *N*-nitro-2,3-dimethylindole (**2b″**; 18±1 %) products was observed (Scheme 4B, Pathway 1).[69] Note that our previous studies have clearly determined that heme superoxo adducts do not directly react with indole substrates under these circumstances.[60] All stable nitrated indole products have been thoroughly characterized utilizing ^{1}H and ^{13}C NMR, FT-IR, and ESI/LC-MS methods (Figures S7–S14).[70] This report therefore offers the first fully characterized series of organic products from any synthetic mimic of TxtE, where the direct and single-step conversion of indole substrates to nitroindoles is unequivocally determined. Interestingly, no further increase in nitration was observed following stirring of reaction mixture for hours at RT, indicating the majority of nitration occurring at cryogenic temperatures.[71] Similar yields of nitrated indoles were also obtained using the other superoxo complexes, $[(TMPP)Fe^{III}(O_2^{-\bullet})]$ and $[(F_{20}TPP)Fe^{III}(O_2^{-\bullet})]$ (Table S1), indicating only a negligible impact from ligand electronic effects. Markedly, the final heme species in solution following indole nitration was characterized to be $[(TPP)Fe^{III}(NO_3)]$ (via UV–vis and ^{2}H NMR; Figure S15), which was further authenticated using QUANTOFIX nitrite/nitrate test strips (~70±12.5 % yield of nitrate).[72,73]

Mechanistic Studies. First, we carried out a series of control experiments that shed further light on the nature of active heme species that is responsible for indole nitration: (i) bubbling excess $NO_{(g)}$ into a final reaction product mixture had no effect on the nitrated indole products or their relative yields, indicating that heme cannot mediate nitration at room temperature by having only $NO_{(g)}$ in solution; (ii) addition of excess $NO_{(g)}$ into a solution containing $[(THF)_2(TPP)Fe^{II}]$ at −80 °C in the presence of **1b**, and the subsequent warm up to RT did not yield any nitrated indoles (only the formation of $[(TPP)Fe^{II}(NO)]$ was evidenced); (iii) the warm up of a −80 °C mixture of $[(TPP)Fe^{III}(NO_3)]$ and **1b** to RT gave no nitrated indoles; and (iv) introduction of excess $^{\bullet}NO_{2(g)}$ into a solution of **1b** with or without the presence of $[(THF)_2(TPP)Fe^{II}]$ at −80 °C, followed by the warm up of that mixture to RT only yielded modest amounts of nitrated products. These observations taken together, further implicate an extremely strong heme-based nitrating agent, similar to a heme peroxynitrite intermediate, that competently mediates the nitration of indoles at cryogenic temperatures. As mentioned above, heme peroxynitrite adducts, $[(Por)Fe^{III}(OONO)]$, have been proposed to generate from the rapid reactivity between the corresponding heme superoxide, $[(Por)Fe^{III}(O_2^{-\bullet})]$, with $NO_{(g)}$.[74] They have the propensity to undergo homolytic O–O bond cleavage to form a couple of caged radical intermediates (heterolytic O–O cleavage has been shown to be energetically uphill.[75]), namely Compound II and nitrogen dioxide, $[(Por)Fe^{IV}{=}O)+{}^{\bullet}NO_2]$, which can recombine (i.e., rebound reaction) to form heme nitrate complexes, $[(Por)Fe^{III}(NO_3)]$.[57,68,76] However, previous studies have indicated evidence for instances where cage escape occurs, and $^{\bullet}NO_2$ diffuses away from the heme site to induce exogenous substrate nitration chemistries.[57,66] In this case, we hypothesize that a cage-escaped $^{\bullet}NO_2$ radical abstracts the N–H hydrogen from the indole ring to form an indolyl radical, where the unpaired electron would be resonance delocalized throughout the ring conjugated system (Scheme 4B, Pathway 1). In support, (1) literature reports on systems where melatonin (i.e., another 3-alkyl substituted biological indole-containing compound) or tryptophan are substrates suggest that hydrogen atom abstraction from indole is likely feasible due to the notable stability of the indolyl radical, in particular, the nitrogen-centered radical;[77–79] and (2) *N*-methyltryptophan did not yield any productive nitration chemistry by TxtE enzyme;[19] similarly, (3) in our model studies, neither 1,3-dimethylindole nor *N*-methylindole yielded any nitration chemistry (Figure S6). So formed indolyl radical intermediate (and its resonance forms) will then react with a second equivalent of $^{\bullet}NO_2$ resulting in the observed nitroindole products (Scheme 4B, Pathway 1; see below for supporting computational studies). In further support, when indole was employed as a substrate, all of 3-, 4-, and 6-nitroindole products were observed as products (see Supporting Information).[69b] According to this mechanism, maximum expected cumulative yield of nitroindoles would be 50 %, which is in agreement with our experimental findings (~40 %).[80] Interestingly, minor amounts of $[(TPP)Fe^{III}(OH)]$ (as also observed during phenol nitration in nitric oxide dioxygenase (NOD) heme model systems[66,81]) were also found within the final product mixture (see Figure S15B for ^{2}H NMR data), indicating that the Compound II species, to some extent, could be involved in the final proton abstraction leading to rearomatization of the indole ring. Accordingly, our control experiments (see above) only gave modest nitroindole yields when only NO_2 was introduced to indoles in the absence of heme. A logical alternative mechanistic possibility in this case would be the formation of indolyl radical via hydrogen atom abstraction by the ferryl species, which will then react with $^{\bullet}NO_2$ leading to nitroindoles. In fact, similar mechanistic propositions have been put forward in describing the phenol nitration chemistry of heme peroxynitrite adducts that mimic the NOD activity of heme proteins.[82–83] To investigate this possibility further, we have independently generated the Compound II species, $[(TPP)Fe^{IV}{=}O]$, to which, **1b** substrate was subsequently introduced at −80 °C (Figure S15). This control experiment unambiguously reveals that $[(TPP)Fe^{IV}{=}O]$ is unreactive toward **1b**, closely paralleling our previous observations.[84] Surprisingly, **1b**, even in the presence of a mixture of $[(TPP)Fe^{IV}{=}O]$ and $^{\bullet}NO_2$ does not undergo nitration, but the mere formation of $[(TPP)Fe^{III}(NO_3)]$ was observed. Thus, in light of this body of evidence, the ferryl species most likely does not *initiate* indolyl radical formation, but rather has a tendency to undergo a virtually barrierless rebound reaction with $^{\bullet}NO_2$ giving $[(TPP)Fe^{III}(NO_3)]$.[73]

To this end, Pathway 1 in Scheme 4B most likely dictates the indole nitration chemistry of the transient heme peroxynitrite adduct formed here (see below for theoretical findings on Pathway 2). To further substantiate the likelihood of this pathway, we have used ^{18}O-labeled $[(TPP)Fe^{III}(O_2^{-\bullet})]$ and $^{15}NO_{(g)}$ to track the source(s) of $^{\bullet}NO_2$

in the final nitrated indole. The unlabeled reaction between [(TPP)Fe^{III}($O_2^{-\bullet}$)], **1b**, and $NO_{(g)}$ generated the final 4-nitrated product **2b** with the mass of 189.06 *m/z* (Figure 4A). When isotopically labeled $^{15}NO_{(g)}$ was utilized for this reaction, the mass of the corresponding product shifted from 189.06 to 190.06 *m/z*, indicating the incorporation of one ^{15}N atom (i.e., $^{\bullet 15}N^{16}O_2$) into the nitrated indole (Figure 4B). Interestingly, when a 1:1 $^{16}O_{2(g)}$:$^{18}O_{2(g)}$ mixture was used to generate [(TPP)Fe^{III}($O_2^{-\bullet}$)], which was then used to nitrate **1b** along with $^{15}NO_{(g)}$, a 1:1 product ratio of $^{\bullet 15}N^{16}O_2$ and $^{\bullet 15}N^{16}O^{18}O$ incorporated 4-nitro products (i.e., at 190.06 and 192.06 *m/z*, respectively) were observed (Figure 4C). These findings in concert afford strong evidence for the formation of a heme peroxynitrite like intermediate, which subsequently undergoes homolytic O–O bond scission and the resulting $^{\bullet}NO_2$ getting incorporated into the indole substrates. In order to rule out heterolytic O–O cleavage of such a peroxynitrite intermediate (see Scheme 1, B and C; latter generates the strong electrophile NO_2^+), *N*-methyl-3-pivaloyl indole, known to encompass a *very* electronically

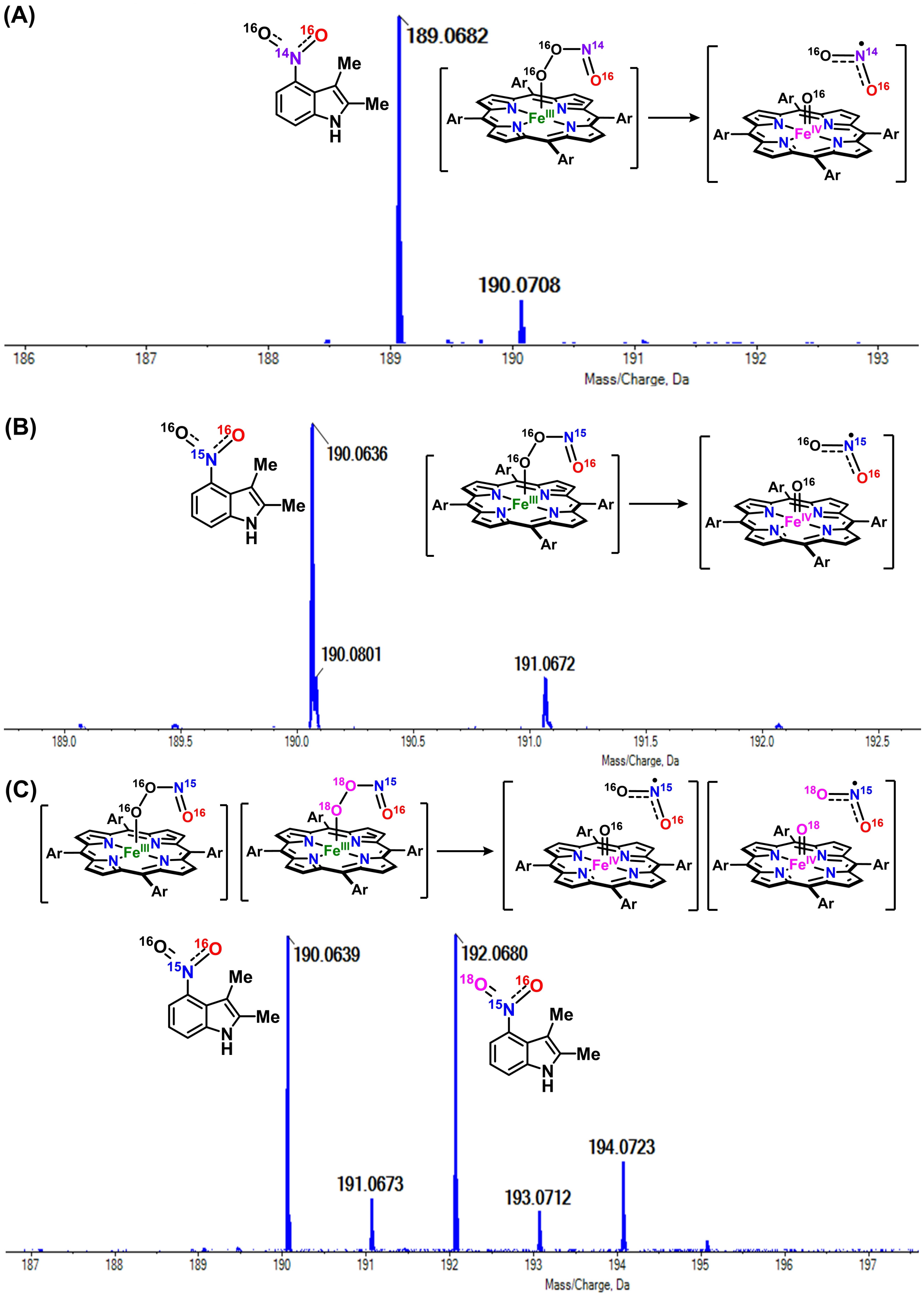


Figure 4. LC–MS spectrum of (A) **2b** showing [M–H]$^+$ m/z=189.06 (calc. 189.06) generated using [(TPP)Fe^{III}($^{16}O_2^{-\bullet}$)] and $^{14}NO_{(g)}$, (B) **2b** showing [M–H]$^+$ m/z=190.06 (calc. 190.06) generated using [(TPP)Fe^{III}($^{16}O_2^{-\bullet}$)] and $^{15}NO_{(g)}$ and (C) **2b** showing [M–H]$^+$ m/z=190.06 and 192.06 (calc. 190.06 and 192.06) generated using 1:1 [(TPP)Fe^{III}($^{16}O_2^{-\bullet}$)] and [(TPP)Fe^{III}($^{18}O_2^{-\bullet}$)] and $^{15}NO_{(g)}$.

rich C_4-position,[85] was utilized as a nitration substrate, which remained unreactive. These findings in concert provide solid evidence into an O–O bond homolytic cleavage process of a heme peroxynitrite type intermediate that predominantly governs the indole nitration chemistry of these heme model systems, strongly reminiscing the analogous mechanistic propositions described for the Cyt P450 TxtE enzyme. To further refine these various mechanistic viewpoints, we then carried out rigorous theoretical interrogations using Density Functional Theory.

Computational Studies and Overall Reaction Landscape. We started the calculations from an iron(III)-superoxo complex embedded into a TPP ligand system with THF as axial ligand and in the presence of substrate (Sub) and NO, and designated the reactant complex as **Re**. The reaction with NO is exothermic and no transition state could be located for the formation of an iron(III)-peroxynitrite complex **IM1**. Consequently, this process is expected to be fast and irreversible; see Figure 5. The doublet spin state ^{2}**IM1** is the ground state over the quartet spin state by ΔE + ZPE = 9.9 kcal mol^{-1}. The electronic configuration of ^{2}**IM1** is $\delta_{x2-y2}{}^2\ \pi^*_{xz}{}^2\ \pi^*_{yz}{}^1$, whereby the δ_{x2-y2} orbital represents a nonbonding orbital in the plane of the heme, while the π^*_{xz} and π^*_{yz} orbitals are antibonding orbitals for the Fe–O interaction. The electronic configuration of ^{4}**IM1** results in the excitation of one electron from π^*_{xz} into the antibonding orbital along the O–Fe-axial ligand axis, i.e. σ^*_{z2}. The spin-state-ordering and relative energies matches previous calculations on iron(III)-peroxynitrite and iron(III)-hydroperoxo heme complexes well.[16,86] Next, the iron(III)-peroxynitrite can cleave off an $^\bullet NO_2$ radical to form a Compound II (Cpd-II) structure, [(THF)(TPP)Fe^{IV}(O)], with a triplet spin on the iron(IV)-oxo coupled to a radical on $^\bullet NO_2$ with either an up- or a down-spin electron. As such, the doublet and quartet spin states of **IM2** are degenerate. We attempted to swap molecular orbitals for the **IM2** intermediates to generate the alternative conformations representing a Compound-I type structure with an NO_2^- anion (Scheme 1, Pathway (B)) or the iron(III)-oxo intermediate with NO_2^+ cation (Scheme 1, Pathway (C)). However, these configurations could not be characterized, hence are significantly higher in energy and inaccessible. Therefore, the iron(III)-peroxynitrite intermediate homolytically cleaves its O–O bond to form Compound-II and $^\bullet NO_2$ radical.

For the conversion of the iron(III)-peroxynitrite structures (^{4,2}**IM1**) into Cpd-II + $^\bullet NO_2$ (^{4,2}**IM2**) we located transition states (^{4,2}**TS1**) that are shown in Figure 5. The low-spin transition state is at ΔE + ZPE = 7.1 kcal mol^{-1} above ^{2}**IM1**, while ^{4}**TS1** is at ΔE + ZPE = 13.9 kcal mol^{-1}. Both transition states are characterized with an imaginary frequency for the O–O stretch vibration with a magnitude of i744 cm^{-1} for ^{4}**TS1** and i561 cm^{-1} for ^{2}**TS1**. The O–O bond has elongated significantly in the transition states; to 1.847 (1.844) Å for ^{4}**TS1** (^{2}**TS1**). These are typical values for imaginary frequencies and structures of O–O cleavage transition states.[87–90] From ^{4,2}**IM2** we studied several pathways but will start with $^\bullet NO_2$ attack on Cpd-II to form nitrate products, i.e., the pathway via transition state **TS4** to form **P2**. Energetically, on both spin states a small barrier is encountered for nitrate formation, namely ^{2}**TS4** is ΔE + ZPE = 2.9 kcal mol^{-1} above ^{2}**IM1** and ^{4}**TS4** is ΔE + ZPE = 3.2 kcal mol^{-1} above ^{4}**IM2**. These barriers are small and therefore the reaction will happen rapidly on both spin states. Moreover, the formation of the iron(III) nitrate product complex is highly exothermic and will be irreversible. The calculated transition state structures are shown in Figure 5. Both show an imaginary frequency for the O–N stretch vibration, and these have a value of i105 cm^{-1} for ^{4}**TS4** and i226 cm^{-1} for ^{2}**TS4**. The O–N interaction is still long for both complexes and consequently, the transition states are reactant-like.

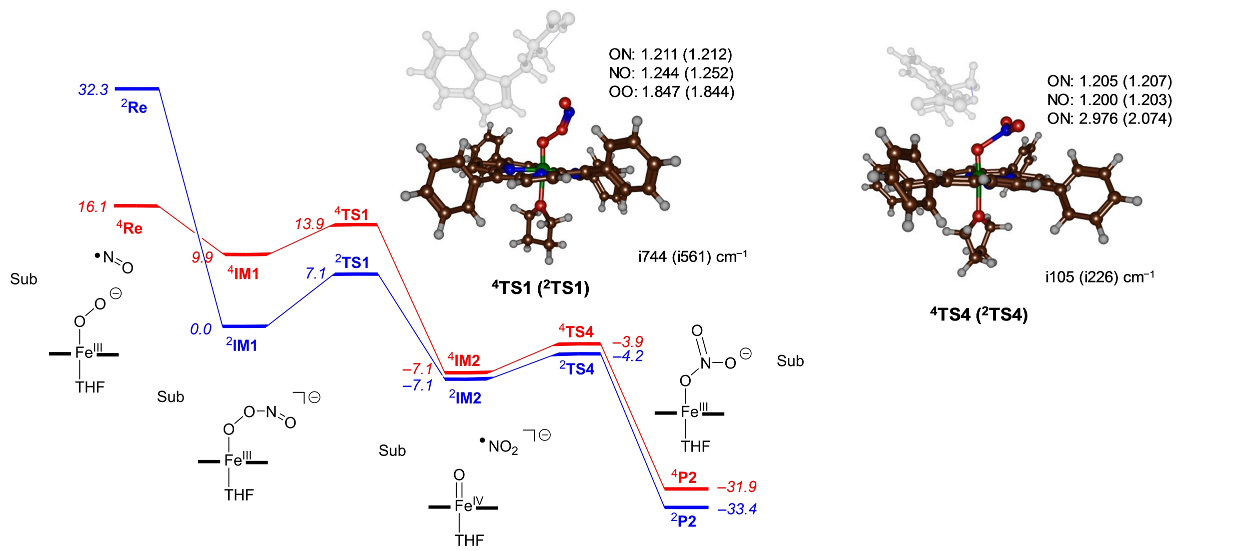


Figure 5. Potential energy landscape with ΔE + ZPE (ΔG) values in kcal mol^{-1} for the reaction of [Fe^{III}(TPP)(O_2)(THF)] with NO to form nitrate and in the presence of indole substrate (Sub). Key transition state structures are given with bond lengths in Å and the imaginary frequency in cm^{-1}.

Next, we explored several cage-escape pathways and started with H• transfer from the indole N–H group to •NO_2 (Figure 6; also see Scheme 4). Interestingly, a small barrier of $\Delta E + ZPE = 0.6\ kcal\,mol^{-1}$ is obtained for hydrogen atom transfer from indole N–H group to •NO_2, whereby the transition state structure has an imaginary frequency of $i1109\ cm^{-1}$ for the N–H–O stretch vibration. The structure is relatively central with an indole N–H distance of 1.271 Å and an H–ONO distance of 1.230 Å. Overall, the hydrogen atom abstraction barrier from indole by •NO_2 is of the same order of magnitude as the nitrate forming transition states ^{4,2}**TS4** and as such, a mixture of products may be expected with partial indolyl radical generation and partial heme nitrate formation. No further reactions between HNO_2 and indolyl radical were observed. The group spin densities of the transition state and the product complex show radical on the indole moiety (spread over the entire system) and not on the HONO group, hence a H• abstraction has taken place in this step to form dehydrogenated indole, i.e., **Sub**. The group spin densities on the indole group are shown in the inset in Figure 6. We identify most spin on the nitrogen atom (about 0.26 unpaired spin density), while there is also spin seen on atoms C_4 (about 0.22 spin) and on C_6 (about 0.16 spin). Based on these spin distributions we expect the NO_2 group to dominantly attack the center with largest unpaired spin density, which is the nitrogen atom of the indole. Indeed, the product distributions experimentally obtained linearly correlate with the unpaired spin densities in the substrate radical. We tested further reactivity within the complex but could not find any low energy channels leading to nitrated indole products. Instead, we located a pathway where HNO_2 is released and where the radical **Sub** interacts with a second •NO_2 radical to form nitroindole (see Figure 6; note that this unequivocally supports Scheme 4, Pathway 1). Noteworthily, we could only obtain a slight energy barrier for N–N or C–N bond formation that we were unable to characterize, as such, these bond formation steps will be fast. Nevertheless, the **[Sub+NO$_2$]** complex collapses giving rise to the very stable **Sub–NO$_2$** product complex. Importantly, even if the attack of •NO_2 on 4- or 6-position on indole is exothermic, the formation of *N*-nitro product was found to be the most favorable, which is in excellent agreement with experimental results, where *N*-nitroindole was found to be the major nitrated indole product (see above). Finally, we also computed the energy profile for Pathway 2 in Scheme 4B (see Figure S16 and corresponding descriptions in the Supporting Information), which however, was found to be less feasible than Pathway 1 in Scheme 4B. It is important to note that despite the overall reaction, precise mechanistic details of these model systems can be different to those of the enzymatic system, warranting further investigation.

Conclusion

Economically impactful TxtE enzyme mediates the unique transformation of tryptophan to 4-nitrotryptophan, however, direct experimental evidence for this pathway is scant. Moreover, nitrated heteroaromatic motifs are of supreme importance in a broad array of industrial applications. Given these crucial considerations, in this work we have investigated the ability of putative synthetic heme peroxynitrite intermediates to nitrate indole substrates for the first time. Our heme model systems predominantly produce three nitrated indole species (i.e., *N*-, 4-, and 6-nitroindole), formation of which, operates via very similar energy barriers as illustrated by our theoretical findings. The 4-nitroindole produced in this model system directly mimics the 4-nitrotryptophan product of TxtE, and ^{15}N and ^{18}O isotope labeling experiments reveal that the *N*-atom and one of *O*-atoms of the nitro group delivered on to the indole originates from nitric oxide, while the other *O*-atom is dioxygen dependent. Interestingly, similar to TxtE, our

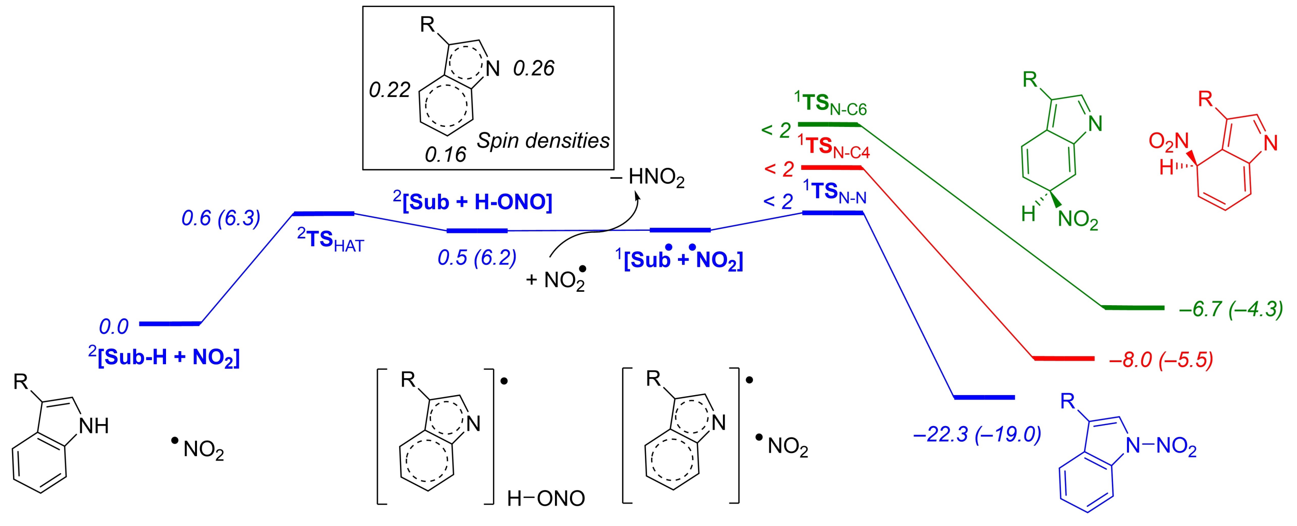


Figure 6. Cage escape pathways calculated for indole activation by •NO_2. Potential energy landscape with $\Delta E + ZPE$ (ΔG) values in $kcal\,mol^{-1}$. Spin densities on the indole group shown in the inset.

model systems only generate nitroindole products if the N–H group of indoles is unsubstituted, which, computations infer to be climacteric for the lowest energy pathway to nitroindole formation (i.e., via the generation of the indolyl radical). This rigorous experimental, spectroscopic, and theoretical investigation therefore not only shed light on numerous important unknowns with direct relevance to the TxtE enzyme, but also impart a fundamental understanding into how economically and environmentally benign facile nitration of heterocyclic moieties maybe achieved, defining new avenues for targeting complex organic frameworks with a myriad of benefits to humans.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords: Heme peroxynitrite · indole nitration · synthetic heme models · TxtE · mechanism

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[70] Please see Supporting Information for characterization details on all the nitroindole products. Note that these results should be viewed within the caveat that $NO_{(g)}$ is present in excess under these conditions.
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Supporting Information for

A Cytochrome P450 TxtE Model System with Mechanistic and Theoretical Evidence for a Heme Peroxynitrite Active Species

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Experimental Section

Materials and Methods. All commercially available chemicals were purchased at the highest available purity and used as received unless otherwise stated. Air-sensitive compounds were handled either under an argon atmosphere using standard Schlenk techniques, or in an Mbraun Unilab Pro SP (<0.1 ppm O_2, <0.1 ppm H_2O) nitrogen-filled glovebox. All organic solvents were purchased at HPLC-grade or better and degassed (bubbling argon gas for 40 min at room temperature) and dried (passing through a 60 cm alumina column) using an Inert Pure Solv MD 5 (2018) solvent purification system. These solvents were then stored in dark glass bottles inside the glovebox over 4 Å molecular sieves at least for 72 hrs prior to use. Benchtop UV-vis experiments were carried out using Agilent Cary 60 spectrophotometer equipped with a liquid nitrogen chilled Unisoku CoolSpek UV USP-203-B cryostat. A 2 mm path length quartz cell cuvette modified with an extended glass neck with a female 14/19 joint and stopcock was used to perform all UV–vis experiments. ^1H and low temperature ^2H NMR spectroscopic studies were carried out on a Bruker AV 400 MHz NMR spectrometer. All spectra were recorded in 5-mm (outer diameter) NMR tubes. The chemical shifts were reported as δ (ppm) values calibrated to natural abundance deuterium or proton solvent peaks. Infrared (IR) vibrational spectra were collected on a Bruker FT-IR spectrometer (Vertex 70) at room temperature. For LC-MS analysis, a SCIEX 5600 Triple-Tof mass spectrometer (SCIEX, Toronto, Canada) was used to analyze the mass profiles of the organic products. The IonSpray voltages for positive modes were ±5000 V, and the declustering potential was 80 V. Ionspray GS1/GS2 and curtain gases were set at 40 and 25 psi, respectively. The interface heater temperature was maintained at 400 °C. ESI-MS data were collected in Waters Xevo G2-XS Qtof (quadrupole time-of-flight) instrument and the conditions are: Capillary voltage 0.8 KV in positive mode, Sampling cone 40 V, Source offset 80, Source temperature 100 °C, Desolvation 350 °C, Cone gas 30 L/h, Desolvation gas 400 L/h, lock spray capillary voltage 0.1 KV, lock mass: 556.2771 in positive mode (leucine enkephalin). The expected cations or $[M + H]^+$ or $[M + Na]^+$ ions were observed in positive ion mode with <5 ppm mass accuracy. X-band electron paramagnetic resonance (EPR) spectra were collected in 4 mm (outer diameter) quartz tubes using a Bruker ELEXSYS E540 X-band (Bruker-Biospin, Billerica, MA) with a bimodal resonator, and an Oxford ESR900 cryostat and Oxford ITC 03 temperature controller for low-temperature spectral analysis (experimental conditions: microwave frequency = 9.41 GHz; microwave power = 0.2 mW; modulation frequency = 100 kHz; modulation amplitude = 10 G; temperature = 7 K). The preparation and purification of $NO_{(g)}$

(or $^{15}NO_{(g)}$) was effected according to published procedures,[1] and a three-way Hamilton gastight syringe was used to administer $NO_{(g)}$ into reaction mixtures. 5,10,15,20-tetraphenylporphyrin iron(III) chloride, [(TPP)Fe^{III}Cl] and 5,10,15,20-tetrakis(4-methoxyphenyl)porphyrin, H_2(TMPP) were purchased from commercial sources. The syntheses of H_2(F_{20}TPP) and H_2(TPP-d_8) were carried out according to previously published methods.[2-3] Metalation of the porphyrinates to generate [(TMPP)Fe^{III}Cl], [(F_{20}TPP)Fe^{III}Cl], and [(TPP-d_8)Fe^{III}Cl] and the subsequent reduction to [$(THF)_2$(Por)Fe^{II}] complexes were carried out by following previously reported procedures.[4] Authentic [(Por)Fe^{III}(NO_3)] complexes were synthesized as previously reported.[5]

Computation. DFT calculations were performed on an [Fe^{III}(TPP)O_2(THF)] complex for its reaction with NO and Trp as models for the reactions studied in this work. The model included the full TPP system with tetrahydrofuran (THF) as the axial ligand. As such the iron(III)-superoxo structure has overall charge 0 and after binding NO the system has even multiplicity (doublet or quartet). The model consisted of 121 atoms and no constraints were used. Reaction mechanisms were explored as described in Scheme S1. All geometries were fully optimized and transition states were characterized with a single imaginary frequency for the correct mode. For a number of transition state geometries, intrinsic reaction coordinate scans were performed that connected them to the two local minima adjacent to the transition state. All computational studies were performed using *Gaussian*-09[6] at the unrestricted B3LYP[7-8] level of theory with an LANL2DZ basis set with core potential on iron and 6-31G* on the rest of the atoms[9-11]: basis set BS1. To improve the energies, single point calculations were performed with the LANL2TZ+ basis set on iron with diffuse d functions and a core potential and 6-31G* on the rest of the atoms (C, N, O, H): basis set BS2. All optimizations, frequencies, and geometry scans included a conductor-like polarizable continuum model (CPCM) with a dielectric constant mimicking THF solvent at a temperature of T = 193.15 K.[12] These methods were previously validated against experimental data and found to reproduce experimentally determined free energies of activation to within a few kcal mol^{-1} and predict the correct product distributions.[13-14] The cage-escape pathways for done for a minimal cluster model of methylindole or deprotonated methylindole in a reaction with NO_2 at UB3LYP/BS2 level of theory.

Formation of the Heme Superoxo Complexes, [(Por)Fe^{III}($O_2^{-\bullet}$)] and their spectroscopic reactivity studies with $NO_{(g)}$. Generation of the superoxo complexes, [(Por)Fe^{III}($O_2^{-\bullet}$)], was carried out following a literature-adapted procedure.[4, 15-16] In a typical experiment, a 50 μM THF solution (1 mL) of [$(THF)_2$(Por)Fe^{II}] was taken into a 2 mm pathlength Schlenk cuvette and was sealed using a rubber septum inside the glovebox. Following cooling down inside a UV–vis cryostat stabilized at –80 °C for 10 min, the solution was bubbled with dry dioxygen gas using a needle, and the complete formation of the superoxo complexes, [(Por)Fe^{III}($O_2^{-\bullet}$)], was monitored by UV-vis spectroscopy. Excess $O_{2(g)}$ was removed by three vacuum/Ar purge cycles, and subsequently 1 mL $NO_{(g)}$ was bubbled to the solution at –80 °C using a three-way gastight syringe. (Figures 2A, S2A and S3).

In situ generation of authentic [(NO)(Por)Fe^{III}(NO_3)] Complexes. In a typical experiment, 50 μM THF solution (1 mL) of authentic [(Por)Fe^{III}(NO_3)] complex was taken in a 2 mm pathlength Schlenk cuvette and was sealed using a rubber septum inside the glovebox. The sample was then cooled to –80 °C in a UV–vis cryostat and 1 mL of $NO_{(g)}$ was directly bubbled into the solution of [(Por)Fe^{III}(NO_3)], resulting in the formation of the [(NO)(Por)Fe^{III}(NO_3)] complex (Figure S2B).

Low-Temperature ^{2}H NMR Spectroscopic Studies. For a typical ^{2}H NMR experiment, [$(THF)_2$(TPP-d_8)Fe^{II}] (15 mg, 0.02 mmol) was dissolved in 0.5 mL of THF in a 5 mm (outer diameter) NMR tube inside the glovebox and was sealed with a rubber septum. This tube was then stabilized at –80 °C using a liquid nitrogen/acetone cold bath, followed by the addition of $O_{2(g)}$ by means of a 9” needle to generate the [(TPP-d_8)Fe^{III}($O_2^{-\bullet}$)] complex. Subsequently, 1 mL $NO_{(g)}$ was bubbled to the solution at –80 °C using a three-way gastight syringe to generate the corresponding reactivity products. For each instance, the NMR tube was immediately transferred into the cryostat of the NMR spectrometer held at –80 °C for data accumulation (Figure 3).

EPR Sample Preparation. EPR Samples were prepared similarly to the UV−vis samples as mentioned earlier; however, samples were made at 2 mM concentrations in THF solution with a total volume of 0.2 mL at −80 °C (acetone/liquid N_2 bath) in a 4 mm outer diameter quartz EPR tube. After the desired complexes were generated, tubes were immediately frozen in liquid N_2, and all spectra were recorded at 7 K (Figure S5).

Semi-Quantitative Analysis of Nitrate Anions. Inside the glove box, [$(THF)_2$(TPP)Fe^{II}] (3.34 mg, 1 mM) was dissolved in 5 mL THF in a 10 mL Schlenk flask (equipped with a magnetic stir bar) and sealed with a rubber septum. The flask was cooled at −80 °C (using acetone/liquid N_2 bath) and dry dioxygen was bubbled to the cold solution to generate [(TPP)Fe^{III}($O_2^{-\bullet}$)]. Excess dioxygen was removed by three cycles of vacuum/Ar and followed by addition of $NO_{(g)}$ by using three-way gas tight syringe to [(TPP)Fe^{III}($O_2^{-\bullet}$)]. The excess $NO_{(g)}$ was removed by several cycles of Ar/vacuum. The reaction mixture was allowed to stir for 20 min at low temperature. The solvent was then removed under vacuum and solid was redissolved in 10 mL dichloromethane and extracted with 10 mL of aqueous NaCl solution. The presence of significant amounts of nitrate ion (~85%) in the aqueous layer was confirmed by semi quantitative QUANTOFIX nitrate/nitrite test strips.

Preparation and Quantification of $NO_{(g)}$-solubilized THF solutions. $NO_{(g)}$-saturated THF solutions were prepared by bubbling $NO_{(g)}$ into 5 mL of degassed/dried THF solvent for 5 min, and this solution was left to equilibrate for 30 min. This was done under close supervision to ensure that there was no formation of brown NO_2 gas (i.e., due to air/O_2 contamination). The $NO_{(g)}$ concentration of this solution was quantified by titrating with a 50 µM solution of [(F_{20}TPP)Fe^{II}] in THF at room temperature (i.e., by conversion of [(F_{20}TPP)Fe^{II}] into [(F_{20}TPP)Fe^{II}(NO)]; see figure S1B), which was found to be 8.9 mM. Appropriate volumes of this solution were then used to add 1 equiv of NO to the bulk reactions, in place of NO gas, in the procedure described below.

Bulk-Scale Nitration of Indole Substrates. The bulk nitration reaction of all the indole substrates using [(Por)Fe^{III}($O_2^{-\bullet}$)] and $NO_{(g)}$ was carried out by a generalized procedure as follows: A 100 mL Schlenk flask containing [(TPP)Fe^{III}($O_2^{-\bullet}$)] (200 mg, 0.3 mmol) in THF (25 mL) was cooled down in an acetone/liquid N_2 bath adjusted to –80 °C. Upon temperature equilibration, dioxygen gas (or labeled $^{18}O_{2(g)}$) was bubbled through to form [(TPP)Fe^{III}($O_2^{-\bullet}$)]. Then substrate **1b** (45 mg, 0.3 mmol; in 2 mL of THF) was added to it, and subsequently, 2 mL of $NO_{(g)}$ (or labeled $^{15}NO_{(g)}$) was bubbled into the solution at –80 °C using a three-way gastight syringe. The solution was stirred at –80 °C for 30 minutes before warming to room temperature and immediately concentrated in vacuum. The final nitrated products (4-, 6-, and *N*-nitro-2,3-dimethylindole) were purified by silica gel column chromatography using DCM:hexane as an eluent, and characterized by ^{1}H and ^{13}C NMR, IR, ESI-MS and LC-MS methodologies (Figures S7-S14).

2a: Yield: 4.7 mg (9±1%); ^{1}H NMR ($CDCl_3$, 298 K): δ = 8.36 (br, 1 H), 7.81 (d, 1H), 7.60 (d, 1H), 7.20-7.19 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm) = 143.18, 139.01, 126.90, 120.59, 120.01, 117.19, 116.88, 111.66, 13.02; FT-IR (ATR, cm^{-1}): 1360, 1315, 1278, 1054, 978, 785, 728; ESI-MS: $[M+H]^+$ *m/z* = 177.06 (calc. 177.06).

2a´: Yield: 4.8 mg (9±1%); ^{1}H NMR ($CDCl_3$, 298 K): δ = 8.41 (br, 1 H), 8.33 (d, 1H), 8.01 (dd, 1H), 7.61 (d, 1H), 7.25-7.28 (m, 1H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm) = 143.29, 134.62, 132.95, 129.91, 127.70, 118.74, 114.73 109.04, 9.45; FT-IR (ATR, cm^{-1}): 1503, 1462, 1317, 1293, 1056, 872, 779, 732; ESI-MS: $[M+H]^+$ *m/z* = 177.06 (calc. 177.06).

2a´´: Yield: 7.8 mg (15±1%); ^{1}H NMR ($CDCl_3$, 298 K): δ = 8.38-8.01 (m, 3H), 7.30–7.56 (m, 2H), 2.30 (s, 3H); FT-IR (ATR, cm^{-1}): 1452, 1351, 1272; ESI-MS: $[M+H]^+$ *m/z* = 177.06 (calc. 177.06).

2b: Yield: 6 mg (10±1%); ^{1}H NMR ($CDCl_3$, 298 K): δ (ppm) = 8.28 (br, 1 H), 7.75 (d, 1H), 7.51 (d, 1H), 7.11 (t, 1H), 2.44 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6, 298 K): δ (ppm) = 137.55, 136.05, 121.22, 119.41, 117.47, 116.97, 115.51, 107.02, 12.08, 11.15; FT-IR (ATR, cm^{-1}): 1501, 1325, 1284, 1052, 824, 726; ESI-MS: $[M+H]^+$ *m/z* = 191.08 (calc. 191.08).

2b´: Yield: 4.7 mg (8±1%); ^{1}H NMR ($CDCl_3$, 298 K): δ (ppm) = 8.92 (br, 1H), 6.87(m, 1H), 6.82 (d, 1H), 6.77 (d, 1H), 3.80 (s, 3 H), 3.55 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6, 298 K): δ (ppm) = 142.23, 138.18, 134.25, 133.48, 117.46, 114.91, 108.86, 107.03, 11.99, 8.31; FT-IR (ATR, cm^{-1}): 1456, 1280, 1052, 887, 811, 754, 730; ESI-MS: $[M+H]^+$ *m/z* = 191.08 (calc. 191.08).

2c: Yield: 7.5 mg (8%); ^{1}H NMR ($CDCl_3$, 298 K): δ (ppm) = 11.80 (br, 1H), 8.28-8.25 (m, 1H), 7.83-7.79 (m, 2H), 7.52 (br, 1H), 7.25 (m, 1H), 4.38 (m, 1H), 3.53 (s, 3H), 3.26-3.01 (m, 2H), 1.77 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6, 298 K): δ (ppm) = 173.00, 169.73, 142.40, 139.61, 130.59, 120.42, 118.88, 118.71, 117.51, 109.31, 53.81, 52.09, 29.44, 22.67; FT-IR (ATR, cm^{-1}): 1729, 1643, 1509, 1431, 1313, 1240, 1107, 1052, 1007, 732; LC-MS: $[M+H]^+$ *m/z* = 306.10 (calc. 306.10).

2c′: Yield: 3.7 mg (4%); ^{1}H NMR (DMSO-d_6, 298 K): δ (ppm) = 11.70 (br, 1H), 8.38 (d, 1H), 8.32 (d, 1H), 7.92-7.89 (dd, 1H), 7.69 (d, 1H), 7.62 (d, 1H), 4.50 (m, 1H), 3.60 (s, 3H), 3.22-3.06 (ddd, 2H), 1.81 (s, 3H); 13C NMR (125 MHz, DMSO-d_6, 298 K): δ (ppm) = 173.97, 172.97, 143.24, 138.01, 130.73, 128.24, 117.85, 116.81, 112.45, 107.87, 56.52, 44.57, 30.14, 21.89; FT-IR (ATR, cm^{-1}): 1865, 1619, 1569, 1498, 1344, 1210, 1025, 973,834, 632; ESI-MS: $[M+Na]^+$ *m/z* = 328.09 (calc. 328.09).

Nitroindole yields produced when 1 equiv of NO was used for bulk reactions instead of NO gas, by means of NO-solubilized in THF (see above for details):

2a: 8±1%; **2a´**: 7±1%

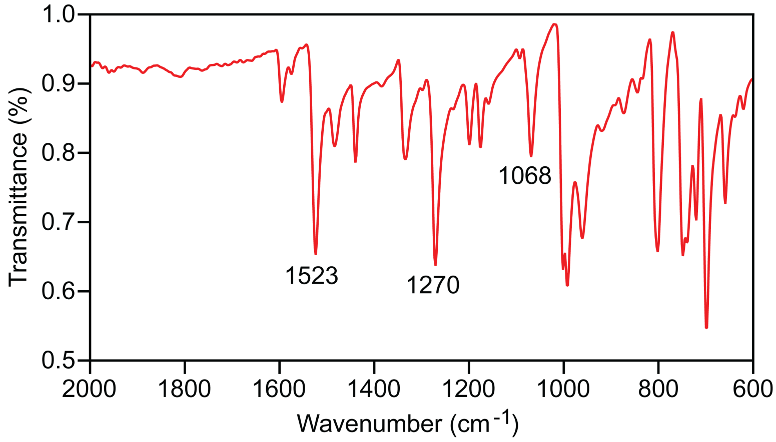
2b: 8±1%; **2b´**: 6±1%

3-Nitroindole: Yield: 2.4 mg (6.5%); ^{1}H NMR (CD_2Cl_2 , 298 K): δ (ppm) = 9.04 (br, 1H), 8.27-8.32(m, 2H), 7.57 (m, 1H), 7.41-7.49 (m, 2H); ^{13}C NMR (125 MHz, CD_2Cl_2, 298 K): δ (ppm) =135.54, 132.11,129.84, 125.94, 123.47, 120.62, 119.39, 110.63; FT-IR (ATR, cm^{-1}): 3225, 3126, 1514, 1440, 1376, 1321, 1210, 1125, 745 ; ESI-MS: $[M+H]^+$ m/z = 163.04 (calc. 163.04).

4-Nitroindole: Yield: 2.1 mg (6%); ^{1}H NMR (CD_2Cl_2, 298 K): δ (ppm) = 8.85 (br, 1H), 8.17 (d, 1H), 7.83 (d, 1H), 7.58 (t, 1H), 7.36 (d, 1H), 7.30-7.33 (m, 1H).

6-Nitroindole: Yield: 2.3 mg (6%); ^{1}H NMR (CD_2Cl_2, 298 K): δ (ppm) = 8.73 (br, 1H), 8.30 (d, 1H), 7.89-7.94 (dd, 1H), 7.60 – 7.64 (d, 1H) ,7.47 (t, 1H), 6.60 (t, 1H).

(A)



(B)

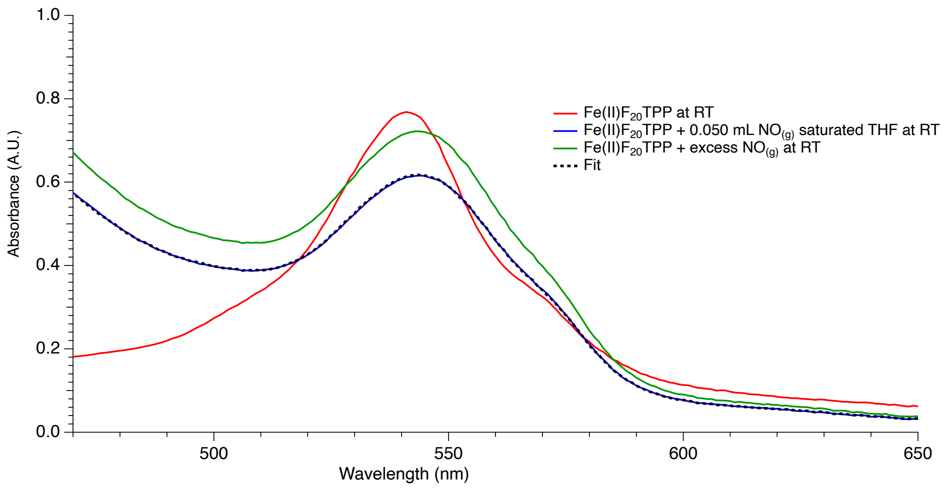


Figure S1. (A) Solid-state FT-IR spectral features corresponding to $[(TPP)Fe^{III}(NO_3)]$ prepared from the reaction between $[(TPP)Fe^{III}(O_2^{-\bullet})]$ and $NO_{(g)}$ ($\nu(NO_3)$: 1523, 1270, 1068 cm^{-1}). (B) Room temperature UV-vis spectra of 50 μM solutions of $[(F_{20}TPP)Fe^{II}]$ (red), $[(F_{20}TPP)Fe^{II}(NO)]$ (green), and $[(F_{20}TPP)Fe^{II}]$ + 50 μL of NO-saturated THF (blue) in THF. The black dashed line shows the fit wave used to deconvolute the $[(F_{20}TPP)Fe^{II}]$ + 50 μL of NO-saturated THF spectrum in order to quantify the NO concentration in THF at room temperature.

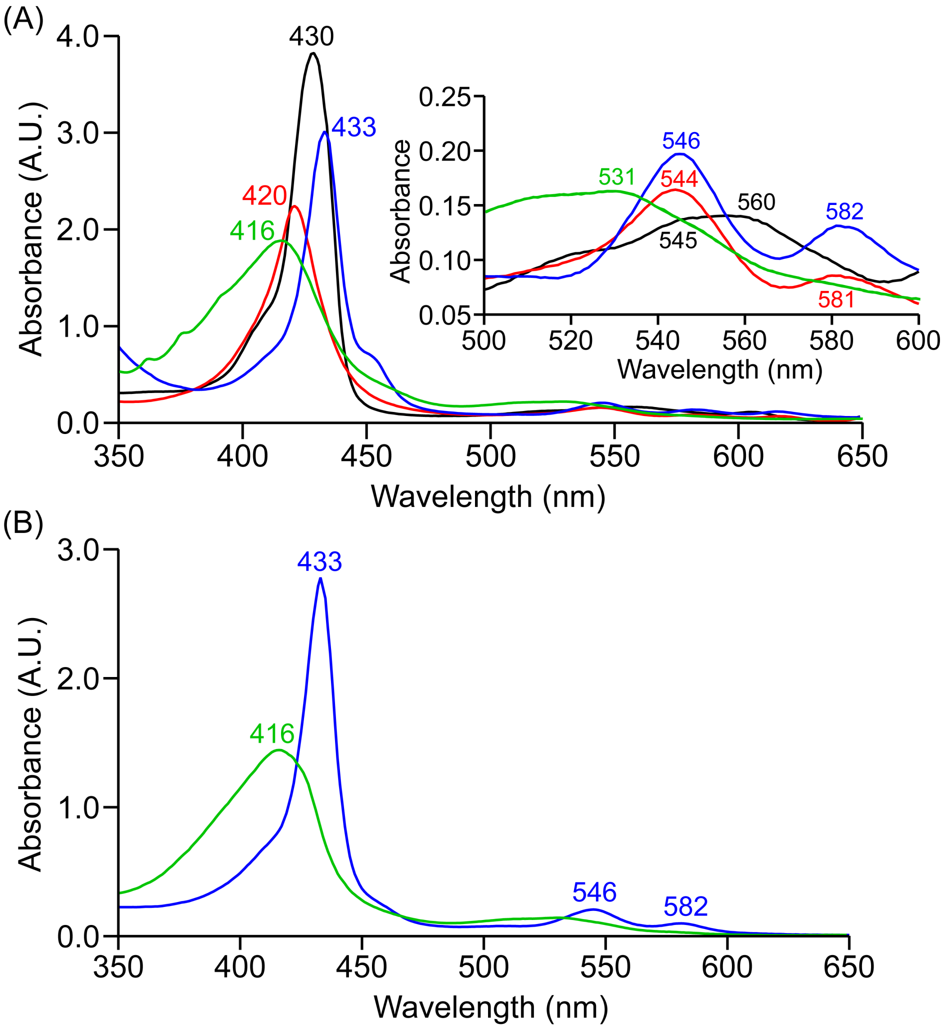


Figure S2. UV–vis spectra (in THF at –80 °C) for 50 μM solutions of (A) [$(THF)_2$(TMPP)Fe^{II}] (black), [(TMPP)Fe^{III}($O_2^{-\bullet}$)] (red), the product after bubbling of 1 mL of $NO_{(g)}$ into [(TMPP)Fe^{III}($O_2^{-\bullet}$)**]** (blue), and the final product at RT after Ar bubbling (green); inset shows the expanded Q-band region; (B) authentic [(TMPP)Fe^{III}(NO_3)] (green) and product after the addition of 1 mL of $NO_{(g)}$; i.e., [(NO)(TMPP)Fe^{III}(NO_3)] (blue).

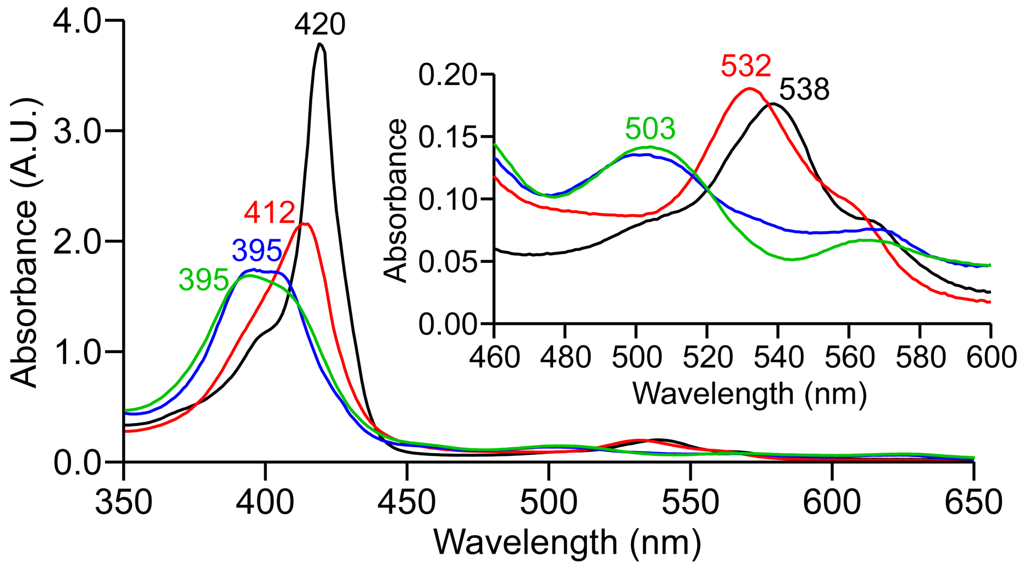


Figure S3. UV–vis spectra (in THF at –80 °C) for 50 µM solutions of (A) [(THF)$_2$(F$_{20}$TPP)Fe^{II}] (black), [(F$_{20}$TPP)Fe^{III}(O$_2^{-•}$)] (red), the product after bubbling of 1 mL of NO$_{(g)}$ into [(F$_{20}$TPP)Fe^{III}(O$_2^{-•}$)] (blue), and authentic [(F$_{20}$TPP)Fe^{III}(NO$_3$)] (green); inset shows the expanded Q-band region.

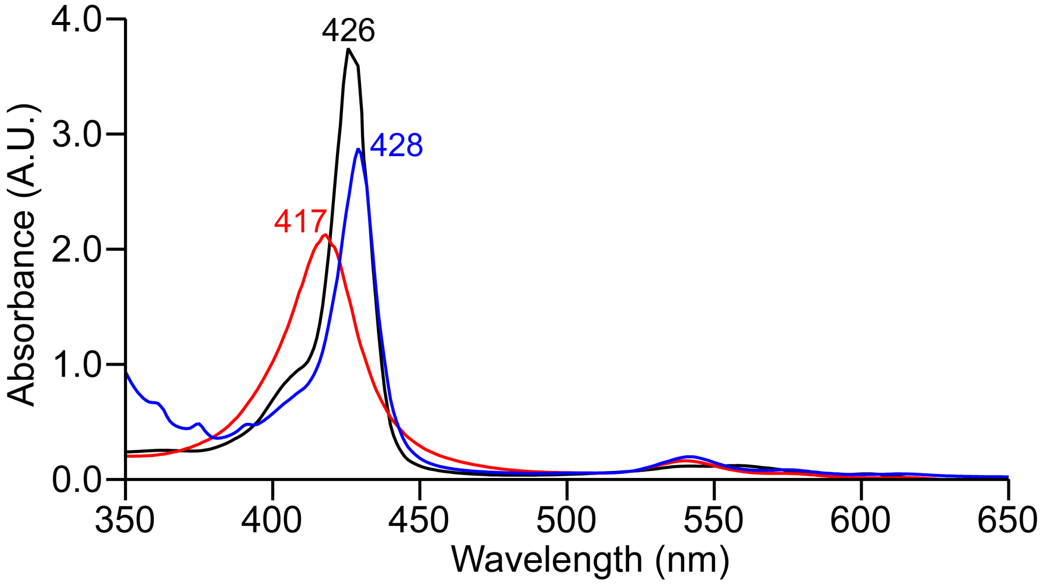


Figure S4. UV–vis spectra (in MeTHF at –135 °C) for 50 µM solutions of (A) [(THF)$_2$(TPP)Fe^{II}] (black), [(TPP)Fe^{III}(O$_2^{-•}$)] (red), the product after bubbling of 1 mL of NO$_{(g)}$ into [(TPP)Fe^{III}(O$_2^{-•}$)] (blue); i.e., [(NO)(TPP)Fe^{III}(NO$_3$)].

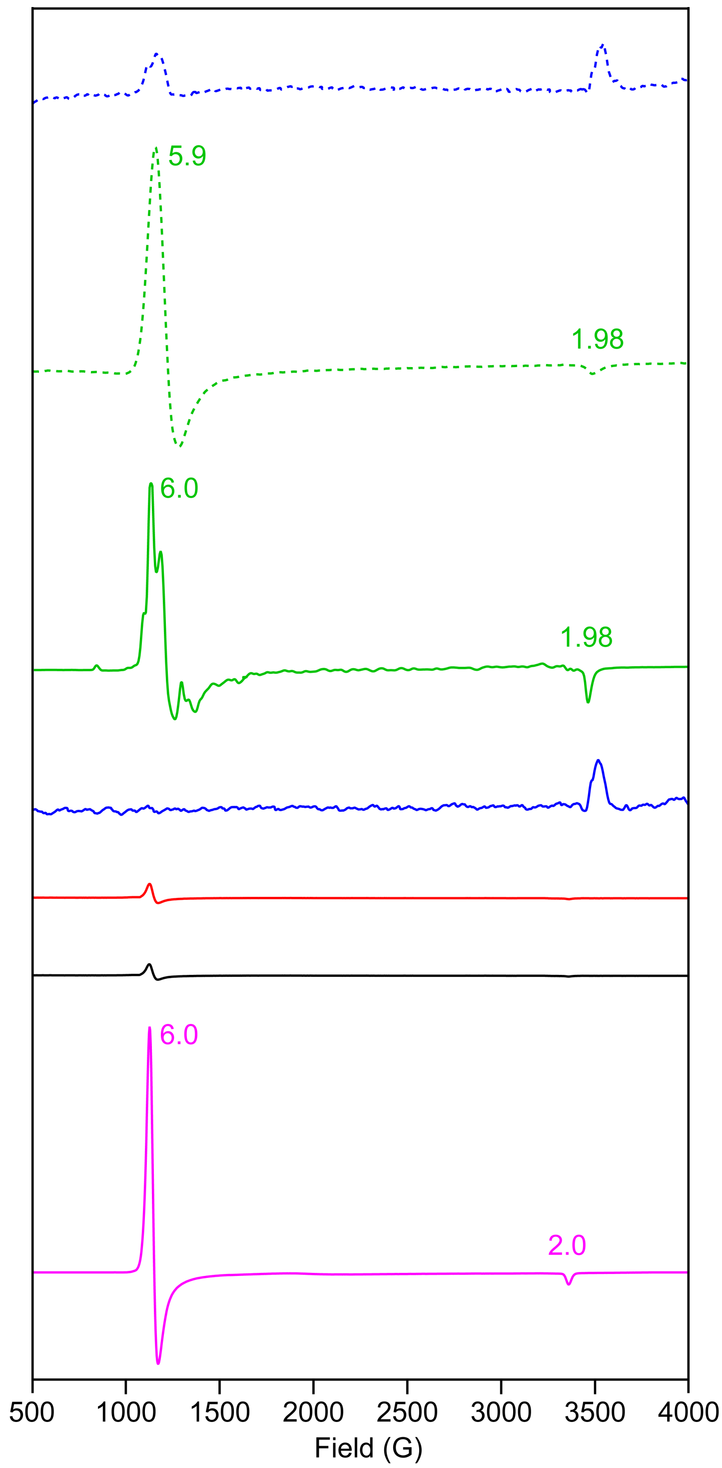


Figure S5. (Bottom to top) EPR spectral features (in frozen THF at 7 K) for 2 mM solutions of [(TPP)Fe^{III}(Cl)] (pink), [$(THF)_2$(TPP)Fe^{II}] (black), [(TPP)Fe^{III}($O_2^{-\bullet}$)] (red), the product after bubbling of 1 mL of $NO_{(g)}$ into [(TPP)Fe^{III}($O_2^{-\bullet}$)] (blue), and the final product at RT after Ar bubbling (green); authentic [(TPP)Fe^{III}(NO_3)] (green dotted) and product after the addition of 1 mL of $NO_{(g)}$ into authentic [(TPP)Fe^{III}(NO_3)] at –80 °C (blue); i.e., [(NO)(TPP)Fe^{III}(NO_3)].

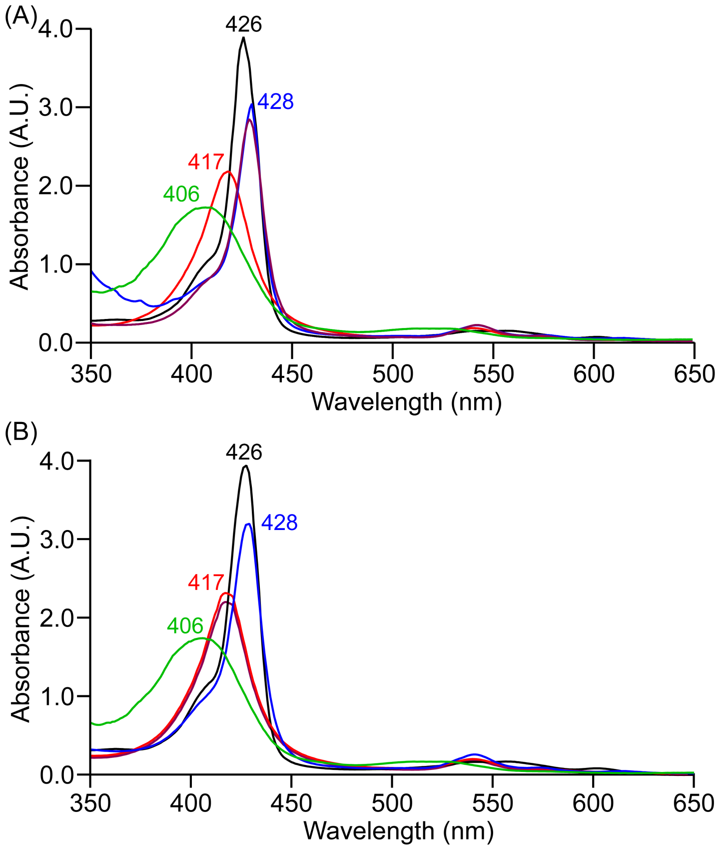


Figure S6. (A) UV–vis spectra (in THF at –80 °C) for 50 μM solutions of (A) $[(THF)_2(TPP)Fe^{II}]$ (black), $[(TPP)Fe^{III}(O_2^{-\bullet})]$ (red), the product after bubbling of 1 mL of $NO_{(g)}$ into $[(TPP)Fe^{III}(O_2^{-\bullet})]$ (blue; i.e., $[(NO)(TPP)Fe^{III}(NO_3)]$), after adding 50 equiv. of **1b** to $[(NO)(TPP)Fe^{III}(NO_3)]$ (purple), and the final product at RT after Ar bubbling (green; i.e., $[(TPP)Fe^{III}(NO_3)]$). (B) $[(THF)_2(TPP)Fe^{II}]$ (black), $[(TPP)Fe^{III}(O_2^{-\bullet})]$ (red), after adding 50 equiv. of 1,3-dimethylindole to $[(TPP)Fe^{III}(O_2^{-\bullet})]$ (purple), the product after bubbling of 1 mL of $NO_{(g)}$ into the mixture of $[(TPP)Fe^{III}(O_2^{-\bullet})]$ and 1,3-dimethylindole (blue; i.e., $[(NO)(TPP)Fe^{III}(NO_3)]$, and the final product at RT after Ar bubbling (green; i.e., $[(TPP)Fe^{III}(NO_3)]$.

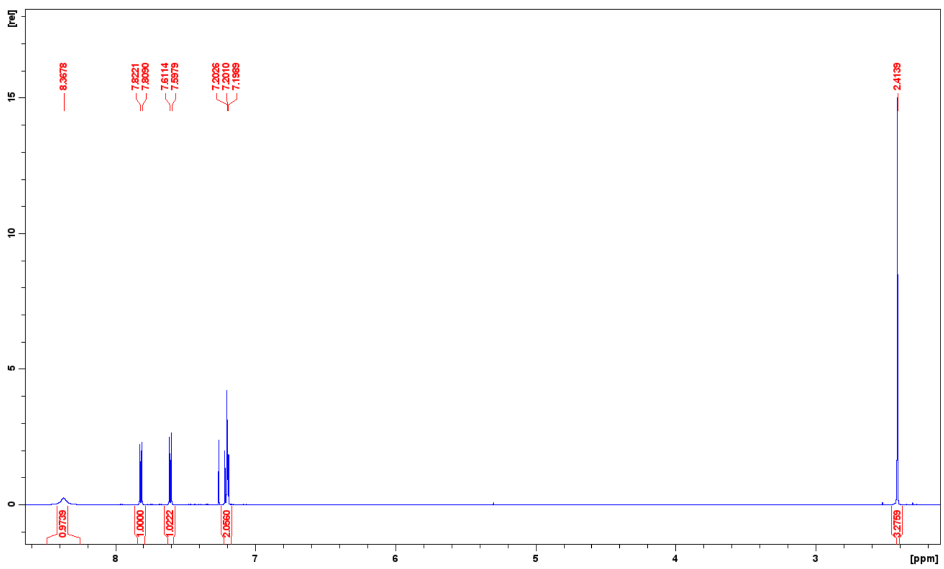


Figure S7. ^1H NMR spectrum (in $CDCl_3$ at 25 °C) of **2a**.

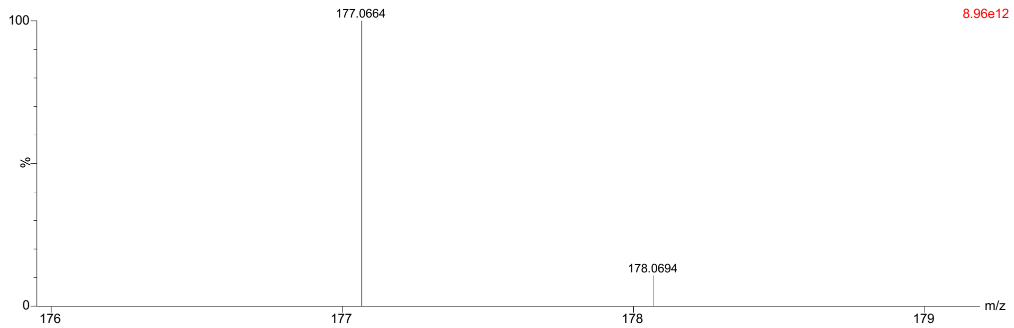


Figure S8. ESI-MS spectrum of **2a** showing $[M+H]^+$ m/z = 177.066 (calc. 177.066).

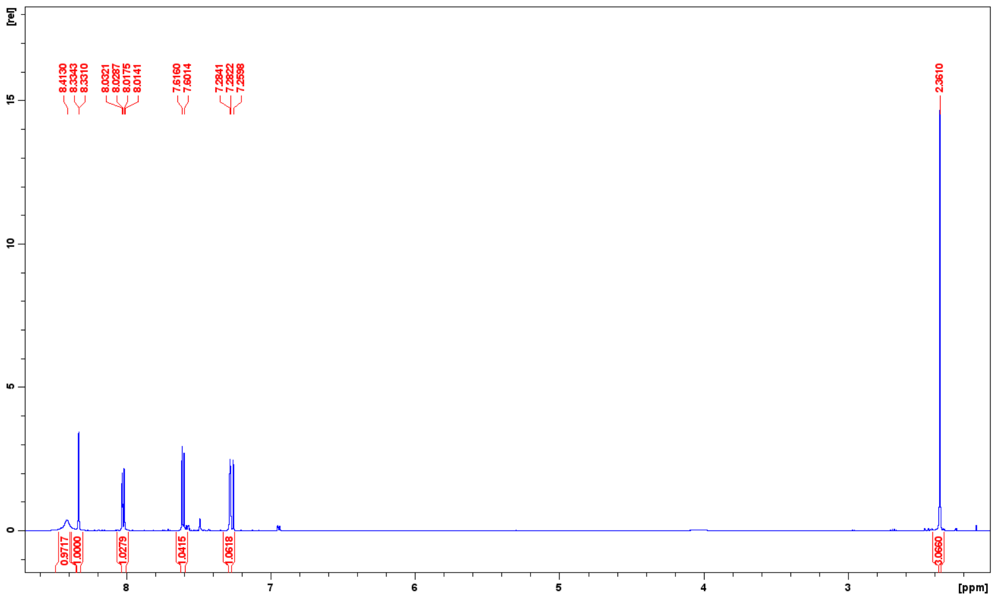


Figure S9. ^{1}H NMR spectrum (in $CDCl_3$ at 25 °C) of **2a′**.

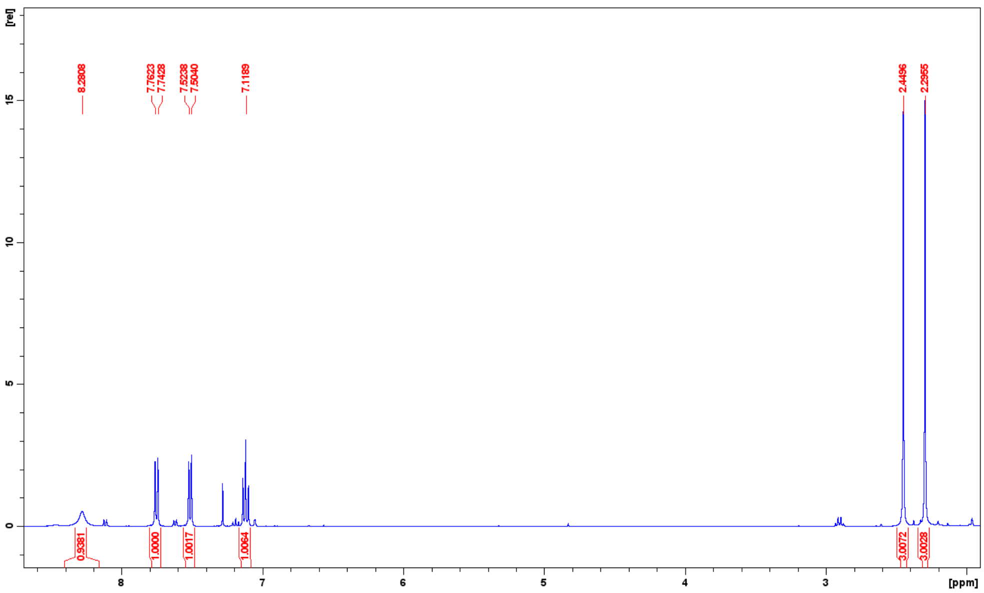


Figure S10. ^{1}H NMR spectrum (in $CDCl_3$ at 25 °C) of **2b**.

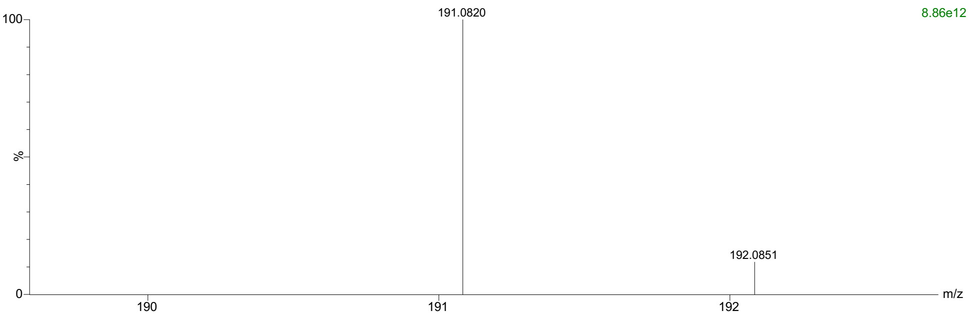


Figure S11. ESI-MS spectrum of **2b** showing $[M+H]^+$ m/z = 191.082 (calc. 191.082).

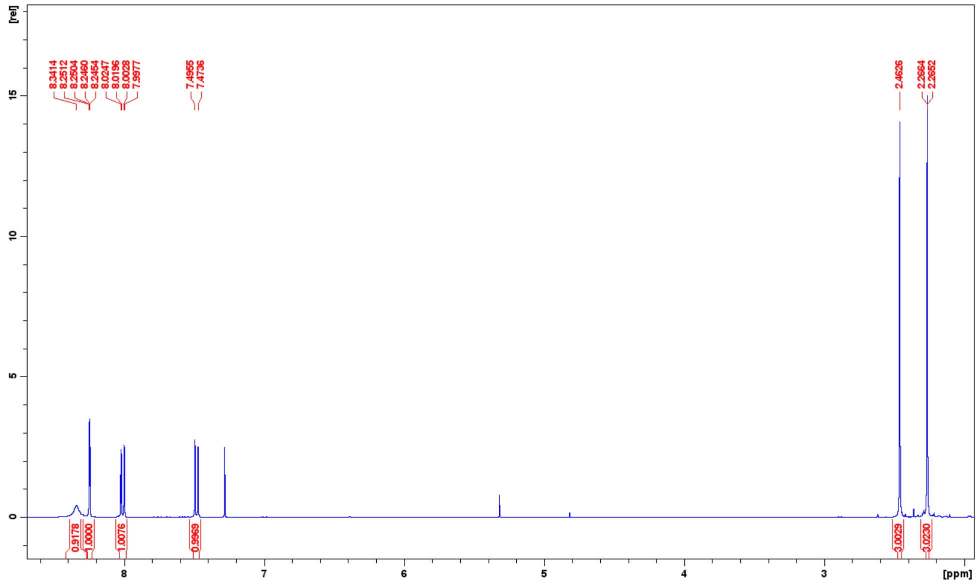


Figure S12. ^{1}H NMR spectrum (in $CDCl_3$ at 25 °C) of **2b′**.

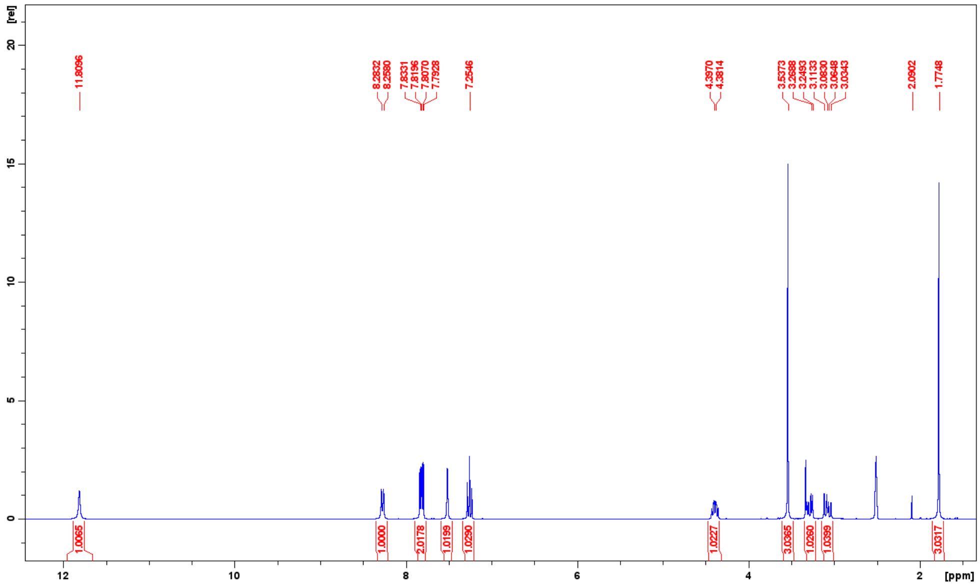


Figure S13. ^{1}H NMR spectrum (in DMSO-d_6 at 25 °C) of **2c**.

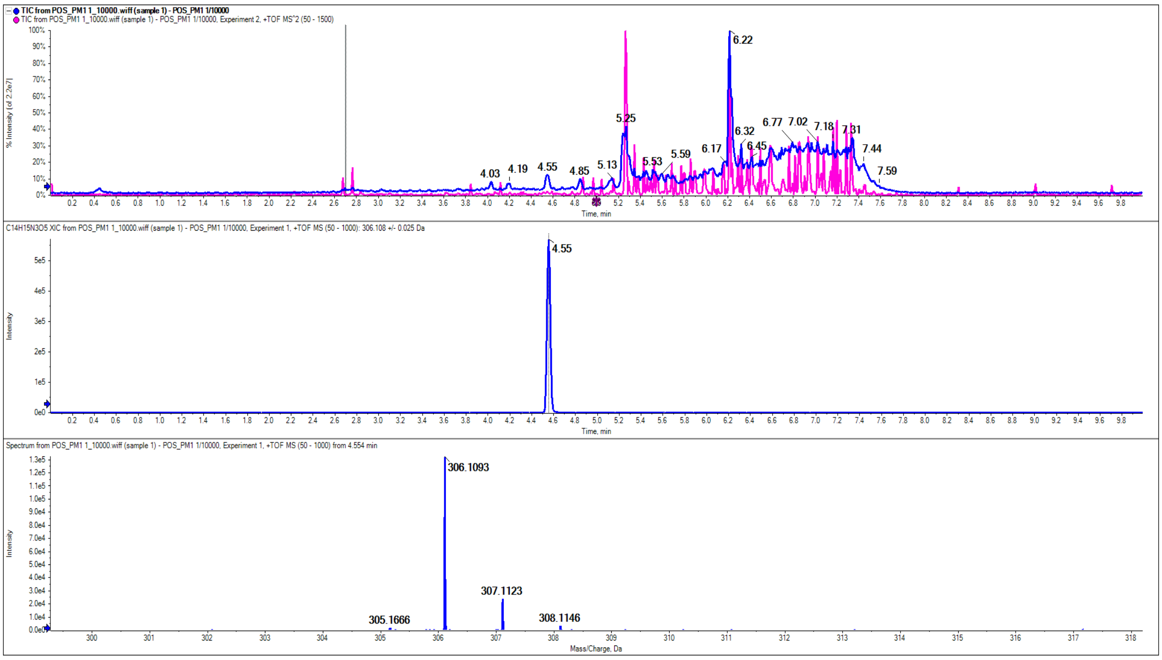
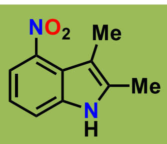
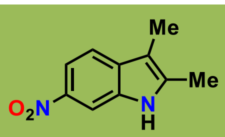
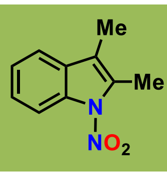


Figure S14. LC-MS spectrum of **2c** showing $[M+H]^+$ = 306.109 *m/z* (calc. 306.109).

Table S1. Product distribution of nitrated indoles from bulk reaction using $[(Por)Fe^{III}(O_2^{-\bullet})]$, $NO_{(g)}$, and **1b** (see experimental section for details on bulk reactions).

$[(Por)Fe^{III}(O_2^{-\bullet})]$			
$[(TPP)Fe^{III}(O_2^{-\bullet})]$	10 %	8 %	18 %
$[(F_{20}TPP)Fe^{III}(O_2^{-\bullet})]$	12 %	10 %	18 %
$[(TMPP)Fe^{III}(O_2^{-\bullet})]$	11 %	9 %	20 %

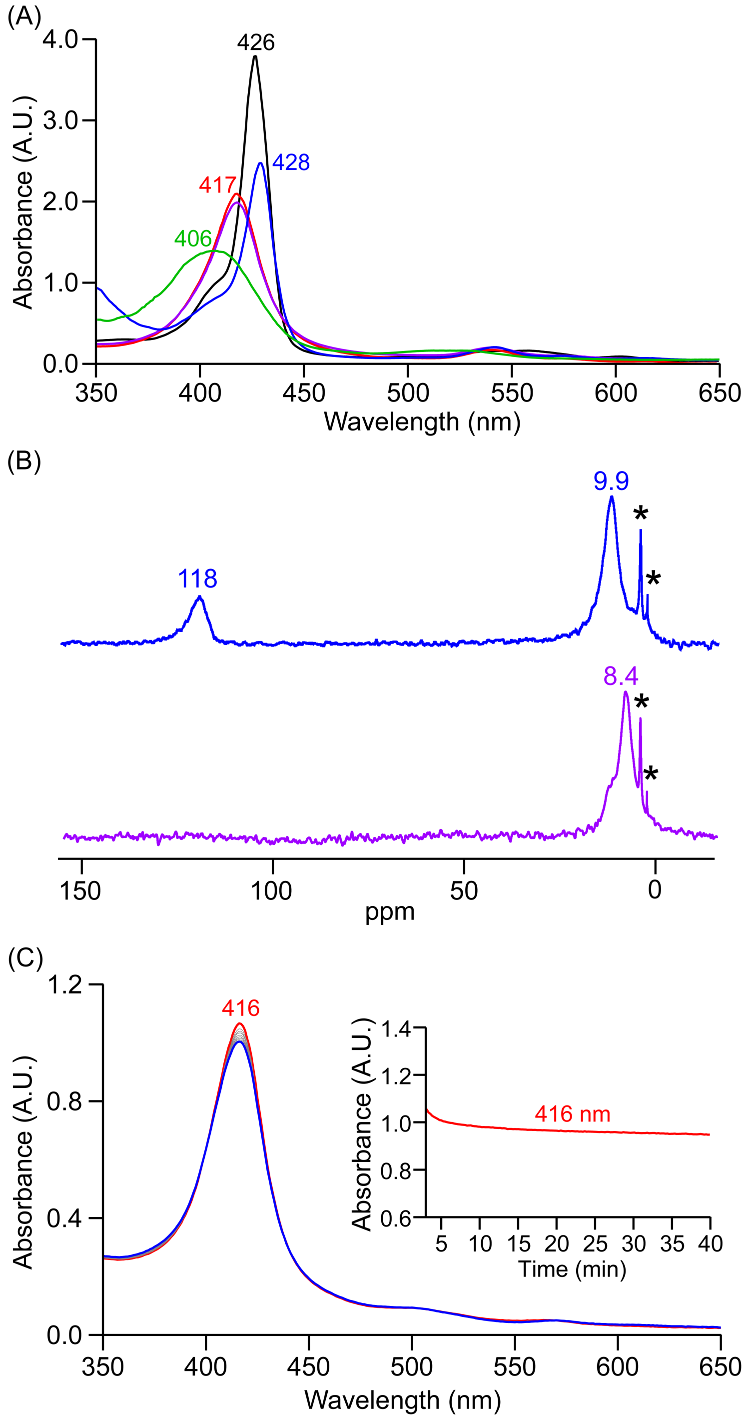


Figure S15. (A) UV–vis spectra (in THF at –80 °C) for 50 μM solutions of [(THF)$_2$(TPP)Fe^{II}] (black), [(TPP)Fe^{III}($O_2^{-\bullet}$)] (red), after adding 50 equiv. of **1b** to [(TPP)Fe^{III}($O_2^{-\bullet}$)] (purple), the product after bubbling of 1 mL of NO$_{(g)}$ into the mixture of [(TPP)Fe^{III}($O_2^{-\bullet}$)] and **1b** (blue; i.e., [(NO)(TPP)Fe^{III}(NO$_3$)], and the final product at RT after Ar bubbling (green; i.e., [(TPP)Fe^{III}(NO$_3$)]. (B) ^{2}H NMR spectra (in THF at –80 °C) of the mixture of [(TPP)Fe^{III}($O_2^{-\bullet}$)] with 50 equiv. of **1b** (purple) and the product after bubbling of 1 mL of NO$_{(g)}$ into the mixture. The peak at 118 ppm indicates the formation of minor amount of [(TPP)Fe^{III}(OH)]. (C) UV–vis spectral changes (in THF at –80 °C) upon the addition of 50 equiv. of **1b** into a 50 μM solution of [(TPP)Fe^{IV}=O]. Inset shows the time trace at 416 nm.

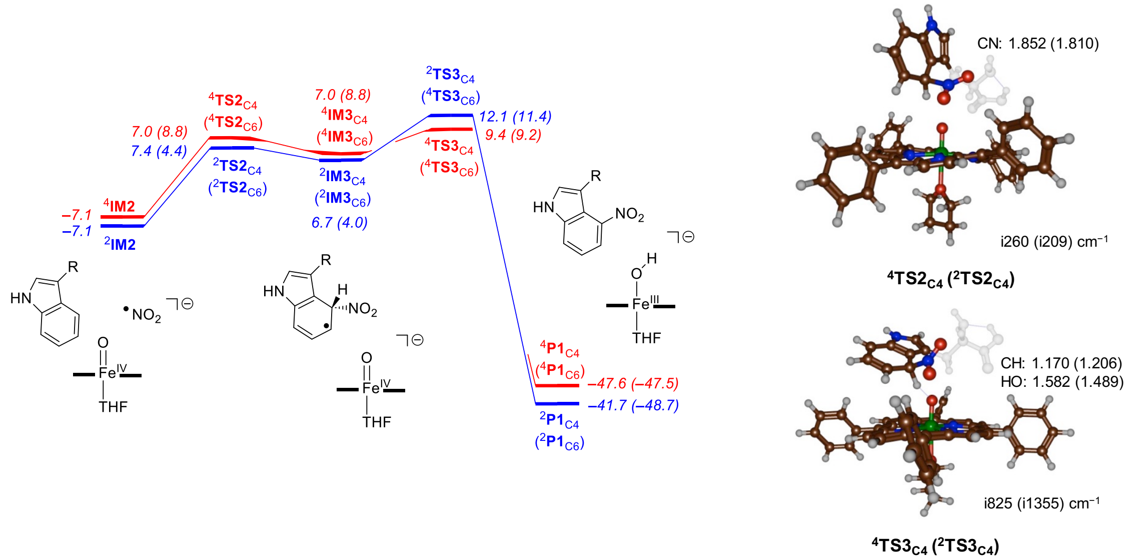
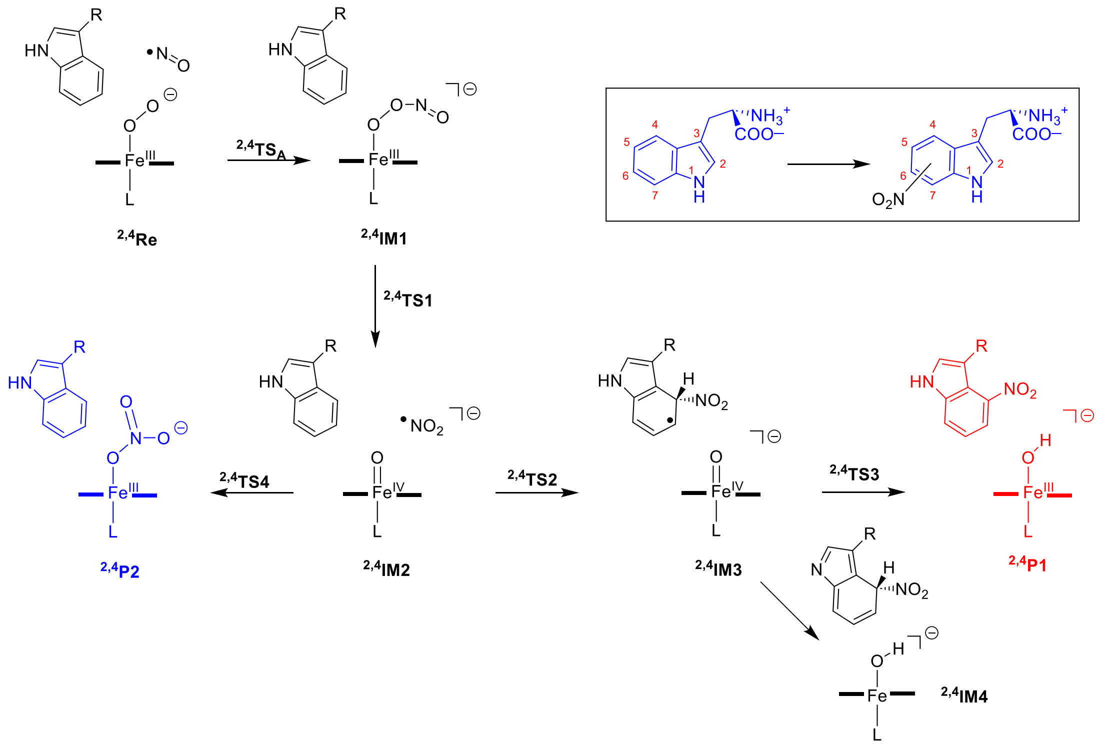


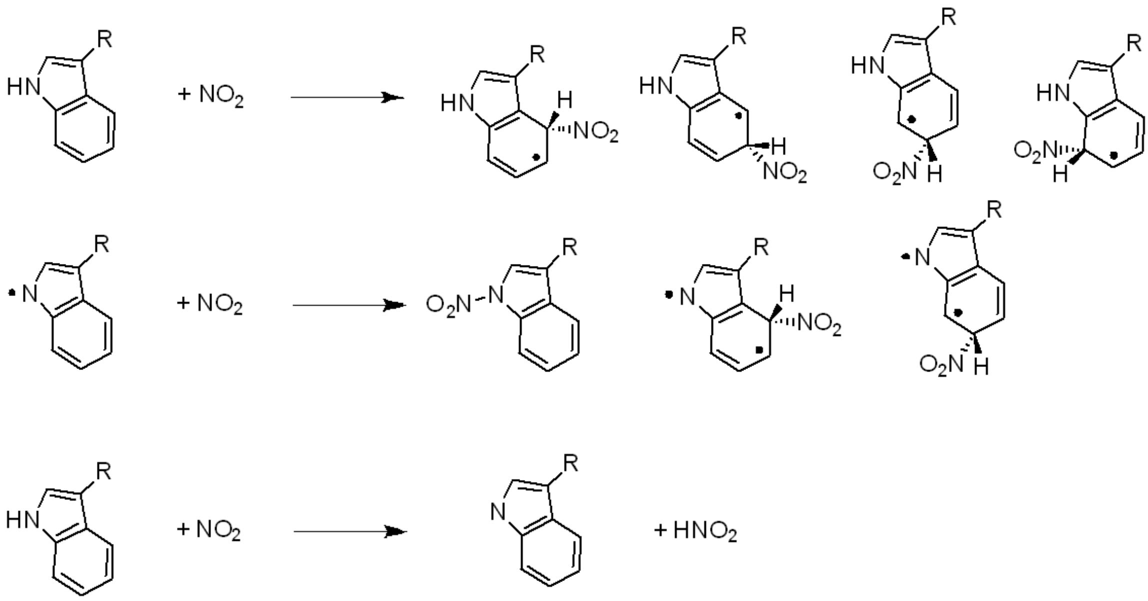
Figure S16. Potential energy landscape with ΔE+ZPE (ΔG) values in kcal mol^{-1} for the reaction of NO_2 with substrate in the presence of [Fe^{IV}(TPP)(O)(THF)] to form 4-nitroindole and 6-nitroindole products. Key transition state structures are given with bond lengths in Å and the imaginary frequency in cm^{-1}.

Figure S16 shows a pathway we investigated starting from ^{4,2}**IM2** for the direct attack of $^{\bullet}NO_2$ on the substrate in the presence of the Cpd-II complex. In particular, we investigated the pathways for $^{\bullet}NO_2$ attack on the C_4 and C_6-positions of the substrate (Figure S16) as well as the C_5-position (Figure S23). The latter pathway is considerably higher in energy than the mechanisms for C_4 and C_6 activation, hence we will focus on C_4 and C_6 positions. The attack of $^{\bullet}NO_2$ on the aromatic ring of the substrate distorts the aromaticity and creates an sp^3 hybridized carbon atom bound to $^{\bullet}NO_2$ in **IM3**. As a strong π-system is distorted, this step requires a substantial amount of energy and we calculated a barrier of 11.5 kcal mol^{-1} via ^{2}**TS2**$_{C6}$ from ^{2}**IM2**, while it is 15.9 kcal mol^{-1} in the quartet spin state. Attack on the C_4-position of substrate proceeds via the barriers ^{4}**TS2**$_{C4}$ and ^{2}**TS2**$_{C4}$ with a magnitude of 14.1 and 14.5 kcal mol^{-1}, respectively. All four pathways lead to a shallow local minimum (**IM3**) that via another barrier (**TS3**) collapses to the 4-nitroindole and 6-nitroindole products. The latter proceeds through a hydrogen atom abstraction from the *ipso*-indole position by the Cpd-II species, that reforms the aromatic system and gives an iron(III)-hydroxo complex (also see Scheme 4, Pathway 1). The hydrogen atom abstraction barriers range from 9.2 – 12.1 kcal mol^{-1} with respect to ^{2}**IM1**. The overall barrier heights for C_4- and C_6-activation are very similar and would predict analogous product distributions. Indeed, the experimental data reported above confirms this with almost equal 4-nitroindole versus 6-nitroindole products. Moreover, the indole C_4- and C_6-activation barriers are higher in energy than the barrier for nitrate formation, which is in line with the experimental observation reported above that supports the notion of nitrate formation is faster than indole nitration.

As an example, we show the transition state geometries for the C_4-activation pathway in Figure S16, while those for the C_6-activation pathways are given in Figure S24. Structurally, they are all very similar. Thus, the **TS2** transition states are characterized with an imaginary frequency of i260 cm^{-1} for ^{4}**TS2**$_{C4}$, whereas a value of i209 cm^{-1} for ^{2}**TS2**$_{C4}$ is calculated. The C−N bond in these transition states is long, namely 1.852 and 1.810 Å, respectively. By contrast, the hydrogen atom abstraction transition states have large imaginary frequencies of i825 cm^{-1} for ^{4}**TS3**$_{C4}$ and i1355 cm^{-1} for ^{2}**TS3**$_{C4}$. As such, these barriers will incur a significant amount of quantum chemical tunneling that will lower the actual barriers.[17] Next, we explored several initial hydrogen atom (H$^•$) transfer pathways, namely (i) H$^•$ transfer from substrate by iron(IV)-oxo complex and (ii) H$^•$ transfer from substrate by $^•NO_2$. Thus, we started with calculations on the H$^•$ transfer from substrate to oxidant in ^{4,2}**IM2**, whereby we ran geometry scans for the O−H distance in the presence of unbound $^•NO_2$. These geometry scans gave maxima that were considerably higher in energy than the values of ^{4,2}**TS4** (Figure 5) and ^{4,2}**TS3** (Figure S16; also see Supporting Information Figure S26). Consequently, we do not expect a H$^•$ from the N−H group of the substrate to be transferred to Cpd-II to form an iron(III) hydroxo species. Even higher H$^•$ transfer barriers were found when we ran a geometry scan for the H$^•$ transfer to Cpd-II in structures ^{4}**IM3**$_{C4}$. Therefore, the caged complex is not expected to lose a H$^•$ from the N−H group of the indole substrate.



Scheme S1. Reaction mechanisms with labelling of the structures of the pathways investigated in this work. Note that the first reaction step from **Re** to **IM1** is highly exothermic and hence **TS**$_A$ is negligible.



Scheme S2. Reaction mechanisms for cage-escape pathways calculated here.

Table S2. Absolute (free) energies of UB3LYP/BS1 optimized geometries along the reaction mechanism of [FeOO(TPP)] + NO + indole as calculated in Gaussian-09.

Species	E [BS1, au]	ZPE [au]	G [au]	E [BS2, au]
^{2}**Re**	-3235.07944	0.95059	-3234.18691	-3235.89928
^{4}**Re**	-3235.10162	0.95016	-3234.20914	-3235.92477
^{2}**IM1**	-3235.13360	0.95288	-3234.23651	-3235.95312
^{2}**TS1**	-3235.11885	0.95104	-3234.22417	-3235.93991
^{2}**IM2**	-3235.13972	0.95176	-3234.24655	-3235.96327
^{2}**TS2**$_{C4}$	-3235.12285	0.95323	-3234.22307	-3235.94164
^{2}**IM3**$_{C4}$	-3235.12367	0.95419	-3234.22338	-3235.94374
^{2}**TS2**$_{C5}$	-3235.11423	0.95290	-3234.21618	-3235.93628
^{2}**IM3**$_{C5}$	-3235.11440	0.95348	-3234.21632	-3235.93544
^{2}**TS2**$_{C6}$	-3235.12113	0.95297	-3234.22278	-3235.94617
^{2}**IM3**$_{C6}$	-3235.12176	0.95398	-3234.22222	-3235.94562
^{2}**TS4**	-3235.13830	0.95216	-3234.24111	-3235.95906
^{2}**P2**	-3235.18544	0.95557	-3234.28540	-3236.00909
^{4}**IM1**	-3235.13071	0.95103	-3234.23810	-3235.93556
^{4}**TS1**	-3235.10377	0.94891	-3234.21407	-3235.92700
^{4}**IM2**	-3235.13980	0.95187	-3234.24704	-3235.96353
^{4}**TS2**$_{C4}$	-3235.12032	0.95283	-3234.22229	-3235.94185
^{4}**IM3**$_{C4}$	-3235.12150	0.95413	-3234.22221	-3235.94185
^{4}**TS2**$_{C5}$	-3235.11162	0.95261	-3234.21532	-3235.93518
^{4}**IM3**$_{C5}$	-3235.11175	0.95329	-3234.21528	-3235.93518
^{4}**TS2**$_{C6}$	-3235.11316	0.95215	-3234.21905	-3235.93841
^{4}**IM3**$_{C6}$	-3235.11394	0.95301	-3234.21945	-3235.93806
^{4}**TS4**	-3235.13982	0.95150	-3234.24650	-3235.96095
^{4}**P2**	-3235.18125	0.95450	-3234.28186	-3236.00562
^{2}**TS3**$_{C4}$	-3235.11165	0.94975	-3234.21434	-3235.93079
^{2}**P1**$_{C4}$	-3235.20546	0.95605	-3234.30342	-3236.02282
^{2}**TS3**$_{C5}$	-3235.10845	0.95071	-3234.21078	-3235.92891
^{2}**P1**$_{C5}$	-3235.21841	0.95626	-3234.31570	-3236.04243
^{2}**TS3**$_{C6}$	-3235.11142	0.95022	-3234.21424	-3235.93224
^{2}**P1**$_{C6}$	-3235.21571	0.95657	-3234.31199	-3236.03444
^{4}**TS3**$_{C4}$	-3235.11249	0.94930	-3234.21964	-3235.93464
^{4}**P1**$_{C4}$	-3235.20355	0.95364	-3234.30684	-3236.02968
^{4}**TS3**$_{C5}$	-3235.10276	0.94871	-3234.20926	-3235.92644
^{4}**P1**$_{C5}$	-3235.20257	0.95284	-3234.30795	-3236.03154
^{4}**TS3**$_{C6}$	-3235.11476	0.94885	-3234.22182	-3235.93658
^{4}**P1**$_{C6}$	-3235.20347	0.95325	-3234.30636	-3236.02921

Table S3. Relative (free) energies of UB3LYP/BS1 optimized geometries along the reaction mechanism of [FeOO(TPP)] + NO + indole as calculated in Gaussian-09.

Species	ΔE [BS1]	ΔE+ZPE [BS1]	ΔG [BS1]	ΔE [BS2]	ΔE+ZPE [BS2]
^{2}**Re**	33.98	32.55	31.13	33.79	32.35
^{4}**Re**	20.07	18.36	17.17	17.80	16.08
^{2}**IM1**	0.00	0.00	0.00	0.00	0.00
^{2}**TS1**	9.26	8.10	7.75	8.29	7.14
^{2}**IM2**	-3.84	-4.54	-6.30	-6.37	-7.07
^{2}**TS2**$_{C4}$	6.75	6.97	8.44	7.21	7.42
^{2}**IM3**$_{C4}$	6.23	7.06	8.24	5.89	6.71
^{2}**TS2**$_{C5}$	12.15	12.17	12.76	10.57	10.58
^{2}**IM3**$_{C5}$	12.05	12.43	12.67	11.10	11.47
^{2}**TS2**$_{C6}$	7.82	7.88	8.62	4.36	4.42
^{2}**IM3**$_{C6}$	7.43	8.12	8.97	4.71	5.40
^{2}**TS4**	-2.95	-3.40	-2.88	-3.72	-4.17
^{2}**P2**	-32.53	-30.84	-30.68	-35.12	-33.43
^{4}**IM1**	1.81	0.66	-1.00	11.02	9.86
^{4}**TS1**	18.72	16.23	14.08	16.39	13.90
^{4}**IM2**	-3.89	-4.52	-6.60	-6.53	-7.17
^{4}**TS2**$_{C4}$	8.33	8.30	8.92	7.07	7.04
^{4}**IM3**$_{C4}$	7.59	8.37	8.97	7.07	7.85
^{4}**TS2**$_{C5}$	13.79	13.63	13.30	11.26	11.09
^{4}**IM3**$_{C5}$	13.71	13.97	13.33	11.26	11.51
^{4}**TS2**$_{C6}$	12.83	12.37	10.96	9.23	8.78
^{4}**IM3**$_{C6}$	12.34	12.42	10.71	9.45	9.53
^{4}**TS4**	-3.90	-4.77	-6.27	-4.91	-3.90
^{4}**P2**	-29.90	-28.89	-28.45	-32.95	-31.93
^{2}**TS3**$_{C4}$	13.78	11.81	13.91	14.01	12.05
^{2}**P1**$_{C4}$	-45.10	-43.10	-41.99	-43.74	-41.75
^{2}**TS3**$_{C5}$	15.78	14.43	16.15	15.20	13.84
^{2}**P1**$_{C5}$	-53.22	-51.10	-49.69	-56.05	-53.92
^{2}**TS3**$_{C6}$	13.92	12.25	13.98	13.10	11.43
^{2}**P1**$_{C6}$	-51.53	-49.21	-47.37	-51.03	-48.71
^{4}**TS3**$_{C4}$	13.24	11.00	10.59	11.60	9.35
^{4}**P1**$_{C4}$	-43.89	-43.42	-44.13	-48.05	-47.57
^{4}**TS3**$_{C5}$	19.35	16.73	17.10	16.74	14.12
^{4}**P1**$_{C5}$	-43.28	-43.30	-44.83	-49.22	-49.24
^{4}**TS3**$_{C6}$	11.82	9.29	9.22	9.23	6.70
^{4}**P1**$_{C6}$	-43.85	-43.61	-43.83	-47.75	-47.51

Table S4. Group spin densities of UB3LYP/BS1 optimized geometries along the reaction mechanism of [FeOO(TPP)] + NO + indole as calculated in Gaussian-09.

Species	Fe	O	NO_2	Indole	TPP	Total
^{2}**IM1**	0.98	0.06	0.00	0.00	-0.05	1.00
^{2}**TS1**	1.06	0.44	-0.45	0.00	-0.03	1.00
^{2}**IM2**	1.26	0.76	-0.98	0.00	-0.05	1.00
^{2}**TS2**$_{C4}$	1.27	0.77	-0.20	-0.79	-0.05	1.00
^{2}**IM3**$_{C4}$	1.28	0.77	-0.09	-0.90	-0.05	1.00
^{2}**TS2**$_{C5}$	1.27	0.77	-0.20	-0.79	-0.05	1.00
^{2}**IM3**$_{C5}$	1.27	0.77	-0.12	-0.87	-0.05	1.00
^{2}**TS2**$_{C6}$	1.33	0.72	-0.24	-0.76	-0.06	1.00
^{2}**IM3**$_{C6}$	1.33	0.72	-0.11	-0.88	-0.06	1.00
^{4}**IM1**	2.77	0.21	0.02	0.00	0.00	3.00
^{4}**TS1**	2.39	0.16	0.51	0.00	-0.06	3.00
^{4}**IM2**	1.29	0.78	0.99	0.00	-0.05	3.00
^{4}**TS2**$_{C4}$	1.28	0.77	0.26	0.74	-0.04	3.00
^{4}**IM3**$_{C4}$	1.28	0.77	0.09	0.91	-0.05	3.00
^{4}**TS2**$_{C5}$	1.27	0.78	0.21	0.78	-0.05	3.00
^{4}**IM3**$_{C5}$	1.27	0.78	0.13	0.87	-0.05	3.00
^{4}**TS2**$_{C6}$	1.27	0.78	0.24	0.76	-0.05	3.00
^{4}**IM3**$_{C6}$	1.27	0.78	0.10	0.90	-0.05	3.00
^{2}**TS3**$_{C4}$	0.97	0.08	0.00	0.00	-0.03	1.00
^{2}**IM4**$_{C4}$	1.13	0.68	-0.03	-0.74	-0.05	1.00
^{2}**TS3**$_{C5}$	0.96	0.09	0.00	0.00	-0.03	1.00
^{2}**IM4**$_{C5}$	1.12	0.66	-0.02	-0.71	-0.04	1.00
^{2}**TS3**$_{C6}$	0.95	0.10	0.00	-0.01	-0.04	1.00
^{2}**IM4**$_{C6}$	0.96	0.09	0.00	0.00	-0.03	1.00
^{4}**TS3**$_{C4}$	2.01	0.41	0.02	0.66	-0.08	3.00
^{4}**IM4**$_{C4}$	2.68	0.31	0.00	0.01	0.01	3.00
^{4}**TS3**$_{C5}$	1.90	0.44	0.04	0.71	-0.07	3.00
^{4}**IM4**$_{C5}$	2.64	0.35	0.00	0.00	0.02	3.00
^{4}**TS3**$_{C6}$	1.93	0.45	0.17	0.53	-0.06	3.00
^{4}**IM4**$_{C6}$	2.63	0.36	0.00	0.00	0.03	3.00
^{2}**TS4**	1.14	0.63	-0.72	0.00	-0.04	1.00
^{2}**P2**	1.04	0.00	0.00	0.00	-0.02	1.00
^{4}**TS4**	1.27	0.79	0.99	0.00	-0.05	3.00
^{4}**P2**	2.91	0.05	0.02	0.00	0.05	3.00

Table S5. Group charges of UB3LYP/BS1 optimized geometries along the reaction mechanism of [FeOO(TPP)] + NO + indole as calculated in Gaussian-09.

Species	Fe	O	NO_2	Indole	TPP	Total
^{2}**IM1**	0.66	-0.36	-0.08	-0.05	-0.18	0.00
^{2}**TS1**	0.66	-0.39	-0.10	-0.05	-0.14	0.00
^{2}**IM2**	0.63	-0.45	0.03	-0.05	-0.16	0.00
^{2}**TS2**$_{C4}$	0.62	-0.46	-0.29	0.35	-0.23	0.00
^{2}**IM3**$_{C4}$	0.63	-0.45	-0.29	0.34	-0.22	0.00
^{2}**TS2**$_{C5}$	0.62	-0.45	-0.30	0.36	-0.23	0.00
^{2}**IM3**$_{C5}$	0.62	-0.45	-0.30	0.35	-0.23	0.00
^{2}**TS2**$_{C6}$	0.67	-0.48	-0.33	0.28	-0.14	0.00
^{2}**IM3**$_{C6}$	0.67	-0.48	-0.32	0.28	-0.14	0.00
^{4}**IM1**	0.75	-0.39	-0.13	-0.06	-0.17	0.00
^{4}**TS1**	0.75	-0.46	-0.07	-0.04	-0.18	0.00
^{4}**IM2**	0.63	-0.46	0.04	-0.05	-0.16	0.00
^{4}**TS2**$_{C4}$	0.63	-0.45	-0.29	0.34	-0.22	0.00
^{4}**IM3**$_{C4}$	0.63	-0.45	-0.28	0.32	-0.21	0.00
^{4}**TS2**$_{C5}$	0.63	-0.45	-0.30	0.34	-0.22	0.00
^{4}**IM3**$_{C5}$	0.64	-0.45	-0.30	0.34	-0.22	0.00
^{4}**TS2**$_{C6}$	0.64	-0.45	-0.30	0.32	-0.21	0.00
^{4}**IM3**$_{C6}$	0.64	-0.45	-0.30	0.31	-0.21	0.00
^{2}**TS3**$_{C4}$	0.57	-0.73	-0.43	0.89	-0.30	0.00
^{2}**IM4**$_{C4}$	0.63	-0.50	-0.28	0.40	-0.25	0.00
^{2}**TS3**$_{C5}$	0.57	-0.72	-0.44	0.88	-0.29	0.00
^{2}**IM4**$_{C5}$	0.63	-0.52	-0.27	0.42	-0.26	0.00
^{2}**TS3**$_{C6}$	0.53	-0.74	-0.23	0.77	-0.33	0.00
^{2}**IM4**$_{C6}$	0.57	-0.72	-0.44	0.88	-0.29	0.00
^{4}**TS3**$_{C4}$	0.71	-0.61	-0.27	0.48	-0.31	0.00
^{4}**IM4**$_{C4}$	0.73	-0.79	-0.43	0.84	-0.34	0.00
^{4}**TS3**$_{C5}$	0.68	-0.57	-0.29	0.48	-0.29	0.00
^{4}**IM4**$_{C5}$	0.72	-0.79	-0.45	0.91	-0.38	0.00
^{4}**TS3**$_{C6}$	0.70	-0.57	-0.52	0.72	-0.33	0.00
^{4}**IM4**$_{C6}$	0.72	-0.80	-0.43	0.88	-0.36	0.00
^{2}**TS4**	0.64	-0.44	-0.05	0.03	-0.19	0.00
^{2}**P2**	0.68	-0.46	-0.07	-0.08	-0.08	0.00
^{4}**TS4**	0.61	-0.45	0.02	0.04	-0.23	0.00
^{4}**P2**	0.79	-0.47	-0.18	-0.07	-0.08	0.00

Table S6. Relative (free) energies of UB3LYP/BS1 optimized geometries along the reaction mechanism of [FeOO(TPP)] + NO + indole as calculated in Gaussian-09.

Species	Fe	O	NO_2	Indole	TPP	Total
^{2}**IM1**	0.66	-0.36	-0.08	-0.05	-0.18	0.00
^{2}**TS1**	0.66	-0.39	-0.10	-0.05	-0.14	0.00
^{2}**IM2**	0.63	-0.45	0.03	-0.05	-0.16	0.00
^{2}**TS2**$_{C4}$	0.62	-0.46	-0.29	0.35	-0.23	0.00
^{2}**IM3**$_{C4}$	0.63	-0.45	-0.29	0.34	-0.22	0.00
^{2}**TS2**$_{C5}$	0.62	-0.45	-0.30	0.36	-0.23	0.00
^{2}**IM3**$_{C5}$	0.62	-0.45	-0.30	0.35	-0.23	0.00
^{2}**TS2**$_{C6}$	0.67	-0.48	-0.33	0.28	-0.14	0.00
^{2}**IM3**$_{C6}$	0.67	-0.48	-0.32	0.28	-0.14	0.00
^{4}**IM1**	0.75	-0.39	-0.13	-0.06	-0.17	0.00
^{4}**TS1**	0.75	-0.46	-0.07	-0.04	-0.18	0.00
^{4}**IM2**	0.63	-0.46	0.04	-0.05	-0.16	0.00
^{4}**TS2**$_{C4}$	0.63	-0.45	-0.29	0.34	-0.22	0.00
^{4}**IM3**$_{C4}$	0.63	-0.45	-0.28	0.32	-0.21	0.00
^{4}**TS2**$_{C5}$	0.63	-0.45	-0.30	0.34	-0.22	0.00
^{4}**IM3**$_{C5}$	0.64	-0.45	-0.30	0.34	-0.22	0.00
^{4}**TS2**$_{C6}$	0.64	-0.45	-0.30	0.32	-0.21	0.00
^{4}**IM3**$_{C6}$	0.64	-0.45	-0.30	0.31	-0.21	0.00
^{2}**TS3**$_{C4}$	0.57	-0.73	-0.43	0.89	-0.30	0.00
^{2}**IM4**$_{C4}$	0.63	-0.50	-0.28	0.40	-0.25	0.00
^{2}**TS3**$_{C5}$	0.57	-0.72	-0.44	0.88	-0.29	0.00
^{2}**IM4**$_{C5}$	0.63	-0.52	-0.27	0.42	-0.26	0.00
^{2}**TS3**$_{C6}$	0.53	-0.74	-0.23	0.77	-0.33	0.00
^{2}**IM4**$_{C6}$	0.57	-0.72	-0.44	0.88	-0.29	0.00
^{4}**TS3**$_{C4}$	0.71	-0.61	-0.27	0.48	-0.31	0.00
^{4}**IM4**$_{C4}$	0.73	-0.79	-0.43	0.84	-0.34	0.00
^{4}**TS3**$_{C5}$	0.68	-0.57	-0.29	0.48	-0.29	0.00
^{4}**IM4**$_{C5}$	0.72	-0.79	-0.45	0.91	-0.38	0.00
^{4}**TS3**$_{C6}$	0.70	-0.57	-0.52	0.72	-0.33	0.00
^{4}**IM4**$_{C6}$	0.72	-0.80	-0.43	0.88	-0.36	0.00
^{2}**TS4**	0.64	-0.44	-0.05	0.03	-0.19	0.00
^{2}**P2**	0.68	-0.46	-0.07	-0.08	-0.08	0.00
^{4}**TS4**	0.61	-0.45	0.02	0.04	-0.23	0.00
^{4}**P2**	0.79	-0.47	-0.18	-0.07	-0.08	0.00

Table S7. Absolute (free) energies of UB3LYP/BS2 optimized geometries along the cage escape reaction mechanism of indole + NO_2 as calculated in Gaussian-09.

Species	E [BS2, au]	ZPE [BS2, au]	G [BS2, au]
^{1}**Re**	-607.7284186	0.152747	-607.600982
^{1}**P$_{C1}$**	-607.7436998	0.15766	-607.607890
^{1}**P$_{C2}$**	-607.7408957	0.157851	-607.604592
^{1}**P$_{C3}$**	-607.7459134	0.157857	-607.609847
^{1}**P$_{C4}$**	-607.7366528	0.157727	-607.600834
^{1}**P$_{N-N}$**	-607.7699448	0.158745	-607.632073
^{2}**Re**	-608.3756582	0.165872	-608.234112
^{2}**TS$_{HNO2}$**	-608.3690608	0.160867	-608.232400
^{2}**IM$_{HNO2}$**	-608.3724322	0.164678	-608.232444
^{2}**P$_{C1}$**	-608.3601945	0.168381	-608.213841
^{2}**P$_{C2}$**	-608.3514105	0.167277	-608.206199
^{2}**P$_{C3}$**	-608.3546802	0.168105	-608.208873
^{2}**P$_{C4}$**	-608.3564504	0.167637	-608.210633
^{3}**Re**	-607.7285188	0.152757	-607.601778
^{3}**P$_{C1}$**	-607.6908102	0.153702	-607.559707
^{3}**P$_{C2}$**	-607.7041975	0.153667	-607.574891
^{3}**P$_{C3}$**	-607.6937706	0.154706	-607.561698
^{3}**P$_{C4}$**	-607.7021555	0.154564	-607.570254
^{3}**P$_{N-N}$**	-607.6864301	0.155365	-607.553251

Table S8. Relative (free) energies of UB3LYP/BS1 optimized geometries along the cage escape reaction mechanism of indole + NO_2 as calculated in Gaussian-09.

Species	ΔE [BS2]	ΔE+ZPE [BS2]	ΔG [BS2]
^{1}**Re**	0.00	0.00	0.50
^{1}**P$_{C1}$**	-9.53	-6.45	-3.84
^{1}**P$_{C2}$**	-7.77	-4.57	-1.77
^{1}**P$_{C3}$**	-10.92	-7.71	-5.06
^{1}**P$_{C4}$**	-5.10	-1.99	0.59
^{1}**P$_{N-N}$**	-26.06	-22.29	-19.01
^{2}**Re**	0.00	0.00	0.00
^{2}**TS$_{HNO2}$**	3.49	0.56	6.30
^{2}**IM$_{HNO2}$**	1.37	0.83	6.27
^{2}**P$_{C1}$**	9.70	11.28	12.72
^{2}**P$_{C2}$**	15.22	16.17	17.52
^{2}**P$_{C3}$**	13.16	14.57	15.84
^{2}**P$_{C4}$**	12.05	13.16	14.73
^{3}**Re**	-0.06	-0.06	0.00
^{3}**P$_{C1}$**	23.09	23.96	26.40
^{3}**P$_{C2}$**	14.69	15.54	16.87
^{3}**P$_{C3}$**	21.32	22.76	25.15
^{3}**P$_{C4}$**	16.06	17.41	19.78
^{3}**P$_{N-N}$**	26.41	28.05	30.45

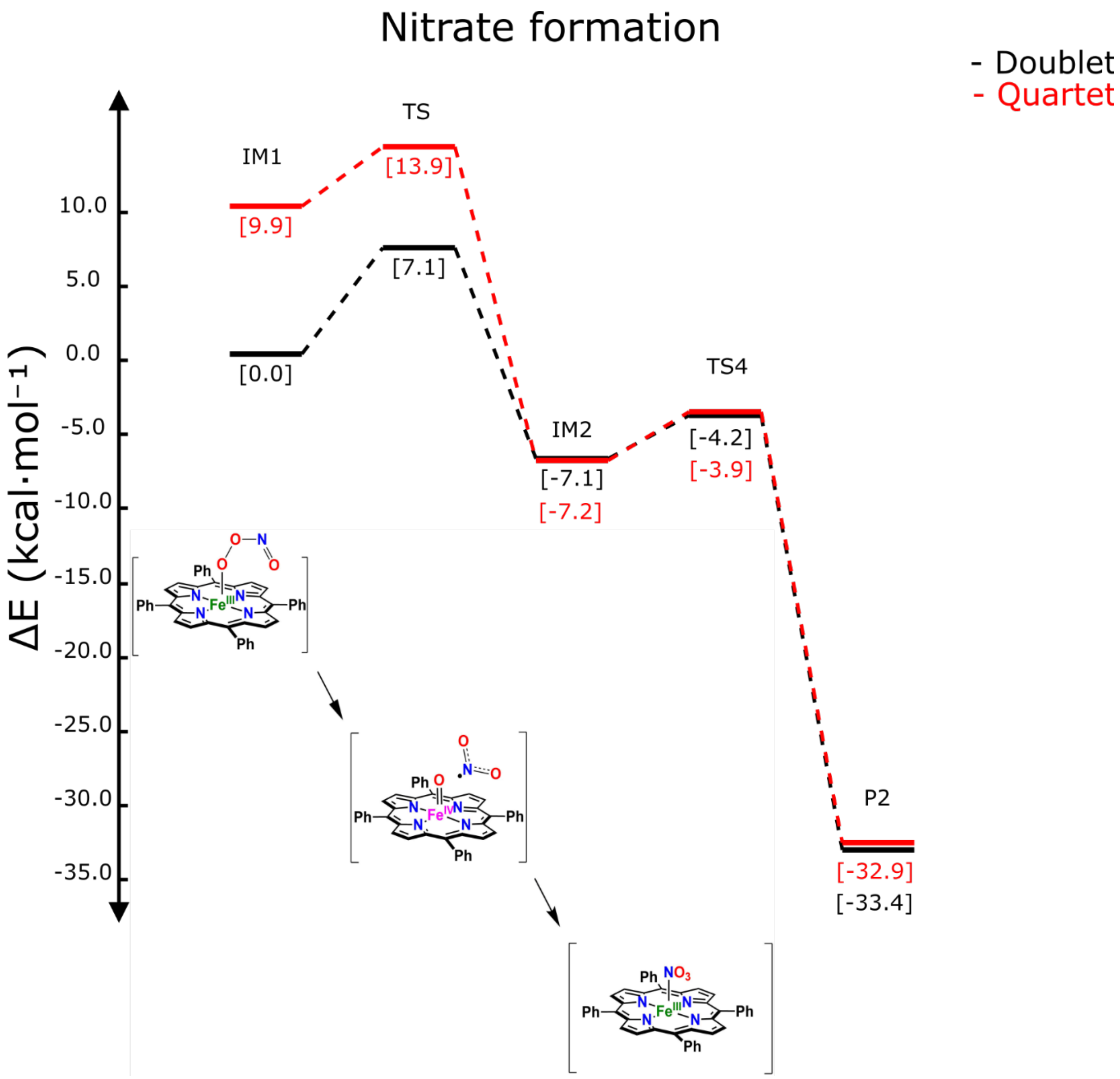


Figure S17. NO_2-transfer reaction profile to [Fe(O)(TPP)] as calculated with DFT. Spin energies shown as ΔE+ZPE values in squared brackets in kcal mol^{-1} with Quartet in red and doublet in black.

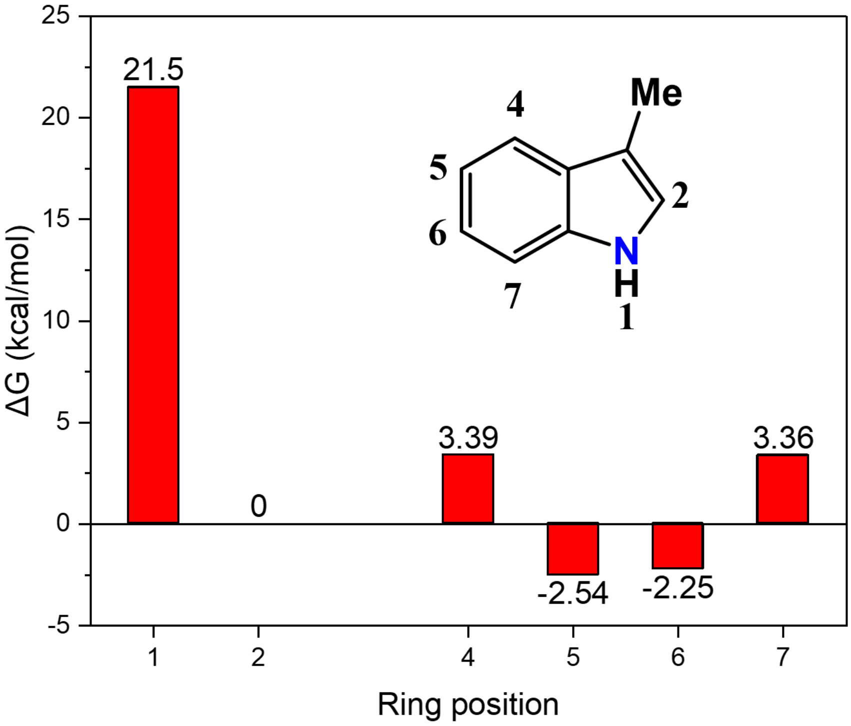
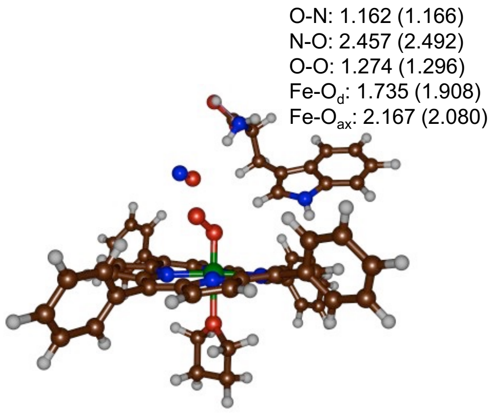


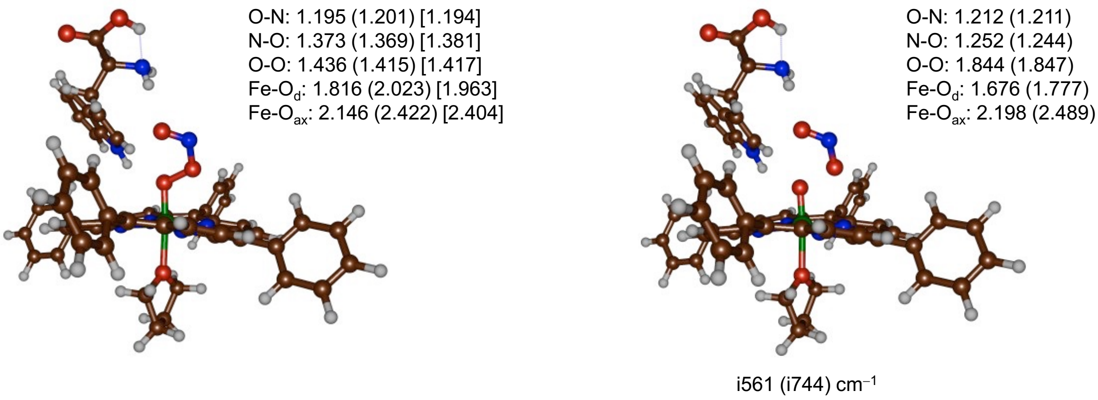
Figure S18. Relative binding energies of nitrated indole groups. Reaction calculated as described in Eq 1 for the addition of NO_2 to an indole molecule at position 1, 2, 4, 5, 6 or 7. Energies are scaled relative to addition of NO_2 at the C2 position. Energies calculated at B3LYP/6-311+G(2d,2p). The calculations show a preferential site of activation of indole and the C5 or C6 position.

$$\text{Indole-NO}_2 \rightarrow \text{Indole}\bullet + \bullet\text{NO}_2 \text{ (Eq 1)}$$



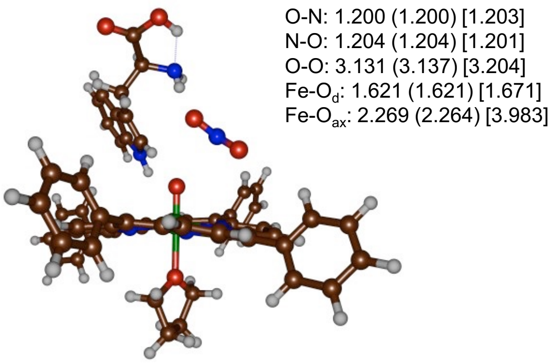
^{2}**Re** (^{4}**Re**)

Figure S19. UB3LYP/BS1 optimized geometries of the reactant complexes. Bond lengths are in angstroms.



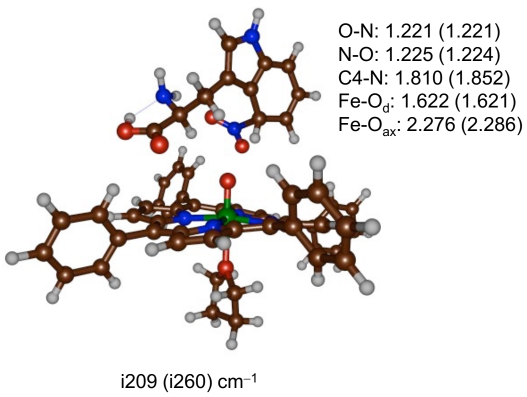
^{2}**IM1** (^{4}**IM1**) [^{6}**IM1**] ^{2}**TS1** (^{4}**TS1**)

Figure S20. UB3LYP/BS1 optimized geometries of iron-peroxynitrite complexes and their NO_2 release transition states. Bond lengths are in angstroms and the imaginary frequency in cm^{-1}.

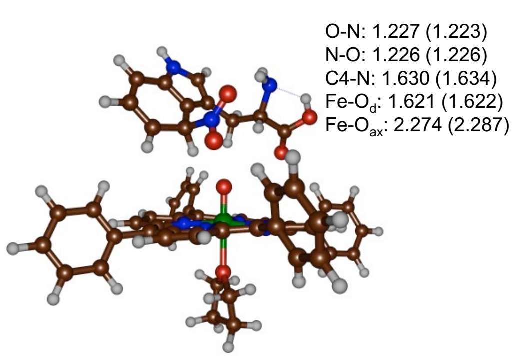


^{2}**IM2** (^{4}**IM2**) [^{6}**IM2**]

Figure S21. UB3LYP/BS1 optimized geometries of iron(IV)-oxo complexes. Bond lengths are in angstroms.



^{2}**TS2$_{C4}$** (^{4}**TS2$_{C4}$**)



^{2}**IM3$_{C4}$** (^{4}**IM3$_{C4}$**)

Figure S22. UB3LYP/BS1 optimized geometries of transition state and NO_2 addition complex for attack on the C4 position of Trp. Bond lengths are in angstroms and the imaginary frequency in cm^{-1}.

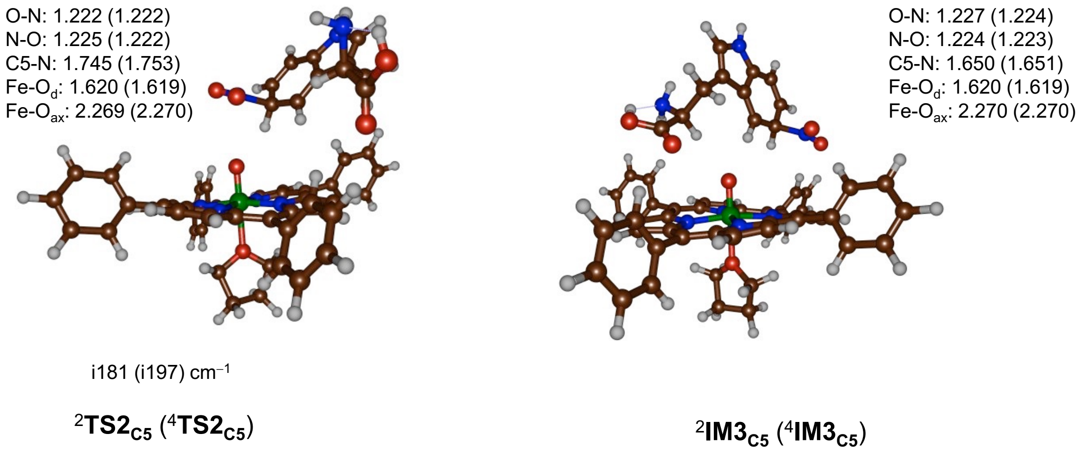


Figure S23. UB3LYP/BS1 optimized geometries of transition state and NO_2 addition complex for attack on the C5 position of Trp. Bond lengths are in angstroms and the imaginary frequency in cm^{-1}.

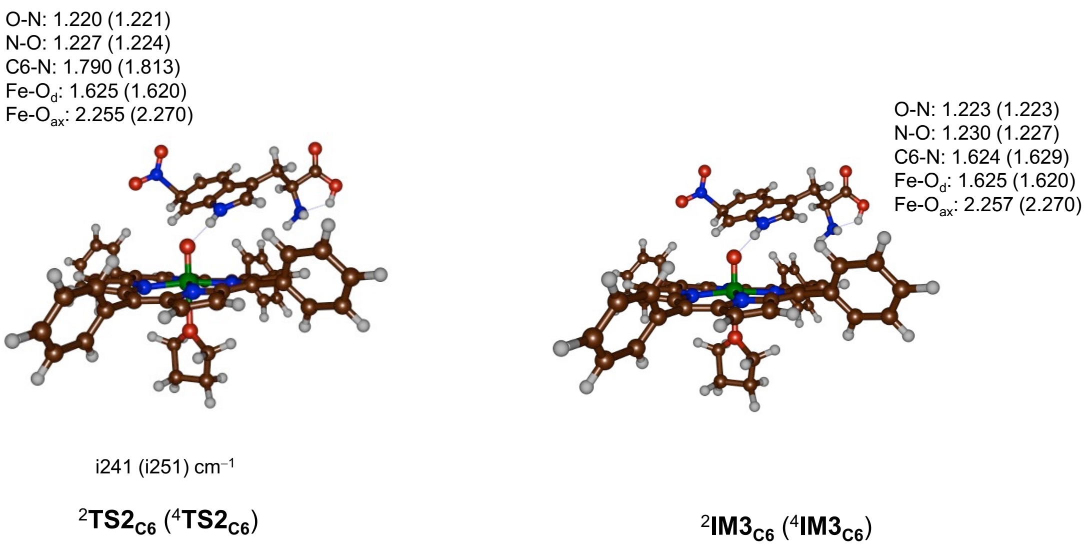
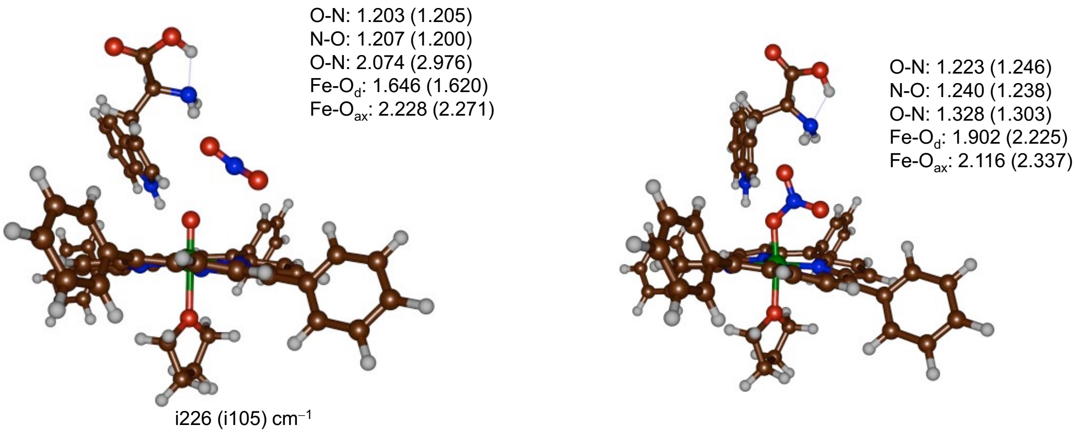


Figure S24. UB3LYP/BS1 optimized geometries of transition state and NO_2 addition complex for attack on the C6 position of Trp. Bond lengths are in angstroms and the imaginary frequency in cm^{-1}.



^{2}**TS4** (^{4}**TS4**) ^{2}**P2** (^{4}**P2**)

Figure S25. UB3LYP/BS1 optimized geometries of transition state and nitrate complex. Bond lengths are in angstroms and the imaginary frequency in cm^{-1}.

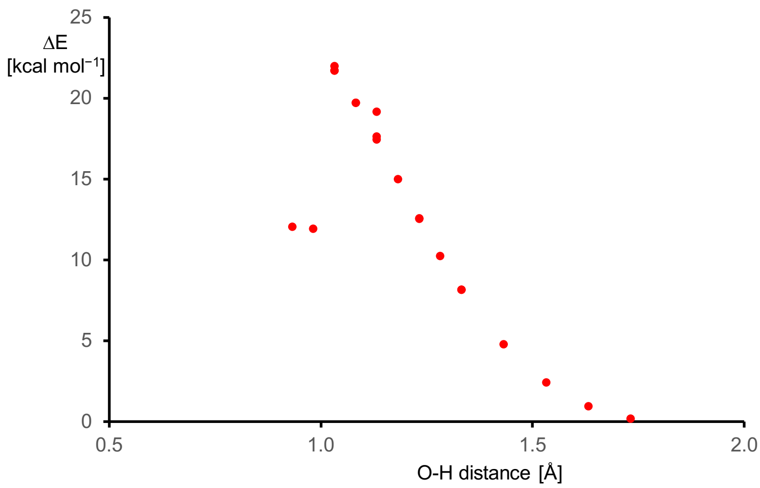


Figure S26. UB3LYP/BS1 calculated constraint geometry scan for proton transfer from the N−H group of substrate to the iron(IV)-oxo species in the presence of NO_2, i.e. from structure ^{4}**IM2**. As can be seen, the proton transfer requires 24 kcal mol^{-1} in energy and hence is considerably higher in energy than NO_2 transfer.

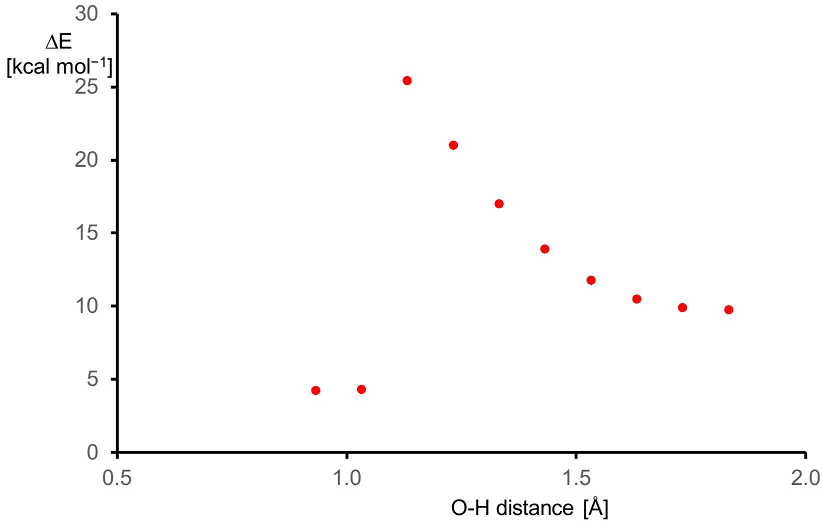


Figure S27. UB3LYP/BS1 calculated constraint geometry scan for proton transfer from the N−H group of substrate to CpdII in the NO_2-bound radical intermediate, i.e. from structure ^{4}**IM3**. As can be seen, the proton transfer requires 26 kcal mol^{-1} in energy and hence is considerably higher in energy than NO_2 transfer.

Cartesian coordinates of optimized geometries.

²Re:

26	0.508686000	0.071391000	0.190949000
7	2.059255000	-0.144107000	-1.039290000
7	0.251211000	-1.906142000	0.236795000
7	-0.958929000	0.290813000	1.561790000
7	0.838370000	2.062155000	0.270099000
6	1.070923000	-2.864303000	-0.322126000
6	0.578416000	-4.180842000	0.000726000
6	-0.571680000	-4.011726000	0.707183000
6	-0.770598000	-2.590273000	0.856212000
6	-1.822651000	-2.027647000	1.593791000
6	-1.878691000	-0.667852000	1.928313000
6	-2.882201000	-0.082769000	2.786355000
6	-2.529127000	1.218728000	2.977502000
6	-1.333036000	1.449982000	2.201583000
6	-0.723443000	2.706326000	2.074979000
6	0.286069000	2.972661000	1.142108000
6	0.852310000	4.281593000	0.910283000
6	1.707880000	4.162318000	-0.139289000
6	1.701608000	2.771629000	-0.531073000
6	2.529314000	2.239355000	-1.529860000
6	2.694961000	0.862902000	-1.735216000
6	3.617527000	0.292402000	-2.686801000
6	3.563535000	-1.058344000	-2.533171000
6	2.580565000	-1.327963000	-1.513588000
6	2.183773000	-2.618074000	-1.136147000
8	-0.593679000	0.317666000	-1.125981000
8	-0.614212000	-0.476599000	-2.121983000
6	-1.227424000	3.824577000	2.934748000
6	-0.979373000	3.821410000	4.316939000
6	-1.964400000	4.886380000	2.384806000
6	-1.449357000	4.856297000	5.128205000
1	-0.410428000	3.005102000	4.753804000
6	-2.435893000	5.920096000	3.196655000
1	-2.178934000	4.891532000	1.319699000
6	-2.178818000	5.908898000	4.569998000
1	-1.243564000	4.840048000	6.195081000
1	-3.009146000	6.731021000	2.755621000
1	-2.546089000	6.713759000	5.200768000
6	-2.899880000	-2.940244000	2.092450000
6	-3.047405000	-3.212135000	3.462650000
6	-3.781539000	-3.553946000	1.187301000
6	-4.052036000	-4.069540000	3.915632000
1	-2.364503000	-2.755007000	4.173388000
6	-4.787455000	-4.409836000	1.640120000
1	-3.678456000	-3.352319000	0.124563000
6	-4.926075000	-4.669782000	3.005797000
1	-4.147816000	-4.271503000	4.979016000
1	-5.463506000	-4.871142000	0.925360000
1	-5.708232000	-5.336452000	3.358305000
6	2.952192000	-3.780212000	-1.683574000
6	4.282381000	-3.998029000	-1.288035000
6	2.372552000	-4.666651000	-2.606385000
6	5.010513000	-5.076271000	-1.794516000
1	4.743328000	-3.319917000	-0.575013000
6	3.101179000	-5.743712000	-3.114787000
1	1.348959000	-4.503317000	-2.931752000
6	4.421758000	-5.952897000	-2.709218000
1	6.036607000	-5.231561000	-1.472354000

1	2.637579000	-6.415981000	-3.831625000
1	4.988258000	-6.791477000	-3.104619000
6	3.304248000	3.195989000	-2.381771000
6	4.700628000	3.302127000	-2.277290000
6	2.633328000	4.018317000	-3.301856000
6	5.407956000	4.205445000	-3.073332000
1	5.230648000	2.678175000	-1.562901000
6	3.340742000	4.919624000	-4.099725000
1	1.553568000	3.939604000	-3.395731000
6	4.730001000	5.016220000	-3.987166000
1	6.487770000	4.277848000	-2.975719000
1	2.806083000	5.544155000	-4.810224000
1	5.280381000	5.718803000	-4.606821000
1	4.226961000	0.856953000	-3.376844000
1	4.115467000	-1.810030000	-3.077951000
1	1.048697000	-5.109575000	-0.286329000
1	-1.218479000	-4.774941000	1.114279000
1	-3.729858000	-0.607298000	3.202014000
1	-3.035627000	1.963565000	3.573937000
1	0.613203000	5.171214000	1.474071000
1	2.311485000	4.933257000	-0.595411000
8	1.886957000	-0.115662000	1.852012000
6	1.789778000	-1.125767000	2.889315000
6	3.092724000	0.676739000	2.020705000
6	2.796568000	-0.694239000	3.952929000
1	0.755291000	-1.151698000	3.235782000
6	3.898217000	-0.043272000	3.102943000
1	3.600484000	0.732886000	1.056192000
1	2.798847000	1.685147000	2.330604000
1	4.538047000	-0.812923000	2.656261000
1	4.533377000	0.644929000	3.667713000
1	3.151985000	-1.538765000	4.550148000
1	2.347812000	0.041887000	4.629911000
1	2.047263000	-2.098979000	2.456259000
1	-3.333822000	2.847850000	-3.957992000
7	-4.248045000	3.198544000	-4.243473000
1	-4.939808000	2.553882000	-3.870824000
1	-5.541122000	4.696555000	-3.597994000
1	-3.899244000	5.951930000	-2.190611000
6	-4.460277000	4.561200000	-3.728716000
6	-3.756704000	4.883885000	-2.389852000
6	-4.253875000	4.053048000	-1.243042000
6	-4.053764000	5.562243000	-4.829506000
8	-3.895527000	4.994869000	-6.030998000
1	-4.049159000	4.022340000	-5.851887000
8	-3.914876000	6.755328000	-4.644303000
1	-2.677143000	4.732909000	-2.520638000
1	-2.652668000	2.544345000	-0.890954000
6	-3.618257000	2.977411000	-0.665564000
7	-4.405258000	2.437736000	0.332718000
1	-4.115806000	1.699436000	0.960914000
1	-8.576874000	3.833824000	1.821522000
6	-7.714868000	3.920754000	1.165571000
6	-7.682522000	4.945632000	0.195108000
6	-6.596325000	5.088997000	-0.661461000
6	-5.515235000	4.193555000	-0.552753000
1	-6.582453000	5.886789000	-1.400101000
1	-8.521175000	5.632613000	0.119476000
1	-6.685451000	2.232784000	2.047212000
6	-6.662180000	3.020722000	1.299335000
6	-5.570785000	3.167082000	0.434150000
7	-0.979652000	0.993988000	-4.056358000

8	-1.098352000	2.058741000	-3.606969000

[4]Re:

26	0.513871000	0.032432000	0.250279000
7	2.022107000	-0.144637000	-1.043561000
7	0.254196000	-1.947097000	0.281661000
7	-0.992193000	0.218582000	1.573155000
7	0.787579000	2.024286000	0.256255000
6	1.097739000	-2.883788000	-0.273401000
6	0.637287000	-4.211552000	0.056501000
6	-0.518802000	-4.069834000	0.758780000
6	-0.754007000	-2.654673000	0.900931000
6	-1.821416000	-2.111246000	1.627189000
6	-1.903444000	-0.747991000	1.942304000
6	-2.923778000	-0.165052000	2.777403000
6	-2.589836000	1.144290000	2.954819000
6	-1.390255000	1.383174000	2.189239000
6	-0.798492000	2.647551000	2.053246000
6	0.208911000	2.926912000	1.121374000
6	0.736322000	4.247442000	0.872315000
6	1.586569000	4.143645000	-0.184707000
6	1.619860000	2.752578000	-0.562289000
6	2.439967000	2.235925000	-1.574952000
6	2.623700000	0.862739000	-1.771375000
6	3.536541000	0.294570000	-2.731216000
6	3.514510000	-1.053298000	-2.549489000
6	2.557827000	-1.325367000	-1.503871000
6	2.197684000	-2.618640000	-1.100020000
8	-0.749905000	0.349164000	-1.143714000
8	-0.772733000	-0.539849000	-2.086533000
6	-1.325948000	3.763871000	2.902036000
6	-1.070121000	3.782283000	4.282603000
6	-2.093410000	4.799210000	2.343591000
6	-1.561816000	4.814167000	5.084733000
1	-0.478413000	2.985572000	4.725421000
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1	-2.314159000	4.785766000	1.279780000
6	-2.321549000	5.840840000	4.518637000
1	-1.349792000	4.815584000	6.150496000
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6	-2.883568000	-3.038626000	2.128458000
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6	-4.728727000	-4.561314000	1.678178000
1	-3.621608000	-3.508601000	0.157888000
6	-4.882580000	-4.796238000	3.046746000
1	-4.144968000	-4.339293000	5.022861000
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1	-5.654375000	-5.473827000	3.401216000
6	2.989877000	-3.768545000	-1.640616000
6	4.326601000	-3.951871000	-1.250013000
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6	5.077371000	-5.016880000	-1.751571000
1	4.775154000	-3.257052000	-0.545191000
6	3.177824000	-5.739051000	-3.057220000
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6	4.504801000	-5.914188000	-2.656405000
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1	2.726774000	-6.427520000	-3.766635000
1	5.088830000	-6.742386000	-3.048159000
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6	5.245599000	4.249317000	-3.186345000
1	5.128086000	2.733999000	-1.658074000
6	3.145657000	4.906263000	-4.184846000
1	1.393158000	3.891776000	-3.442520000
6	4.534063000	5.035211000	-4.096391000
1	6.325013000	4.346677000	-3.108241000
1	2.585431000	5.510803000	-4.892881000
1	5.057923000	5.743482000	-4.732324000
1	4.120854000	0.859066000	-3.442619000
1	4.071076000	-1.804101000	-3.090735000
1	1.131733000	-5.129079000	-0.225853000
1	-1.146878000	-4.847447000	1.167758000
1	-3.769514000	-0.694898000	3.190040000
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1	0.473624000	5.135972000	1.427113000
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8	1.851656000	-0.131900000	1.834924000
6	1.697538000	-1.046445000	2.959002000
6	3.086989000	0.632311000	1.956845000
6	2.747065000	-0.598226000	3.972873000
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6	3.868539000	-0.063680000	3.068471000
1	3.582009000	0.622271000	0.985529000
1	2.823261000	1.661601000	2.219379000
1	4.459008000	-0.892034000	2.661052000
1	4.547385000	0.623148000	3.581361000
1	3.067395000	-1.420310000	4.618865000
1	2.350842000	0.203601000	4.606178000
1	1.880715000	-2.063069000	2.597029000
1	-3.307308000	2.871635000	-4.030914000
7	-4.195172000	3.306764000	-4.281711000
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6	-4.093385000	4.038083000	-1.243071000
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[2]IM1:

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7	0.824618000	2.153517000	0.481163000
6	0.939222000	-2.729326000	-0.378634000
6	0.423220000	-4.049047000	-0.111452000
6	-0.712763000	-3.890446000	0.619645000
6	-0.878554000	-2.474503000	0.842392000
6	-1.901961000	-1.928588000	1.630262000
6	-1.921055000	-0.588228000	2.039609000
6	-2.886006000	-0.037298000	2.961013000
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6	1.660215000	4.270364000	0.097283000
6	1.652588000	2.892272000	-0.332540000
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6	3.398454000	-0.858766000	-2.569282000
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1	3.113273000	-1.677599000	4.520824000
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6	-7.318100000	5.152526000	-0.004454000
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1	-6.243770000	5.757912000	-1.770945000
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[4]IM1:

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7	0.925608000	2.179441000	0.481323000
6	0.918117000	-2.684518000	-0.474959000
6	0.416379000	-4.003226000	-0.191877000
6	-0.683204000	-3.852254000	0.596448000
6	-0.846864000	-2.441779000	0.828069000
6	-1.852785000	-1.901790000	1.639198000
6	-1.875792000	-0.555517000	2.021057000
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6	-2.485420000	1.304620000	3.139273000
6	-1.307680000	1.553091000	2.348746000
6	-0.661140000	2.791960000	2.285762000
6	0.385693000	3.058895000	1.398301000
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1	-2.814425000	4.021872000	-3.085970000
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6	-3.689857000	2.663845000	-0.887620000
7	-4.391895000	2.395618000	0.272998000
1	-4.115505000	1.721395000	0.973887000
1	-8.216329000	4.462186000	1.913007000
6	-7.436246000	4.343467000	1.165740000
6	-7.432112000	5.179161000	0.028123000
6	-6.449834000	5.056457000	-0.949248000
6	-5.446679000	4.080718000	-0.795461000
1	-6.457102000	5.710623000	-1.817873000
1	-8.210043000	5.929975000	-0.082742000
1	-6.458793000	2.728238000	2.225374000
6	-6.457673000	3.370745000	1.348971000
6	-5.471314000	3.249438000	0.362361000
7	-1.426090000	0.178600000	-3.425337000
8	-1.692489000	1.348424000	-3.476551000

[6]IM1:

26	0.456103000	0.276620000	0.172113000
7	2.133886000	0.028887000	-1.017022000
7	0.140325000	-1.762552000	0.144973000
7	-0.974332000	0.452530000	1.673493000
7	0.982842000	2.251120000	0.476479000
6	0.887839000	-2.693218000	-0.543721000
6	0.360967000	-4.010044000	-0.276074000
6	-0.714732000	-3.856433000	0.549030000
6	-0.853080000	-2.444723000	0.812770000
6	-1.824284000	-1.881090000	1.666257000
6	-1.863865000	-0.526898000	2.056594000
6	-2.830919000	0.044332000	2.966124000
6	-2.486945000	1.352745000	3.150850000
6	-1.327784000	1.610989000	2.327130000
6	-0.684233000	2.859527000	2.214929000
6	0.390625000	3.137702000	1.348001000
6	1.007692000	4.433698000	1.194056000
6	1.964126000	4.314271000	0.228815000
6	1.946023000	2.944089000	-0.225248000
6	2.811528000	2.410626000	-1.202937000
6	2.877360000	1.049394000	-1.566573000
6	3.751481000	0.502955000	-2.578741000
6	3.536380000	-0.843204000	-2.613300000
6	2.517785000	-1.139486000	-1.632104000
6	1.982712000	-2.421706000	-1.390034000
8	-0.755245000	0.768007000	-1.292813000
8	-0.869491000	-0.235796000	-2.285708000
6	-1.192480000	3.984264000	3.067975000
6	-0.439427000	4.440697000	4.161504000
6	-2.422663000	4.601396000	2.790489000
6	-0.905589000	5.487346000	4.959824000
1	0.512907000	3.968646000	4.387646000
6	-2.888397000	5.648045000	3.589446000
1	-3.012394000	4.261516000	1.943924000
6	-2.131735000	6.093784000	4.675967000
1	-0.311391000	5.825933000	5.804253000
1	-3.841685000	6.115759000	3.359046000
1	-2.494773000	6.908214000	5.296752000
6	-2.870004000	-2.799805000	2.220479000
6	-2.912595000	-3.105080000	3.590959000
6	-3.828493000	-3.378851000	1.372369000
6	-3.889228000	-3.963232000	4.100022000
1	-2.170906000	-2.673080000	4.257064000
6	-4.806698000	-4.234850000	1.881964000
1	-3.808595000	-3.149076000	0.310578000
6	-4.840065000	-4.529421000	3.247236000
1	-3.903661000	-4.191716000	5.162197000
1	-5.543753000	-4.668731000	1.211807000
1	-5.600790000	-5.196244000	3.643534000
6	2.614329000	-3.576603000	-2.104233000
6	3.938553000	-3.951291000	-1.821898000
6	1.901732000	-4.303648000	-3.072387000
6	4.532672000	-5.026045000	-2.485940000
1	4.499715000	-3.400159000	-1.072290000
6	2.497302000	-5.376021000	-3.739078000
1	0.880229000	-4.018668000	-3.308341000
6	3.813913000	-5.741226000	-3.447112000
1	5.555928000	-5.305101000	-2.249838000
1	1.932926000	-5.922789000	-4.489508000
1	4.276564000	-6.576502000	-3.965468000
6	3.743557000	3.360052000	-1.891377000
6	5.132301000	3.272185000	-1.699527000
6	3.243691000	4.360552000	-2.741274000
6	5.997866000	4.160981000	-2.339883000
1	5.531730000	2.508377000	-1.038095000
6	4.109575000	5.247705000	-3.383480000
1	2.171974000	4.435869000	-2.902999000
6	5.489021000	5.151023000	-3.184194000
1	7.068951000	4.081482000	-2.175205000
1	3.705304000	6.011866000	-4.041642000
1	6.162559000	5.842295000	-3.683094000
1	4.435035000	1.074774000	-3.188847000
1	4.010610000	-1.567369000	-3.259237000
1	0.764026000	-4.934622000	-0.662216000
1	-1.344888000	-4.632583000	0.957816000
1	-3.652722000	-0.488635000	3.421210000
1	-2.977072000	2.077633000	3.784304000
1	0.741741000	5.321131000	1.749427000
1	2.626002000	5.084774000	-0.138074000
8	1.971501000	-0.183102000	1.980309000
6	1.774028000	-1.196681000	2.995416000
6	3.202669000	0.538149000	2.219963000
6	2.830051000	-0.916792000	4.066707000
1	0.746485000	-1.121291000	3.359048000
6	3.970256000	-0.300284000	3.241745000
1	3.716571000	0.655882000	1.263517000
1	2.957652000	1.532157000	2.614469000
1	4.546106000	-1.085513000	2.738047000
1	4.661063000	0.302521000	3.838243000
1	3.123369000	-1.822693000	4.604861000
1	2.452578000	-0.191558000	4.796916000
1	1.913504000	-2.181553000	2.533699000
1	-3.737192000	2.023581000	-4.211966000
7	-4.683353000	2.356681000	-4.401290000
1	-5.315235000	1.786394000	-3.845770000
1	-5.870596000	3.964900000	-3.827040000
1	-4.039898000	5.354829000	-2.815185000
6	-4.812513000	3.781057000	-4.053233000
6	-3.963247000	4.262286000	-2.853768000
6	-4.377306000	3.654681000	-1.544570000
6	-4.519745000	4.612438000	-5.319153000
8	-4.533261000	3.887436000	-6.444186000
1	-4.687524000	2.954018000	-6.117370000
8	-4.326139000	5.812370000	-5.315834000
1	-2.910524000	4.030211000	-3.058553000
1	-2.841626000	2.095152000	-1.122391000
6	-3.745023000	2.635906000	-0.869324000
7	-4.436941000	2.334931000	0.289210000
1	-4.139698000	1.662948000	0.983909000
1	-8.296992000	4.298785000	1.971141000
6	-7.518160000	4.205948000	1.218953000
6	-7.537010000	5.055963000	0.092082000
6	-6.556940000	4.966585000	-0.890926000
6	-5.532622000	4.010604000	-0.753539000
1	-6.581608000	5.631996000	-1.750590000
1	-8.331005000	5.791584000	-0.005619000
1	-6.501965000	2.598601000	2.253823000
6	-6.518695000	3.251812000	1.385596000
6	-5.534527000	3.163939000	0.393159000
7	-1.430607000	0.210840000	-3.465636000
8	-1.723718000	1.368294000	-3.496699000

^{2}TS1:

26	0.422137000	0.233240000	0.278686000

7	1.949506000	0.052207000	-0.992470000
7	0.140400000	-1.740326000	0.221094000
7	-0.980763000	0.390742000	1.724059000
7	0.861238000	2.181878000	0.518413000
6	0.924279000	-2.679773000	-0.413075000
6	0.402024000	-4.000403000	-0.163879000
6	-0.733000000	-3.847023000	0.569203000
6	-0.892633000	-2.434141000	0.812235000
6	-1.913201000	-1.896954000	1.608489000
6	-1.921552000	-0.564039000	2.039738000
6	-2.882266000	-0.014499000	2.966298000
6	-2.481578000	1.256961000	3.246364000
6	-1.308768000	1.515894000	2.446123000
6	-0.656384000	2.754374000	2.390966000
6	0.339160000	3.048778000	1.452700000
6	0.887358000	4.369252000	1.253854000
6	1.709075000	4.299591000	0.172981000
6	1.690683000	2.930370000	-0.283127000
6	2.468249000	2.449518000	-1.344516000
6	2.587992000	1.087189000	-1.643849000
6	3.473200000	0.556986000	-2.652098000
6	3.396775000	-0.798444000	-2.576269000
6	2.434655000	-1.110331000	-1.548571000
6	2.022443000	-2.411744000	-1.238459000
8	-0.735643000	0.611030000	-0.873219000
8	-0.685553000	-0.460078000	-2.373787000
6	-1.092170000	3.842249000	3.325982000
6	-0.266997000	4.224468000	4.395448000
6	-2.317285000	4.504775000	3.148108000
6	-0.659183000	5.240745000	5.269394000
1	0.684118000	3.719566000	4.541690000
6	-2.709145000	5.520630000	4.022534000
1	-2.961667000	4.225933000	2.319106000
6	-1.881951000	5.890982000	5.085769000
1	-0.009675000	5.521919000	6.093922000
1	-3.659499000	6.024416000	3.868677000
1	-2.187308000	6.681770000	5.765399000
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6	-3.139754000	-3.175285000	3.412596000
6	-3.920827000	-3.336425000	1.132327000
6	-4.160284000	-4.035357000	3.822616000
1	-2.432611000	-2.788157000	4.140974000
6	-4.942809000	-4.194603000	1.542775000
1	-3.829431000	-3.063480000	0.084550000
6	-5.065745000	-4.546300000	2.889247000
1	-4.244032000	-4.309292000	4.870765000
1	-5.643295000	-4.585967000	0.810123000
1	-5.860245000	-5.214958000	3.208762000
6	2.747372000	-3.554569000	-1.877752000
6	4.079177000	-3.832558000	-1.528893000
6	2.122983000	-4.359911000	-2.844471000
6	4.766012000	-4.892049000	-2.124994000
1	4.574118000	-3.216853000	-0.782771000
6	2.810780000	-5.417446000	-3.442709000
1	1.097393000	-4.147961000	-3.133468000
6	4.133691000	-5.687699000	-3.083552000
1	5.794260000	-5.095698000	-1.838751000
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1	4.668486000	-6.511107000	-3.548789000
6	3.244812000	3.439871000	-2.156417000
6	4.644614000	3.511274000	-2.070151000
6	2.576504000	4.325792000	-3.016931000
6	5.358088000	4.442203000	-2.827845000
1	5.172885000	2.837753000	-1.400930000
6	3.290293000	5.254756000	-3.776718000
1	1.493677000	4.279386000	-3.093881000
6	4.682942000	5.315668000	-3.684133000
1	6.440658000	4.486555000	-2.745471000
1	2.757376000	5.928804000	-4.441729000
1	5.238180000	6.039506000	-4.274240000
1	4.079211000	1.151122000	-3.319822000
1	3.921634000	-1.527635000	-3.175550000
1	0.844971000	-4.920258000	-0.515473000
1	-1.392124000	-4.617474000	0.941019000
1	-3.731074000	-0.545003000	3.371468000
1	-2.942927000	1.963799000	3.920070000
1	0.652196000	5.234534000	1.855886000
1	2.288665000	5.094002000	-0.273647000
8	1.860962000	-0.136576000	1.898915000
6	1.708625000	-1.151643000	2.927602000
6	3.079218000	0.625040000	2.108253000
6	2.772218000	-0.822149000	3.974504000
1	0.685147000	-1.102725000	3.303240000
6	3.881714000	-0.187374000	3.122353000
1	3.569413000	0.745031000	1.140723000
1	2.810247000	1.612545000	2.499195000
1	4.466752000	-0.963534000	2.615558000
1	4.567948000	0.438315000	3.700001000
1	3.099585000	-1.711320000	4.520622000
1	2.385582000	-0.096733000	4.699503000
1	1.875250000	-2.132125000	2.468635000
1	-3.335754000	1.967841000	-4.233083000
7	-4.278117000	2.295432000	-4.450588000
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1	-3.671194000	5.332871000	-2.926292000
6	-4.416706000	3.727782000	-4.140537000
6	-3.596819000	4.239525000	-2.933554000
6	-4.046098000	3.668696000	-1.619450000
6	-4.095846000	4.528096000	-5.419649000
8	-4.085885000	3.775527000	-6.526477000
1	-4.247188000	2.850465000	-6.179440000
8	-3.901364000	5.727723000	-5.441765000
1	-2.539883000	3.999654000	-3.105629000
1	-2.544385000	2.094523000	-1.129291000
6	-3.443648000	2.655802000	-0.909051000
7	-4.161925000	2.392986000	0.242389000
1	-3.897806000	1.723165000	0.952536000
1	-8.029315000	4.444968000	1.797050000
6	-7.235699000	4.325382000	1.064340000
6	-7.218571000	5.150522000	-0.080891000
6	-6.219056000	5.026425000	-1.040347000
6	-5.211422000	4.059809000	-0.860404000
1	-6.216459000	5.672247000	-1.915195000
1	-8.000118000	5.894283000	-0.211847000
1	-6.264334000	2.727235000	2.155238000
6	-6.253128000	3.362059000	1.273396000
6	-5.249126000	3.239497000	0.304731000
7	-1.064173000	0.127030000	-3.413310000
8	-1.369481000	1.299644000	-3.442143000

^{2}IM2:

26	0.412995000	0.351537000	0.253717000
7	1.995620000	0.160894000	-0.973007000

7	0.109877000	-1.631163000	0.177536000
7	-0.970457000	0.482047000	1.712152000
7	0.922536000	2.268949000	0.561272000
6	0.872068000	-2.562873000	-0.491432000
6	0.318013000	-3.880748000	-0.293116000
6	-0.811931000	-3.729852000	0.447178000
6	-0.937602000	-2.323264000	0.742680000
6	-1.941338000	-1.789294000	1.560284000
6	-1.919605000	-0.467422000	2.022460000
6	-2.859706000	0.074080000	2.973903000
6	-2.440746000	1.335658000	3.271818000
6	-1.276632000	1.596879000	2.459703000
6	-0.612599000	2.829275000	2.423695000
6	0.396881000	3.126271000	1.502109000
6	0.974016000	4.440008000	1.344611000
6	1.821981000	4.376650000	0.284337000
6	1.788586000	3.018159000	-0.201576000
6	2.586524000	2.546988000	-1.251711000
6	2.680467000	1.190372000	-1.582030000
6	3.569335000	0.660678000	-2.587830000
6	3.441550000	-0.692161000	-2.556912000
6	2.446925000	-1.000298000	-1.557390000
6	1.984210000	-2.296115000	-1.298770000
8	-0.637356000	0.689406000	-0.933282000
8	-0.329825000	-1.174050000	-3.685380000
6	-1.041834000	3.906079000	3.374885000
6	-0.224410000	4.254411000	4.461675000
6	-2.254282000	4.590939000	3.195221000
6	-0.611583000	5.259759000	5.350395000
1	0.716776000	3.731666000	4.609526000
6	-2.641133000	5.596058000	4.084206000
1	-2.892992000	4.337839000	2.353587000
6	-1.821596000	5.932848000	5.164390000
1	0.031795000	5.514588000	6.188192000
1	-3.581629000	6.117575000	3.928778000
1	-2.123031000	6.715202000	5.855450000
6	-3.051315000	-2.693505000	1.998755000
6	-3.173072000	-3.099599000	3.337792000
6	-3.989776000	-3.163266000	1.065357000
6	-4.209044000	-3.947958000	3.733467000
1	-2.446677000	-2.754507000	4.068380000
6	-5.027140000	-4.009737000	1.461465000
1	-3.906084000	-2.856834000	0.026222000
6	-5.140035000	-4.404233000	2.796905000
1	-4.285072000	-4.255364000	4.772898000
1	-5.747290000	-4.358526000	0.726367000
1	-5.946512000	-5.063690000	3.105358000
6	2.671692000	-3.439102000	-1.979354000
6	3.982867000	-3.793567000	-1.622969000
6	2.028348000	-4.168511000	-2.992745000
6	4.631986000	-4.854364000	-2.258085000
1	4.491446000	-3.236475000	-0.840793000
6	2.678540000	-5.227259000	-3.629637000
1	1.018802000	-3.895129000	-3.286297000
6	3.981379000	-5.574362000	-3.263082000
1	5.644784000	-5.118136000	-1.965879000
1	2.167927000	-5.777439000	-4.415343000
1	4.486578000	-6.398855000	-3.758565000
6	3.409757000	3.537099000	-2.015953000
6	4.808814000	3.562350000	-1.896884000
6	2.789104000	4.468762000	-2.863843000
6	5.567537000	4.492913000	-2.609653000
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6	3.548043000	5.397762000	-3.578455000
1	1.707432000	4.458212000	-2.966395000
6	4.939412000	5.412677000	-3.453163000
1	6.648778000	4.500942000	-2.501961000
1	3.051288000	6.107619000	-4.234153000
1	5.529971000	6.136409000	-4.008059000
1	4.210646000	1.252833000	-3.223610000
1	3.952054000	-1.421510000	-3.168230000
1	0.740069000	-4.796378000	-0.679660000
1	-1.488007000	-4.498241000	0.791965000
1	-3.707061000	-0.455856000	3.382832000
1	-2.882974000	2.034028000	3.966922000
1	0.741842000	5.296199000	1.960592000
1	2.430553000	5.167530000	-0.128593000
8	1.874469000	-0.108750000	1.926710000
6	1.694582000	-1.150032000	2.919666000
6	3.112096000	0.608257000	2.161230000
6	2.757792000	-0.880914000	3.985036000
1	0.669785000	-1.091704000	3.291847000
6	3.888813000	-0.249806000	3.158975000
1	3.612558000	0.740184000	1.200128000
1	2.871764000	1.594523000	2.575293000
1	4.459014000	-1.026086000	2.635441000
1	4.586132000	0.342433000	3.758436000
1	3.058168000	-1.793522000	4.507694000
1	2.384035000	-0.166935000	4.728107000
1	1.841389000	-2.121205000	2.433452000
1	-3.560150000	1.516332000	-3.996823000
7	-4.497657000	1.846904000	-4.226690000
1	-5.139089000	1.387114000	-3.586184000
1	-5.623815000	3.561908000	-3.887994000
1	-3.743395000	5.017527000	-3.087745000
6	-4.575294000	3.310484000	-4.092607000
6	-3.695995000	3.927830000	-2.980635000
6	-4.107211000	3.506823000	-1.599744000
6	-4.270035000	3.937100000	-5.468236000
8	-4.318732000	3.056478000	-6.475414000
1	-4.500858000	2.186326000	-6.016872000
8	-4.037639000	5.117284000	-5.641704000
1	-2.652362000	3.640964000	-3.164286000
1	-2.587136000	1.993030000	-0.982620000
6	-3.485255000	2.572319000	-0.803484000
7	-4.173042000	2.432348000	0.386940000
1	-3.896390000	1.829146000	1.150771000
1	-8.005668000	4.633698000	1.816568000
6	-7.230184000	4.438916000	1.080604000
6	-7.243543000	5.141368000	-0.143826000
6	-6.267658000	4.919369000	-1.109862000
6	-5.253617000	3.976005000	-0.856492000
1	-6.287636000	5.472386000	-2.045893000
1	-8.029748000	5.867957000	-0.331166000
1	-6.227809000	2.961865000	2.305915000
6	-6.240330000	3.502274000	1.363261000
6	-5.260250000	3.280690000	0.387774000
7	-1.163202000	-0.327306000	-3.519819000
8	-1.330573000	0.770542000	-3.985176000

^{4}IM2:

26	0.358512000	0.239064000	0.252608000
7	1.907984000	0.065602000	-1.021911000
7	0.133862000	-1.758353000	0.255893000

7	-0.985514000	0.365862000	1.749637000
7	0.793595000	2.189570000	0.471982000
6	0.908837000	-2.681874000	-0.409627000
6	0.434212000	-4.014828000	-0.125483000
6	-0.663533000	-3.885364000	0.665606000
6	-0.850394000	-2.474108000	0.899725000
6	-1.859552000	-1.949134000	1.716798000
6	-1.899751000	-0.603648000	2.102381000
6	-2.887005000	-0.044610000	2.993586000
6	-2.537669000	1.254236000	3.208052000
6	-1.355990000	1.509213000	2.419866000
6	-0.747953000	2.767077000	2.322290000
6	0.257367000	3.060586000	1.395106000
6	0.841189000	4.370115000	1.229327000
6	1.687582000	4.295875000	0.168499000
6	1.652655000	2.933138000	-0.304302000
6	2.436624000	2.457945000	-1.363559000
6	2.541259000	1.098785000	-1.679045000
6	3.394554000	0.571422000	-2.716394000
6	3.299984000	-0.783076000	-2.656670000
6	2.363430000	-1.095517000	-1.604013000
6	1.963868000	-2.398610000	-1.284905000
8	-0.745140000	0.488294000	-0.907887000
8	-0.570382000	-1.242220000	-3.662716000
6	-1.253106000	3.863858000	3.208158000
6	-1.006684000	3.832837000	4.590039000
6	-1.993037000	4.933428000	2.677960000
6	-1.482362000	4.849382000	5.420938000
1	-0.434958000	3.010113000	5.010910000
6	-2.470866000	5.948188000	3.509517000
1	-2.200421000	4.961788000	1.611815000
6	-2.215941000	5.909614000	4.882799000
1	-1.277957000	4.812866000	6.487535000
1	-3.046276000	6.765723000	3.083948000
1	-2.587659000	6.699824000	5.529245000
6	-2.911795000	-2.881144000	2.230711000
6	-3.003989000	-3.188409000	3.598347000
6	-3.826292000	-3.475017000	1.345076000
6	-3.986351000	-4.062359000	4.067926000
1	-2.295872000	-2.745809000	4.293391000
6	-4.810345000	-4.346799000	1.815020000
1	-3.766769000	-3.244795000	0.284861000
6	-4.893423000	-4.642879000	3.177857000
1	-4.039266000	-4.292221000	5.128599000
1	-5.512943000	-4.792106000	1.115939000
1	-5.658565000	-5.322088000	3.543480000
6	2.661827000	-3.536704000	-1.963241000
6	4.001665000	-3.829946000	-1.661752000
6	1.999012000	-4.323207000	-2.919615000
6	4.659896000	-4.886217000	-2.294902000
1	4.525683000	-3.228627000	-0.923777000
6	2.658211000	-5.377191000	-3.555234000
1	0.966007000	-4.098780000	-3.170204000
6	3.989985000	-5.662703000	-3.243621000
1	5.695162000	-5.102235000	-2.045322000
1	2.131711000	-5.971896000	-4.296745000
1	4.502439000	-6.483487000	-3.737808000
6	3.225809000	3.449025000	-2.161055000
6	4.628640000	3.477958000	-2.098530000
6	2.569676000	4.377468000	-2.985811000
6	5.355957000	4.408287000	-2.843506000
1	5.148615000	2.772024000	-1.456889000
6	3.297134000	5.305640000	-3.733307000
1	1.484834000	4.364363000	-3.045066000
6	4.692392000	5.323899000	-3.664087000
1	6.440598000	4.419253000	-2.779032000
1	2.772818000	6.012244000	-4.370798000
1	5.258539000	6.047087000	-4.244551000
1	3.990855000	1.166269000	-3.392143000
1	3.798629000	-1.511766000	-3.278543000
1	0.883698000	-4.925318000	-0.492876000
1	-1.281584000	-4.669094000	1.078051000
1	-3.724664000	-0.583271000	3.411136000
1	-3.038297000	1.982958000	3.828600000
1	0.620727000	5.230098000	1.844103000
1	2.301290000	5.080662000	-0.248387000
8	1.888158000	-0.110926000	1.885080000
6	1.776862000	-1.117809000	2.922956000
6	3.097435000	0.668588000	2.061613000
6	2.845310000	-0.754521000	3.954107000
1	0.757210000	-1.092921000	3.312157000
6	3.930842000	-0.109624000	3.079104000
1	3.573035000	0.778657000	1.085222000
1	2.821881000	1.660880000	2.437182000
1	4.525831000	-0.881739000	2.577506000
1	4.611330000	0.539121000	3.637966000
1	3.196993000	-1.628992000	4.509004000
1	2.452805000	-0.026528000	4.673630000
1	1.961770000	-2.100194000	2.473414000
1	-3.265560000	2.012717000	-4.066148000
7	-4.169587000	2.411872000	-4.320234000
1	-4.875995000	1.895152000	-3.803491000
1	-5.270938000	4.105925000	-3.829906000
1	-3.418568000	5.370242000	-2.706492000
6	-4.217017000	3.845675000	-3.990898000
6	-3.410609000	4.274950000	-2.743510000
6	-3.941522000	3.692219000	-1.466241000
6	-3.789794000	4.641265000	-5.241138000
8	-3.784090000	3.907348000	-6.360558000
1	-4.023927000	2.990512000	-6.039716000
8	-3.513256000	5.824724000	-5.232850000
1	-2.364015000	3.975411000	-2.886950000
1	-2.532259000	2.037339000	-0.957085000
6	-3.418339000	2.630224000	-0.763853000
7	-4.208590000	2.354841000	0.335524000
1	-3.986720000	1.675848000	1.051680000
1	-8.056129000	4.519891000	1.777471000
6	-7.233028000	4.391130000	1.079687000
6	-7.125699000	5.253199000	-0.033068000
6	-6.085569000	5.119811000	-0.946955000
6	-5.127939000	4.106012000	-0.752896000
1	-6.012513000	5.795019000	-1.796256000
1	-7.868756000	6.033611000	-0.174490000
1	-6.383190000	2.716954000	2.157566000
6	-6.302770000	3.379803000	1.300243000
6	-5.258159000	3.247238000	0.377253000
7	-1.292343000	-0.287353000	-3.591597000
8	-1.211005000	0.846134000	-3.989015000

[6]IM2:

26	0.400370000	0.654644000	-0.091796000
7	2.162199000	0.272099000	-1.165880000
7	0.096000000	-1.431888000	-0.074031000
7	-0.727424000	0.704922000	1.689178000

7	1.355304000	2.400455000	0.615266000
6	0.677575000	-2.341356000	-0.923967000
6	0.099398000	-3.648822000	-0.713261000
6	-0.854322000	-3.510596000	0.247839000
6	-0.870291000	-2.116153000	0.627701000
6	-1.752786000	-1.550453000	1.568941000
6	-1.703415000	-0.212171000	2.012398000
6	-2.669359000	0.395056000	2.897343000
6	-2.255493000	1.676224000	3.120824000
6	-1.032539000	1.860567000	2.376064000
6	-0.261212000	3.041203000	2.379170000
6	0.885586000	3.252733000	1.587784000
6	1.746601000	4.409524000	1.681354000
6	2.714493000	4.261243000	0.735838000
6	2.451859000	3.013191000	0.055940000
6	3.213770000	2.510976000	-1.019602000
6	3.033215000	1.243805000	-1.608488000
6	3.758517000	0.762324000	-2.761219000
6	3.332699000	-0.508933000	-2.997503000
6	2.343803000	-0.817104000	-1.990945000
6	1.687906000	-2.056551000	-1.865534000
8	-0.669882000	1.216826000	-1.246053000
8	-1.670054000	-0.962341000	-3.371189000
6	-0.687723000	4.147585000	3.289166000
6	-0.694807000	3.967943000	4.682788000
6	-1.086339000	5.388742000	2.764790000
6	-1.086212000	5.005597000	5.529987000
1	-0.379245000	3.016356000	5.100929000
6	-1.487296000	6.421658000	3.613276000
1	-1.092922000	5.537105000	1.688837000
6	-1.485862000	6.234104000	4.997779000
1	-1.076511000	4.853681000	6.605660000
1	-1.802140000	7.371843000	3.191176000
1	-1.794191000	7.040030000	5.657757000
6	-2.816876000	-2.431374000	2.140076000
6	-2.840476000	-2.724575000	3.514148000
6	-3.810168000	-2.982929000	1.313342000
6	-3.830142000	-3.552034000	4.046568000
1	-2.072191000	-2.312265000	4.161895000
6	-4.805118000	-3.801736000	1.849489000
1	-3.807090000	-2.757983000	0.250715000
6	-4.816600000	-4.090418000	3.216431000
1	-3.828262000	-3.776783000	5.109438000
1	-5.571590000	-4.212415000	1.198305000
1	-5.589200000	-4.731156000	3.632021000
6	2.083616000	-3.152319000	-2.802564000
6	3.373105000	-3.706943000	-2.759449000
6	1.163421000	-3.643115000	-3.743959000
6	3.731650000	-4.733930000	-3.634173000
1	4.089390000	-3.339293000	-2.030231000
6	1.527673000	-4.663098000	-4.624220000
1	0.168460000	-3.209799000	-3.791757000
6	2.811006000	-5.213064000	-4.569650000
1	4.729764000	-5.159838000	-3.582766000
1	0.808624000	-5.026271000	-5.353191000
1	3.092202000	-6.009880000	-5.252481000
6	4.291816000	3.387632000	-1.570735000
6	5.639717000	2.997510000	-1.498930000
6	3.974428000	4.619080000	-2.168361000
6	6.644831000	3.821502000	-2.007355000
1	5.898329000	2.051547000	-1.031914000
6	4.980203000	5.436904000	-2.685328000
1	2.935253000	4.927518000	-2.237545000
6	6.317883000	5.041900000	-2.603982000
1	7.682992000	3.509634000	-1.935353000
1	4.717128000	6.381575000	-3.152881000
1	7.100533000	5.680914000	-3.003120000
1	4.492443000	1.325399000	-3.318149000
1	3.654861000	-1.176667000	-3.782592000
1	0.397623000	-4.553775000	-1.221401000
1	-1.479780000	-4.282069000	0.671550000
1	-3.546001000	-0.092420000	3.297700000
1	-2.734247000	2.424412000	3.735105000
1	1.634570000	5.218705000	2.387567000
1	3.539170000	4.926398000	0.527377000
8	3.069084000	-0.749143000	2.511110000
6	2.225117000	-1.283123000	3.541636000
6	3.830464000	0.357492000	3.034260000
6	2.056414000	-0.154840000	4.559173000
1	1.287658000	-1.603649000	3.077500000
6	3.445870000	0.500793000	4.516238000
1	4.899817000	0.156775000	2.894142000
1	3.571241000	1.254521000	2.458316000
1	4.145580000	-0.054742000	5.151364000
1	3.444673000	1.543481000	4.847265000
1	1.777172000	-0.516192000	5.553600000
1	1.288054000	0.547976000	4.216139000
1	2.705218000	-2.160681000	4.003053000
1	-3.863051000	1.126475000	-4.236678000
7	-4.875189000	1.195555000	-4.350611000
1	-5.294717000	0.646129000	-3.605222000
1	-6.359763000	2.598053000	-3.969099000
1	-4.831261000	4.533728000	-3.471439000
6	-5.306057000	2.601093000	-4.276553000
6	-4.513238000	3.499108000	-3.298904000
6	-4.698622000	3.117582000	-1.858642000
6	-5.306422000	3.178916000	-5.706257000
8	-5.244833000	2.239592000	-6.658571000
1	-5.159615000	1.387364000	-6.142846000
8	-5.388615000	4.364027000	-5.961913000
1	-3.449810000	3.450390000	-3.567115000
1	-2.804653000	2.081780000	-1.277924000
6	-3.803917000	2.442488000	-1.059157000
7	-4.345059000	2.253241000	0.198104000
1	-3.866461000	1.821341000	0.977559000
1	-8.485502000	3.586009000	1.826746000
6	-7.743976000	3.516081000	1.035363000
6	-8.024337000	4.075955000	-0.229820000
6	-7.099776000	4.006057000	-1.266877000
6	-5.866502000	3.363937000	-1.044716000
1	-7.327815000	4.447559000	-2.234154000
1	-8.978448000	4.570246000	-0.392773000
1	-6.314914000	2.449208000	2.262863000
6	-6.533346000	2.877786000	1.288351000
6	-5.605384000	2.808877000	0.241961000
7	-1.144611000	0.067550000	-3.695503000
8	-1.556089000	1.084601000	-4.188900000

^{2}TS2$_{C4}$:

26	0.496583000	-0.131408000	0.731085000
7	1.991850000	-0.279685000	-0.605127000
7	0.307281000	-2.128911000	0.747526000
7	-0.777703000	-0.023363000	2.285218000
7	0.934736000	1.812765000	0.951720000

6	1.076654000	-3.041291000	0.060256000
6	0.618167000	-4.379536000	0.343810000
6	-0.464349000	-4.264575000	1.158158000
6	-0.653464000	-2.856572000	1.411735000
6	-1.624819000	-2.347561000	2.283482000
6	-1.645187000	-1.010867000	2.699326000
6	-2.535159000	-0.488753000	3.708078000
6	-2.167698000	0.801060000	3.932332000
6	-1.087413000	1.097195000	3.022845000
6	-0.479801000	2.353899000	2.912394000
6	0.452085000	2.668370000	1.916544000
6	0.966668000	3.998420000	1.692292000
6	1.722569000	3.946535000	0.563984000
6	1.698456000	2.580222000	0.102710000
6	2.411478000	2.122174000	-1.011895000
6	2.554668000	0.762114000	-1.310003000
6	3.384974000	0.244334000	-2.370455000
6	3.351062000	-1.111738000	-2.274243000
6	2.465636000	-1.435752000	-1.182087000
6	2.107384000	-2.743872000	-0.837462000
8	-0.650162000	0.107565000	-0.390919000
8	-1.363583000	2.629727000	-3.399702000
6	-0.884816000	3.435878000	3.867531000
6	0.002019000	3.864310000	4.868135000
6	-2.145212000	4.048080000	3.778936000
6	-0.362429000	4.876473000	5.758651000
1	0.980671000	3.398521000	4.946940000
6	-2.510640000	5.059451000	4.669815000
1	-2.838927000	3.730951000	3.004975000
6	-1.620339000	5.476527000	5.662524000
1	0.336115000	5.193282000	6.528397000
1	-3.489278000	5.523963000	4.584261000
1	-1.904347000	6.264040000	6.355122000
6	-2.642411000	-3.296326000	2.837053000
6	-2.636123000	-3.660397000	4.193615000
6	-3.620832000	-3.852235000	1.996697000
6	-3.586006000	-4.551172000	4.697461000
1	-1.877655000	-3.247295000	4.852794000
6	-4.572053000	-4.741569000	2.500689000
1	-3.635946000	-3.579773000	0.944954000
6	-4.557903000	-5.093213000	3.852687000
1	-3.562821000	-4.824368000	5.748955000
1	-5.324614000	-5.157702000	1.836414000
1	-5.297418000	-5.786020000	4.244744000
6	2.809455000	-3.873689000	-1.527576000
6	4.138159000	-4.188082000	-1.202136000
6	2.155589000	-4.625940000	-2.517401000
6	4.798108000	-5.238434000	-1.844083000
1	4.652494000	-3.608826000	-0.439785000
6	2.818846000	-5.673690000	-3.160085000
1	1.135927000	-4.367203000	-2.789529000
6	4.139215000	-5.984742000	-2.824217000
1	5.825249000	-5.472781000	-1.577478000
1	2.303878000	-6.244607000	-3.928322000
1	4.652401000	-6.801208000	-3.325180000
6	3.072925000	3.134843000	-1.894228000
6	4.470869000	3.255313000	-1.947080000
6	2.288446000	3.991295000	-2.685471000
6	5.072440000	4.207196000	-2.772934000
1	5.086497000	2.604711000	-1.331862000
6	2.892626000	4.940342000	-3.512892000
1	1.205748000	3.903180000	-2.652033000
6	4.284708000	5.051695000	-3.559290000
1	6.155658000	4.290547000	-2.798299000
1	2.273598000	5.592501000	-4.123366000
1	4.752614000	5.791868000	-4.202718000
1	3.930097000	0.846078000	-3.082485000
1	3.855131000	-1.835903000	-2.897250000
1	1.063657000	-5.282812000	-0.045885000
1	-1.068905000	-5.056190000	1.575790000
1	-3.319330000	-1.048702000	4.195543000
1	-2.595451000	1.499091000	4.636533000
1	0.754566000	4.857489000	2.311585000
1	2.260635000	4.751664000	0.085670000
8	2.105180000	-0.471580000	2.305586000
6	2.062744000	-1.496562000	3.329605000
6	3.313861000	0.317746000	2.427502000
6	3.187332000	-1.142244000	4.303199000
1	1.067352000	-1.487359000	3.778345000
6	4.213717000	-0.470803000	3.378037000
1	3.730455000	0.454379000	1.427675000
1	3.050988000	1.299162000	2.839626000
1	4.784496000	-1.227607000	2.827205000
1	4.920910000	0.173877000	3.907837000
1	3.578296000	-2.023179000	4.820358000
1	2.831974000	-0.430671000	5.057654000
1	2.228222000	-2.469859000	2.853552000
1	-1.987612000	-0.200624000	-5.749922000
7	-1.265093000	0.081989000	-5.088114000
1	-1.340264000	1.089863000	-4.971768000
1	-0.995154000	0.063714000	-3.029942000
1	-2.914366000	-1.228259000	-2.346504000
6	-1.466081000	-0.573381000	-3.787490000
6	-2.930046000	-0.839636000	-3.370714000
6	-3.854903000	0.342880000	-3.469780000
6	-0.651518000	-1.879710000	-3.782723000
8	0.294910000	-1.913913000	-4.726852000
1	0.141963000	-1.067745000	-5.239721000
8	-0.822289000	-2.791033000	-2.994213000
1	-3.330890000	-1.645769000	-3.997870000
1	-5.180220000	-0.251746000	-5.172312000
6	-4.891738000	0.438737000	-4.392087000
7	-5.600422000	1.589057000	-4.175047000
1	-6.435567000	1.860073000	-4.674464000
1	-5.295594000	4.600337000	-0.658643000
6	-4.894058000	3.771240000	-1.234394000
6	-3.786634000	3.095882000	-0.765529000
6	-3.147486000	2.029142000	-1.549437000
6	-3.945186000	1.510462000	-2.654650000
1	-2.562723000	1.304909000	-0.978689000
1	-3.307555000	3.402047000	0.157462000
1	-6.415043000	3.935658000	-2.791718000
6	-5.543341000	3.397531000	-2.433466000
6	-5.061078000	2.258985000	-3.097502000
7	-1.693466000	2.855088000	-2.241524000
8	-1.103909000	3.614544000	-1.488438000

^{2}IM3$_{C4}$:

26	0.592846000	-0.114950000	0.641690000
7	2.172395000	-0.264284000	-0.601086000
7	0.398467000	-2.116350000	0.640770000
7	-0.783836000	-0.006231000	2.111006000
7	1.003813000	1.839978000	0.878039000
6	1.173046000	-3.022679000	-0.048730000

6	0.695394000	-4.362040000	0.194178000
6	-0.396952000	-4.254804000	0.995541000
6	-0.582051000	-2.850134000	1.269831000
6	-1.583209000	-2.348948000	2.110555000
6	-1.646546000	-1.006956000	2.503027000
6	-2.612368000	-0.484000000	3.438990000
6	-2.307543000	0.826295000	3.633286000
6	-1.179778000	1.127486000	2.785283000
6	-0.610037000	2.400267000	2.673053000
6	0.402808000	2.710790000	1.759634000
6	0.911982000	4.045985000	1.555822000
6	1.798610000	3.979645000	0.527782000
6	1.849046000	2.602230000	0.103061000
6	2.682109000	2.136010000	-0.919568000
6	2.826499000	0.777855000	-1.221606000
6	3.732909000	0.265418000	-2.220685000
6	3.638639000	-1.089952000	-2.183019000
6	2.653941000	-1.416678000	-1.180230000
6	2.238164000	-2.722662000	-0.903359000
8	-0.484248000	0.119844000	-0.547201000
8	-1.981147000	2.635001000	-3.860541000
6	-1.144263000	3.501292000	3.540006000
6	-0.402460000	3.963097000	4.638327000
6	-2.388642000	4.092378000	3.269695000
6	-0.893758000	4.988593000	5.449324000
1	0.562119000	3.512850000	4.857119000
6	-2.880184000	5.117729000	4.080722000
1	-2.968009000	3.748131000	2.417090000
6	-2.134490000	5.568163000	5.173042000
1	-0.307602000	5.332027000	6.297450000
1	-3.844266000	5.566103000	3.856284000
1	-2.517144000	6.365922000	5.803690000
6	-2.607203000	-3.305283000	2.639912000
6	-2.634668000	-3.659442000	3.998677000
6	-3.558574000	-3.874059000	1.777507000
6	-3.590356000	-4.554918000	4.482987000
1	-1.898585000	-3.234198000	4.675361000
6	-4.515371000	-4.768317000	2.261852000
1	-3.548101000	-3.608115000	0.724031000
6	-4.534378000	-5.111081000	3.616104000
1	-3.593732000	-4.820339000	5.536711000
1	-5.246583000	-5.194976000	1.580612000
1	-5.278381000	-5.807535000	3.992900000
6	2.925307000	-3.850661000	-1.612705000
6	4.210580000	-4.259452000	-1.225200000
6	2.294401000	-4.508880000	-2.681292000
6	4.851462000	-5.310376000	-1.885436000
1	4.705840000	-3.753550000	-0.400515000
6	2.938762000	-5.557671000	-3.341504000
1	1.307129000	-4.181888000	-2.997498000
6	4.216094000	-5.962739000	-2.944878000
1	5.844994000	-5.618591000	-1.570969000
1	2.442574000	-6.056551000	-4.169877000
1	4.714168000	-6.779913000	-3.459723000
6	3.470442000	3.137206000	-1.707834000
6	4.859470000	3.256251000	-1.542008000
6	2.824313000	3.976676000	-2.630235000
6	5.587054000	4.192308000	-2.280148000
1	5.368165000	2.614779000	-0.827419000
6	3.553856000	4.910747000	-3.369225000
1	1.750466000	3.888161000	-2.770778000
6	4.935827000	5.021951000	-3.196342000
1	6.661117000	4.274092000	-2.136593000
1	3.040977000	5.550273000	-4.082686000
1	5.501485000	5.750014000	-3.771396000
1	4.360764000	0.871434000	-2.856990000
1	4.169634000	-1.811367000	-2.786487000
1	1.140254000	-5.260272000	-0.207791000
1	-1.015307000	-5.049203000	1.386609000
1	-3.406027000	-1.055441000	3.896791000
1	-2.804086000	1.534651000	4.279753000
1	0.614701000	4.915470000	2.123423000
1	2.375900000	4.782567000	0.093481000
8	2.100935000	-0.448951000	2.310463000
6	2.002911000	-1.478296000	3.326545000
6	3.301420000	0.339764000	2.501805000
6	3.060439000	-1.117739000	4.369773000
1	0.981291000	-1.479345000	3.711598000
6	4.140845000	-0.443709000	3.510695000
1	3.779599000	0.468805000	1.529031000
1	3.014079000	1.323932000	2.890136000
1	4.748096000	-1.199695000	2.999227000
1	4.810457000	0.204585000	4.083147000
1	3.421450000	-1.996322000	4.912117000
1	2.654205000	-0.407023000	5.098957000
1	2.206870000	-2.448564000	2.859101000
1	-3.256409000	-0.564173000	-5.422275000
7	-2.330322000	-0.189631000	-5.217805000
1	-2.415216000	0.824525000	-5.216838000
1	-1.174993000	0.115464000	-3.522503000
1	-2.448053000	-1.051833000	-1.873479000
6	-1.866121000	-0.646670000	-3.898681000
6	-2.958128000	-0.895332000	-2.829331000
6	-3.985299000	0.198304000	-2.711788000
6	-1.003019000	-1.906490000	-4.105903000
8	-0.606820000	-2.073441000	-5.371141000
1	-1.065544000	-1.327899000	-5.858094000
8	-0.687080000	-2.671281000	-3.213651000
1	-3.475101000	-1.832744000	-3.068787000
1	-5.794805000	-0.763030000	-3.615981000
6	-5.301419000	0.076352000	-3.146267000
7	-5.984018000	1.230645000	-2.868914000
1	-6.970024000	1.377199000	-3.031627000
1	-4.647321000	4.953521000	-0.440324000
6	-4.420809000	4.015899000	-0.940885000
6	-3.161064000	3.481183000	-0.813458000
6	-2.747099000	2.235456000	-1.535004000
6	-3.876097000	1.502052000	-2.147408000
1	-2.061338000	1.607459000	-0.954199000
1	-2.395109000	3.994676000	-0.243009000
1	-6.436062000	3.808688000	-1.761885000
6	-5.445777000	3.373799000	-1.677486000
6	-5.140896000	2.119091000	-2.237892000
7	-1.703360000	2.759720000	-2.672405000
8	-0.687968000	3.299397000	-2.248409000

^{4}TS2$_{C4}$:

26	0.219422000	0.387885000	0.333429000
7	1.632300000	0.121421000	-1.084701000
7	-0.019196000	-1.607712000	0.465162000
7	-0.962173000	0.615212000	1.953143000
7	0.713035000	2.342746000	0.416176000
6	0.616159000	-2.569120000	-0.290892000
6	0.164484000	-3.881528000	0.101870000

6	-0.770201000	-3.706042000	1.071772000
6	-0.889686000	-2.285362000	1.290203000
6	-1.737090000	-1.719378000	2.249561000
6	-1.748616000	-0.350781000	2.543765000
6	-2.579773000	0.246811000	3.561114000
6	-2.273758000	1.570256000	3.597070000
6	-1.278383000	1.801304000	2.578642000
6	-0.741754000	3.060798000	2.291190000
6	0.175766000	3.289561000	1.260092000
6	0.655080000	4.601620000	0.897515000
6	1.474409000	4.442833000	-0.174797000
6	1.512960000	3.031799000	-0.470335000
6	2.263937000	2.478957000	-1.512265000
6	2.301409000	1.106467000	-1.778652000
6	3.109700000	0.516671000	-2.817631000
6	2.919383000	-0.826765000	-2.753262000
6	1.999491000	-1.070589000	-1.668534000
6	1.560338000	-2.345976000	-1.298415000
8	-0.991958000	0.609676000	-0.721056000
8	-3.508380000	-2.324250000	-1.211248000
6	-1.184574000	4.232148000	3.115493000
6	-0.308359000	4.818952000	4.042353000
6	-2.474577000	4.768224000	2.976038000
6	-0.712005000	5.912127000	4.811865000
1	0.692295000	4.412009000	4.160300000
6	-2.878656000	5.861807000	3.744983000
1	-3.160352000	4.326887000	2.257944000
6	-1.998640000	6.436515000	4.665436000
1	-0.021561000	6.351522000	5.526724000
1	-3.879758000	6.265972000	3.621470000
1	-2.312972000	7.287354000	5.263604000
6	-2.655698000	-2.628557000	3.006834000
6	-2.475539000	-2.857897000	4.380685000
6	-3.712239000	-3.279080000	2.347300000
6	-3.331813000	-3.711667000	5.078845000
1	-1.655315000	-2.369891000	4.899990000
6	-4.569564000	-4.130901000	3.047413000
1	-3.859245000	-3.108203000	1.284595000
6	-4.382390000	-4.349837000	4.414461000
1	-3.174450000	-3.881052000	6.140643000
1	-5.384606000	-4.622344000	2.522883000
1	-5.048807000	-5.013944000	4.958028000
6	2.115683000	-3.529911000	-2.029820000
6	3.454305000	-3.915491000	-1.853641000
6	1.309609000	-4.275594000	-2.904987000
6	3.973197000	-5.019657000	-2.533001000
1	4.087289000	-3.348408000	-1.176477000
6	1.828854000	-5.378621000	-3.585821000
1	0.273682000	-3.983926000	-3.054127000
6	3.161875000	-5.754206000	-3.401400000
1	5.010286000	-5.306354000	-2.381105000
1	1.191748000	-5.941605000	-4.262471000
1	3.565598000	-6.612809000	-3.930904000
6	3.092004000	3.392215000	-2.365957000
6	4.266184000	3.970346000	-1.857515000
6	2.713045000	3.674770000	-3.688281000
6	5.046997000	4.812007000	-2.652601000
1	4.569260000	3.753846000	-0.836460000
6	3.495859000	4.517562000	-4.481050000
1	1.796096000	3.244931000	-4.081887000
6	4.663836000	5.087205000	-3.967665000
1	5.954997000	5.248592000	-2.245177000
1	3.189103000	4.731679000	-5.501530000
1	5.270907000	5.741712000	-4.587361000
1	3.736701000	1.068203000	-3.502238000
1	3.357033000	-1.590957000	-3.378122000
1	0.523991000	-4.810914000	-0.313860000
1	-1.322252000	-4.464176000	1.606729000
1	-3.291549000	-0.286112000	4.173712000
1	-2.685846000	2.329245000	4.245223000
1	0.382542000	5.520290000	1.395523000
1	2.005714000	5.204724000	-0.725672000
8	1.918947000	0.092049000	1.833579000
6	1.917132000	-0.884048000	2.905624000
6	3.140574000	0.870743000	1.861231000
6	3.104928000	-0.514681000	3.795813000
1	0.952298000	-0.830326000	3.413783000
6	4.083896000	0.104873000	2.787233000
1	3.503787000	0.966810000	0.836531000
1	2.911372000	1.869516000	2.251636000
1	4.611249000	-0.680546000	2.233176000
1	4.829450000	0.757911000	3.250021000
1	3.512487000	-1.383442000	4.320623000
1	2.807428000	0.229577000	4.543646000
1	2.031965000	-1.881237000	2.465778000
1	-3.850887000	4.480040000	-3.160291000
7	-3.166582000	4.191410000	-2.462210000
1	-3.664164000	4.108726000	-1.580047000
1	-2.277896000	2.380437000	-1.918001000
1	-2.832026000	1.055446000	-3.886753000
6	-2.538567000	2.913152000	-2.840429000
6	-3.390340000	1.984158000	-3.738166000
6	-4.755872000	1.697892000	-3.182345000
6	-1.187011000	3.225378000	-3.511878000
8	-0.794145000	4.492259000	-3.352679000
1	-1.554882000	4.910064000	-2.852013000
8	-0.521677000	2.401408000	-4.112072000
1	-3.496119000	2.451021000	-4.725749000
1	-6.109577000	2.768235000	-4.607235000
6	-5.947183000	2.164921000	-3.724852000
7	-7.001674000	1.733726000	-2.964646000
1	-7.972227000	1.954544000	-3.135813000
1	-6.982702000	-0.608159000	1.045870000
6	-6.468243000	-0.205905000	0.177675000
6	-5.090337000	-0.285837000	0.110729000
6	-4.348206000	0.176647000	-1.058652000
6	-5.115737000	0.948151000	-2.023662000
1	-3.317093000	0.481377000	-0.872561000
1	-4.533102000	-0.746026000	0.918144000
1	-8.310693000	0.474154000	-0.772549000
6	-7.228924000	0.413875000	-0.837497000
6	-6.525511000	0.990411000	-1.905199000
7	-3.793651000	-1.367406000	-1.918513000
8	-3.677390000	-1.328367000	-3.133178000

^{4}IM3$_{C4}$:

26	0.206950000	0.377161000	0.333610000
7	1.620729000	0.114115000	-1.084772000
7	-0.022535000	-1.619484000	0.469944000
7	-0.973932000	0.602084000	1.954215000
7	0.691433000	2.334647000	0.411046000
6	0.611872000	-2.579034000	-0.289275000
6	0.164845000	-3.892730000	0.104243000
6	-0.765185000	-3.720172000	1.079104000

6	-0.887530000	-2.299879000	1.298578000
6	-1.732897000	-1.736540000	2.261221000
6	-1.751424000	-0.367167000	2.551439000
6	-2.583881000	0.228648000	3.568716000
6	-2.288269000	1.554583000	3.597479000
6	-1.297657000	1.788597000	2.575126000
6	-0.772111000	3.050956000	2.280192000
6	0.144078000	3.281691000	1.248343000
6	0.612730000	4.595647000	0.879254000
6	1.436905000	4.437712000	-0.189442000
6	1.488831000	3.025357000	-0.476630000
6	2.247842000	2.473053000	-1.513301000
6	2.291125000	1.099913000	-1.776553000
6	3.105614000	0.510575000	-2.811013000
6	2.915781000	-0.832919000	-2.747914000
6	1.991660000	-1.077591000	-1.667181000
6	1.553730000	-2.353633000	-1.298291000
8	-1.007218000	0.591553000	-0.719655000
8	-3.468387000	-2.188713000	-1.177045000
6	-1.224835000	4.223042000	3.098004000
6	-0.353016000	4.823788000	4.020082000
6	-2.520055000	4.746040000	2.957056000
6	-0.765939000	5.917808000	4.783426000
1	0.651573000	4.427014000	4.139195000
6	-2.933379000	5.840516000	3.719790000
1	-3.202628000	4.293959000	2.242577000
6	-2.057637000	6.429173000	4.635487000
1	-0.078749000	6.368011000	5.494685000
1	-3.938407000	6.234458000	3.595166000
1	-2.379213000	7.280669000	5.228845000
6	-2.641959000	-2.649025000	3.025901000
6	-2.454953000	-2.870100000	4.400237000
6	-3.695787000	-3.311639000	2.374140000
6	-3.301642000	-3.727143000	5.106006000
1	-1.636705000	-2.372959000	4.913941000
6	-4.543591000	-4.166836000	3.081556000
1	-3.848506000	-3.148084000	1.311149000
6	-4.349518000	-4.377212000	4.448973000
1	-3.138817000	-3.889836000	6.168017000
1	-5.356553000	-4.667447000	2.562543000
1	-5.008504000	-5.043869000	4.998417000
6	2.109023000	-3.536476000	-2.031717000
6	3.446459000	-3.925109000	-1.853532000
6	1.303452000	-4.278132000	-2.910705000
6	3.964767000	-5.028308000	-2.534936000
1	4.079031000	-3.361175000	-1.173356000
6	1.822093000	-5.380229000	-3.593525000
1	0.268376000	-3.984114000	-3.061207000
6	3.153997000	-5.758829000	-3.407242000
1	5.000977000	-5.317395000	-2.381591000
1	1.185411000	-5.940117000	-4.273136000
1	3.557289000	-6.616659000	-3.938322000
6	3.077696000	3.387108000	-2.363920000
6	4.232063000	3.991648000	-1.840626000
6	2.721986000	3.644266000	-3.697992000
6	5.015866000	4.833834000	-2.632094000
1	4.517501000	3.795001000	-0.810537000
6	3.507804000	4.487525000	-4.487167000
1	1.819923000	3.195232000	-4.104116000
6	4.655892000	5.083300000	-3.958776000
1	5.908324000	5.290706000	-2.212760000
1	3.218698000	4.681800000	-5.516720000
1	5.265334000	5.738128000	-4.575788000
1	3.735816000	1.062295000	-3.492416000
1	3.357145000	-1.596679000	-3.370664000
1	0.524781000	-4.820914000	-0.313811000
1	-1.312246000	-4.480102000	1.616597000
1	-3.289852000	-0.306829000	4.185771000
1	-2.704432000	2.313406000	4.243201000
1	0.330406000	5.514868000	1.370727000
1	1.962483000	5.201193000	-0.743515000
8	1.909217000	0.092293000	1.833676000
6	1.914877000	-0.885318000	2.904328000
6	3.128545000	0.874798000	1.857545000
6	3.103815000	-0.512156000	3.791334000
1	0.951371000	-0.836377000	3.415482000
6	4.077408000	0.111766000	2.780252000
1	3.488242000	0.972212000	0.831764000
1	2.897359000	1.872730000	2.248922000
1	4.605988000	-0.671323000	2.224068000
1	4.821954000	0.767205000	3.241259000
1	3.516177000	-1.379788000	4.314258000
1	2.805717000	0.230417000	4.540605000
1	2.032623000	-1.881445000	2.462868000
1	-3.797156000	4.495738000	-3.162715000
7	-3.102836000	4.196747000	-2.478971000
1	-3.583882000	4.122077000	-1.586995000
1	-2.241744000	2.366432000	-1.952173000
1	-2.848265000	1.063716000	-3.925895000
6	-2.504315000	2.907731000	-2.869137000
6	-3.388056000	1.999770000	-3.758599000
6	-4.747634000	1.735434000	-3.177004000
6	-1.156266000	3.196157000	-3.558093000
8	-0.744818000	4.458928000	-3.414441000
1	-1.491739000	4.889349000	-2.903293000
8	-0.508788000	2.358129000	-4.158522000
1	-3.504229000	2.478493000	-4.739390000
1	-6.095967000	2.918833000	-4.518741000
6	-5.932938000	2.276553000	-3.664618000
7	-6.978859000	1.859100000	-2.885265000
1	-7.943358000	2.131672000	-3.009136000
1	-6.944919000	-0.551144000	1.081759000
6	-6.439027000	-0.173247000	0.197231000
6	-5.077356000	-0.328326000	0.092802000
6	-4.317078000	0.105055000	-1.117529000
6	-5.105760000	0.952671000	-2.043095000
1	-3.328996000	0.509150000	-0.863761000
1	-4.519009000	-0.815913000	0.882190000
1	-8.279666000	0.604160000	-0.690789000
6	-7.205239000	0.491217000	-0.791032000
6	-6.501655000	1.055933000	-1.871211000
7	-3.797066000	-1.241784000	-1.883509000
8	-3.702816000	-1.218487000	-3.102515000

^{2}TS2$_{C5}$:

26	0.601560000	0.287380000	0.414685000
7	2.130570000	0.182354000	-0.891789000
7	0.388635000	-1.713837000	0.341335000
7	-0.696153000	0.343103000	1.950293000
7	1.011408000	2.237971000	0.692516000
6	1.078752000	-2.580606000	-0.476138000
6	0.493343000	-3.896716000	-0.404489000
6	-0.576968000	-3.810307000	0.428394000
6	-0.625813000	-2.451183000	0.913251000

6	-1.537718000	-1.988894000	1.869672000
6	-1.500120000	-0.685985000	2.385526000
6	-2.271157000	-0.257486000	3.527036000
6	-1.931200000	1.034797000	3.773733000
6	-0.973178000	1.419233000	2.765812000
6	-0.454624000	2.713577000	2.635085000
6	0.436499000	3.080468000	1.617820000
6	0.855613000	4.438973000	1.369956000
6	1.678837000	4.410969000	0.288430000
6	1.777566000	3.034439000	-0.130236000
6	2.604300000	2.595013000	-1.170714000
6	2.781303000	1.242378000	-1.483550000
6	3.700458000	0.757352000	-2.485638000
6	3.610008000	-0.598740000	-2.483409000
6	2.609741000	-0.952700000	-1.505553000
6	2.154334000	-2.259400000	-1.308831000
8	-0.512151000	0.560608000	-0.729747000
8	-4.906352000	2.209234000	1.901434000
6	-0.901915000	3.768287000	3.599465000
6	0.019329000	4.358069000	4.481052000
6	-2.240482000	4.194407000	3.641555000
6	-0.384864000	5.345722000	5.381256000
1	1.056276000	4.034032000	4.461784000
6	-2.643262000	5.183687000	4.541126000
1	-2.968285000	3.747440000	2.969553000
6	-1.717900000	5.762487000	5.413241000
1	0.341533000	5.786185000	6.058893000
1	-3.681661000	5.503631000	4.557306000
1	-2.033239000	6.531651000	6.112920000
6	-2.578267000	-2.924349000	2.399476000
6	-2.225033000	-4.075810000	3.122946000
6	-3.941634000	-2.653793000	2.189546000
6	-3.206218000	-4.939069000	3.614073000
1	-1.175899000	-4.288511000	3.308254000
6	-4.921738000	-3.519025000	2.679479000
1	-4.232030000	-1.761541000	1.641195000
6	-4.557909000	-4.664923000	3.391249000
1	-2.913295000	-5.822223000	4.175384000
1	-5.970686000	-3.296924000	2.502765000
1	-5.321679000	-5.337125000	3.772572000
6	2.805252000	-3.362152000	-2.092361000
6	3.976449000	-3.971626000	-1.618609000
6	2.255619000	-3.794152000	-3.309956000
6	4.588249000	-4.995708000	-2.345645000
1	4.407355000	-3.641842000	-0.676781000
6	2.869231000	-4.818938000	-4.034763000
1	1.351590000	-3.319400000	-3.683077000
6	4.035427000	-5.421863000	-3.555682000
1	5.494645000	-5.459534000	-1.965681000
1	2.435521000	-5.144758000	-4.976596000
1	4.510571000	-6.218447000	-4.121917000
6	3.358583000	3.620830000	-1.960499000
6	4.747760000	3.766521000	-1.817661000
6	2.682996000	4.460942000	-2.860162000
6	5.443866000	4.724455000	-2.557964000
1	5.281557000	3.127338000	-1.119685000
6	3.378675000	5.418750000	-3.600872000
1	1.607820000	4.357749000	-2.980088000
6	4.761327000	5.552877000	-3.452226000
1	6.518527000	4.824953000	-2.432421000
1	2.840061000	6.057648000	-4.295517000
1	5.302780000	6.298116000	-4.028387000
1	4.332892000	1.380292000	-3.100702000
1	4.147497000	-1.303578000	-3.100790000
1	0.847148000	-4.761435000	-0.946408000
1	-1.266897000	-4.593889000	0.703306000
1	-2.960871000	-0.879050000	4.078151000
1	-2.296211000	1.676638000	4.561266000
1	0.550298000	5.297678000	1.949116000
1	2.186596000	5.240324000	-0.181584000
8	2.172312000	-0.095576000	2.007101000
6	2.134420000	-1.177322000	2.972188000
6	3.361227000	0.710752000	2.195505000
6	3.235957000	-0.856178000	3.982856000
1	1.132643000	-1.212617000	3.405207000
6	4.262303000	-0.112144000	3.114873000
1	3.792298000	0.912667000	1.213137000
1	3.069548000	1.661185000	2.657855000
1	4.857311000	-0.824554000	2.531529000
1	4.947097000	0.515326000	3.692586000
1	3.637376000	-1.757106000	4.455654000
1	2.853473000	-0.196466000	4.770337000
1	2.326128000	-2.118715000	2.445042000
1	-1.926035000	2.061581000	-5.429882000
7	-1.093641000	1.545185000	-5.150701000
1	-0.450985000	2.219038000	-4.740490000
1	-1.172961000	0.763865000	-3.156594000
1	-3.092203000	-0.706983000	-3.530079000
6	-1.435430000	0.487361000	-4.183605000
6	-2.940692000	0.115401000	-4.238482000
6	-3.866635000	1.258223000	-3.940537000
6	-0.612099000	-0.767282000	-4.529833000
8	0.047969000	-0.673243000	-5.686163000
1	-0.177818000	0.252788000	-6.002409000
8	-0.583659000	-1.764127000	-3.830917000
1	-3.167623000	-0.279340000	-5.236880000
1	-4.976919000	1.568638000	-5.844093000
6	-4.764079000	1.822201000	-4.814722000
7	-5.469735000	2.833746000	-4.184009000
1	-6.186935000	3.396268000	-4.619269000
1	-5.084924000	4.481884000	0.133848000
6	-4.828002000	3.785315000	-0.656960000
6	-3.850000000	2.719743000	-0.342808000
6	-3.395997000	1.875568000	-1.448293000
6	-4.025413000	1.967933000	-2.683254000
1	-2.585181000	1.180158000	-1.260250000
1	-3.060099000	3.035451000	0.342856000
1	-6.160625000	4.644390000	-2.089559000
6	-5.427481000	3.870318000	-1.880452000
6	-5.041985000	2.949611000	-2.889812000
7	-4.660157000	1.697249000	0.815983000
8	-4.962086000	0.561045000	0.482696000

^{2}IM3$_{C5}$:

26	0.582037000	0.255666000	0.426868000
7	2.089631000	0.143943000	-0.903937000
7	0.380313000	-1.747787000	0.380888000
7	-0.693062000	0.319871000	1.981308000
7	0.986151000	2.210841000	0.679181000
6	1.058244000	-2.617826000	-0.442930000
6	0.464311000	-3.930007000	-0.369515000
6	-0.593999000	-3.839982000	0.478396000
6	-0.629830000	-2.481431000	0.965435000
6	-1.527461000	-2.015367000	1.933372000

6	-1.483563000	-0.709283000	2.440483000
6	-2.235625000	-0.274592000	3.592186000
6	-1.899791000	1.022339000	3.819513000
6	-0.963232000	1.402556000	2.790010000
6	-0.458718000	2.699532000	2.634265000
6	0.415624000	3.060621000	1.600725000
6	0.821985000	4.418848000	1.331549000
6	1.634306000	4.383316000	0.242051000
6	1.738023000	3.002525000	-0.161296000
6	2.557614000	2.555658000	-1.204235000
6	2.736519000	1.200472000	-1.505893000
6	3.657066000	0.708798000	-2.503434000
6	3.572543000	-0.647546000	-2.486915000
6	2.569942000	-0.995401000	-1.509271000
6	2.121825000	-2.301832000	-1.293358000
8	-0.551088000	0.511495000	-0.702474000
8	-4.870995000	2.063792000	1.880022000
6	-0.906886000	3.763189000	3.588067000
6	0.015262000	4.375472000	4.453028000
6	-2.249762000	4.174785000	3.635941000
6	-0.392458000	5.371155000	5.342802000
1	1.055531000	4.062578000	4.429433000
6	-2.656191000	5.172119000	4.524830000
1	-2.977169000	3.709460000	2.976018000
6	-1.729810000	5.773381000	5.380582000
1	0.334608000	5.829246000	6.007914000
1	-3.697940000	5.480673000	4.545680000
1	-2.047761000	6.548764000	6.072163000
6	-2.557942000	-2.949281000	2.484544000
6	-2.190666000	-4.099385000	3.203220000
6	-3.925189000	-2.679200000	2.300042000
6	-3.161989000	-4.961684000	3.715136000
1	-1.138093000	-4.311586000	3.368518000
6	-4.895320000	-3.543814000	2.810552000
1	-4.226180000	-1.788874000	1.754197000
6	-4.517743000	-4.688079000	3.517815000
1	-2.858151000	-5.843621000	4.272550000
1	-5.947562000	-3.322596000	2.653285000
1	-5.273973000	-5.359535000	3.915165000
6	2.760606000	-3.414122000	-2.072071000
6	3.721778000	-4.240075000	-1.470513000
6	2.401655000	-3.647497000	-3.409447000
6	4.319943000	-5.276057000	-2.191906000
1	4.002280000	-4.066454000	-0.434878000
6	3.000194000	-4.685267000	-4.128074000
1	1.644620000	-3.020166000	-3.873123000
6	3.960911000	-5.500237000	-3.523252000
1	5.065581000	-5.905626000	-1.713688000
1	2.712718000	-4.858357000	-5.161855000
1	4.425293000	-6.306148000	-4.085192000
6	3.303040000	3.576622000	-2.008693000
6	4.693377000	3.724875000	-1.880051000
6	2.618269000	4.410639000	-2.907150000
6	5.381533000	4.678296000	-2.633455000
1	5.234465000	3.091022000	-1.182854000
6	3.305890000	5.364074000	-3.660901000
1	1.541765000	4.307359000	-3.014744000
6	4.689805000	5.500138000	-3.526715000
1	6.457233000	4.780560000	-2.518749000
1	2.759962000	5.998112000	-4.354284000
1	5.225034000	6.241875000	-4.113107000
1	4.289353000	1.327423000	-3.122916000
1	4.116901000	-1.355765000	-3.094071000
1	0.804459000	-4.794416000	-0.920711000
1	-1.285918000	-4.619774000	0.759169000
1	-2.911302000	-0.894960000	4.161760000
1	-2.254238000	1.669933000	4.607195000
1	0.516938000	5.282436000	1.903564000
1	2.131678000	5.210426000	-0.242746000
8	2.179010000	-0.104223000	1.999088000
6	2.160376000	-1.177781000	2.973689000
6	3.362989000	0.713808000	2.168456000
6	3.263606000	-0.833702000	3.974656000
1	1.161564000	-1.221696000	3.412606000
6	4.277374000	-0.089208000	3.092462000
1	3.786235000	0.906029000	1.180651000
1	3.066588000	1.667937000	2.619844000
1	4.876716000	-0.802223000	2.514345000
1	4.958721000	0.552123000	3.658912000
1	3.676992000	-1.724881000	4.455563000
1	2.878310000	-0.168985000	4.756563000
1	2.361114000	-2.121448000	2.453879000
1	-1.847068000	2.355839000	-5.351409000
7	-0.993364000	1.862619000	-5.095233000
1	-0.389992000	2.536812000	-4.629585000
1	-1.076080000	0.948035000	-3.157150000
1	-2.901086000	-0.591934000	-3.671544000
6	-1.296119000	0.726310000	-4.207278000
6	-2.776139000	0.275387000	-4.329792000
6	-3.773973000	1.347599000	-4.002730000
6	-0.394662000	-0.454659000	-4.612612000
8	0.280866000	-0.249057000	-5.745459000
1	0.007460000	0.681059000	-6.007433000
8	-0.322594000	-1.491975000	-3.979096000
1	-2.950720000	-0.075864000	-5.354653000
1	-4.829600000	1.707755000	-5.929113000
6	-4.668613000	1.913471000	-4.879841000
7	-5.449159000	2.849101000	-4.223253000
1	-6.179461000	3.397679000	-4.654129000
1	-5.319249000	4.274781000	0.190090000
6	-4.993209000	3.638762000	-0.625739000
6	-3.944950000	2.619554000	-0.320853000
6	-3.425047000	1.841808000	-1.465292000
6	-4.014612000	1.976312000	-2.715333000
1	-2.590235000	1.173752000	-1.283593000
1	-3.154899000	3.018685000	0.325472000
1	-6.320642000	4.491793000	-2.059596000
6	-5.548514000	3.752510000	-1.864212000
6	-5.074059000	2.912876000	-2.908171000
7	-4.621244000	1.589553000	0.776831000
8	-4.856235000	0.438706000	0.433948000

^{4}TS2$_{C5}$:

26	0.378425000	1.016208000	0.884671000
7	1.732930000	0.824692000	-0.590071000
7	-0.443489000	-0.738116000	0.358957000
7	-0.784242000	1.042911000	2.528139000
7	1.402333000	2.596000000	1.577020000
6	-0.006413000	-1.603075000	-0.621177000
6	-0.861747000	-2.765262000	-0.660866000
6	-1.849025000	-2.564270000	0.252032000
6	-1.580694000	-1.299899000	0.892196000
6	-2.334928000	-0.797639000	1.961366000
6	-1.922101000	0.293949000	2.734785000

6	-2.595730000	0.746081000	3.928659000
6	-1.834318000	1.737907000	4.462279000
6	-0.719240000	1.941618000	3.568899000
6	0.245775000	2.940802000	3.740650000
6	1.214467000	3.243553000	2.776951000
6	2.104354000	4.376383000	2.866357000
6	2.799462000	4.428425000	1.699155000
6	2.357800000	3.314420000	0.895302000
6	2.890243000	2.999156000	-0.361258000
6	2.589935000	1.808740000	-1.034665000
6	3.194183000	1.405696000	-2.280761000
6	2.729784000	0.159007000	-2.561641000
6	1.807263000	-0.195888000	-1.510048000
6	1.060559000	-1.382492000	-1.501768000
8	-0.644365000	1.907765000	0.000923000
8	-1.839485000	2.500580000	-3.320309000
6	0.204597000	3.776000000	4.985191000
6	1.169826000	3.597816000	5.988651000
6	-0.784758000	4.755034000	5.168092000
6	1.145033000	4.376614000	7.147698000
1	1.941239000	2.843663000	5.857903000
6	-0.810288000	5.533577000	6.327208000
1	-1.532316000	4.908630000	4.394578000
6	0.154430000	5.346424000	7.320398000
1	1.898713000	4.223428000	7.915379000
1	-1.581632000	6.288889000	6.451022000
1	0.134961000	5.952820000	8.221755000
6	-3.608118000	-1.501331000	2.314701000
6	-3.736812000	-2.220669000	3.514236000
6	-4.701698000	-1.461363000	1.433864000
6	-4.928626000	-2.877255000	3.827430000
1	-2.894781000	-2.271183000	4.198972000
6	-5.893867000	-2.116864000	1.747911000
1	-4.615127000	-0.908176000	0.502355000
6	-6.011370000	-2.826011000	2.945972000
1	-5.008214000	-3.432623000	4.758031000
1	-6.731066000	-2.070824000	1.056691000
1	-6.938835000	-3.336699000	3.190029000
6	1.391501000	-2.430574000	-2.517406000
6	2.641616000	-3.072301000	-2.484528000
6	0.478052000	-2.792867000	-3.521014000
6	2.966088000	-4.052071000	-3.424570000
1	3.357492000	-2.804793000	-1.712000000
6	0.802742000	-3.772344000	-4.461731000
1	-0.492859000	-2.310980000	-3.577684000
6	2.047179000	-4.405471000	-4.416449000
1	3.935596000	-4.541017000	-3.378690000
1	0.073140000	-4.028092000	-5.224179000
1	2.300333000	-5.168219000	-5.147954000
6	3.857704000	3.958846000	-0.980970000
6	5.213788000	3.627143000	-1.134877000
6	3.421406000	5.222260000	-1.412703000
6	6.108449000	4.532956000	-1.708175000
1	5.567493000	2.657580000	-0.795389000
6	4.315595000	6.127405000	-1.987633000
1	2.374327000	5.490183000	-1.301440000
6	5.661878000	5.785366000	-2.137280000
1	7.155007000	4.260731000	-1.815053000
1	3.958611000	7.098151000	-2.320711000
1	6.358163000	6.489759000	-2.583998000
1	3.888448000	2.000072000	-2.855956000
1	2.964069000	-0.459729000	-3.415112000
1	-0.724876000	-3.616104000	-1.311054000
1	-2.668363000	-3.223013000	0.499432000
1	-3.517074000	0.336954000	4.315551000
1	-2.014385000	2.299373000	5.367006000
1	2.169056000	5.048565000	3.709290000
1	3.554076000	5.143557000	1.406584000
8	1.808919000	-0.223816000	2.136895000
6	1.464010000	-1.461910000	2.806284000
6	3.211320000	0.085679000	2.332043000
6	2.655443000	-1.776328000	3.710890000
1	0.526275000	-1.307368000	3.344055000
6	3.827942000	-1.187210000	2.911951000
1	3.629516000	0.384444000	1.368867000
1	3.287328000	0.928260000	3.029266000
1	4.123994000	-1.870952000	2.107773000
1	4.709390000	-0.977142000	3.524611000
1	2.755673000	-2.848308000	3.903729000
1	2.552730000	-1.262341000	4.673750000
1	1.314220000	-2.238352000	2.047305000
1	-5.461399000	-0.051795000	-6.239991000
7	-4.577553000	-0.465484000	-6.532634000
1	-4.014365000	0.288522000	-6.920337000
1	-3.144426000	-0.437993000	-4.936857000
1	-4.351648000	-2.080525000	-3.534874000
6	-3.897260000	-1.093612000	-5.389711000
6	-4.910420000	-1.518610000	-4.291587000
6	-5.630035000	-0.356428000	-3.676433000
6	-3.166401000	-2.350916000	-5.891336000
8	-3.512865000	-2.715066000	-7.128232000
1	-4.156783000	-1.999834000	-7.408587000
8	-2.373380000	-2.978867000	-5.214930000
1	-5.635548000	-2.211695000	-4.736089000
1	-7.713114000	-0.490768000	-4.451955000
6	-6.943109000	-0.001872000	-3.871133000
7	-7.228139000	1.156789000	-3.166523000
1	-8.130644000	1.609752000	-3.141054000
1	-4.506600000	3.709514000	-0.413217000
6	-4.681545000	2.884559000	-1.094487000
6	-3.528609000	2.033168000	-1.453570000
6	-3.805661000	0.823447000	-2.229107000
6	-5.062148000	0.651175000	-2.799938000
1	-3.004846000	0.108975000	-2.383618000
1	-2.798676000	1.897767000	-0.650827000
1	-6.755319000	3.326046000	-1.369495000
6	-5.921304000	2.679549000	-1.628021000
6	-6.106113000	1.579394000	-2.506874000
7	-2.453049000	3.035732000	-2.408944000
8	-2.332585000	4.199967000	-2.057135000

^{4}IM3$_{C5}$:

26	0.407685000	1.023394000	0.819231000
7	1.800145000	0.819605000	-0.619858000
7	-0.412710000	-0.727428000	0.274915000
7	-0.800116000	1.063430000	2.430956000
7	1.423789000	2.599176000	1.536951000
6	0.036783000	-1.590025000	-0.701704000
6	-0.821426000	-2.749269000	-0.759804000
6	-1.821345000	-2.549759000	0.139415000
6	-1.560359000	-1.287868000	0.787280000
6	-2.334950000	-0.783784000	1.840554000
6	-1.941555000	0.313767000	2.615209000
6	-2.647436000	0.775251000	3.786511000

6	-1.903852000	1.775422000	4.329288000
6	-0.765208000	1.972182000	3.464664000
6	0.196387000	2.970626000	3.657023000
6	1.199275000	3.258172000	2.724484000
6	2.097279000	4.382340000	2.838460000
6	2.837234000	4.416585000	1.698732000
6	2.412435000	3.302085000	0.886594000
6	2.983967000	2.975650000	-0.349396000
6	2.685206000	1.791809000	-1.034668000
6	3.316703000	1.386830000	-2.266426000
6	2.836784000	0.151689000	-2.570557000
6	1.881661000	-0.195354000	-1.545792000
6	1.120079000	-1.372119000	-1.562641000
8	-0.583398000	1.918785000	-0.096569000
8	-2.005844000	2.691905000	-3.320623000
6	0.118027000	3.817291000	4.892036000
6	1.048215000	3.643185000	5.928759000
6	-0.872369000	4.802052000	5.033476000
6	0.988332000	4.431769000	7.079848000
1	1.819980000	2.884514000	5.830085000
6	-0.933021000	5.590378000	6.184684000
1	-1.593002000	4.952036000	4.234144000
6	-0.002991000	5.407313000	7.211186000
1	1.715118000	4.281702000	7.873625000
1	-1.704587000	6.350031000	6.276426000
1	-0.049883000	6.021337000	8.106353000
6	-3.612822000	-1.489152000	2.173942000
6	-3.758429000	-2.207742000	3.371940000
6	-4.692806000	-1.451034000	1.276549000
6	-4.953611000	-2.866597000	3.667104000
1	-2.927074000	-2.255574000	4.069811000
6	-5.888281000	-2.108957000	1.572607000
1	-4.593028000	-0.897130000	0.346823000
6	-6.022662000	-2.818080000	2.768911000
1	-5.046563000	-3.421467000	4.596766000
1	-6.714781000	-2.064800000	0.868499000
1	-6.952675000	-3.330715000	2.998845000
6	1.452769000	-2.413321000	-2.584793000
6	2.693196000	-3.072933000	-2.543269000
6	0.547221000	-2.750746000	-3.604080000
6	3.016278000	-4.045569000	-3.491254000
1	3.402473000	-2.825102000	-1.758197000
6	0.870536000	-3.723315000	-4.552318000
1	-0.416495000	-2.255570000	-3.666723000
6	2.105583000	-4.373999000	-4.499209000
1	3.978186000	-4.548670000	-3.438955000
1	0.147297000	-3.960743000	-5.326764000
1	2.357726000	-5.131285000	-5.236711000
6	3.991199000	3.916215000	-0.934394000
6	5.345873000	3.558735000	-1.032760000
6	3.595774000	5.185354000	-1.387986000
6	6.279588000	4.445468000	-1.572563000
1	5.667088000	2.583951000	-0.676303000
6	4.529072000	6.071389000	-1.929630000
1	2.550236000	5.472982000	-1.319562000
6	5.873757000	5.704024000	-2.023579000
1	7.324359000	4.153595000	-1.636393000
1	4.203985000	7.047130000	-2.280292000
1	6.600291000	6.393746000	-2.444280000
1	4.037029000	1.973121000	-2.817341000
1	3.082356000	-0.464414000	-3.422697000
1	-0.676710000	-3.597920000	-1.411140000
1	-2.645975000	-3.207245000	0.372035000
1	-3.577376000	0.366598000	4.152766000
1	-2.109631000	2.345785000	5.222890000
1	2.137852000	5.060526000	3.678063000
1	3.610495000	5.120868000	1.429506000
8	1.794916000	-0.226474000	2.110685000
6	1.422667000	-1.460604000	2.773296000
6	3.192934000	0.074711000	2.346838000
6	2.587838000	-1.784121000	3.708526000
1	0.473211000	-1.297440000	3.287372000
6	3.785162000	-1.202740000	2.941632000
1	3.640955000	0.372432000	1.396901000
1	3.253907000	0.915513000	3.047701000
1	4.097551000	-1.887719000	2.144726000
1	4.651476000	-0.999317000	3.577663000
1	2.675259000	-2.856980000	3.902686000
1	2.463523000	-1.270493000	4.669009000
1	1.285278000	-2.236609000	2.011608000
1	-5.705631000	-0.171793000	-5.981872000
7	-4.833175000	-0.536022000	-6.361588000
1	-4.367964000	0.240657000	-6.826762000
1	-3.246754000	-0.365083000	-4.927105000
1	-4.174293000	-2.044715000	-3.372460000
6	-3.991914000	-1.084056000	-5.286999000
6	-4.851217000	-1.554244000	-4.080901000
6	-5.601249000	-0.435804000	-3.422333000
6	-3.228083000	-2.298676000	-5.841956000
8	-3.681456000	-2.722492000	-7.024296000
1	-4.403025000	-2.062971000	-7.245702000
8	-2.320434000	-2.848810000	-5.247056000
1	-5.556315000	-2.317403000	-4.433181000
1	-7.729280000	-0.751205000	-4.000218000
6	-6.951412000	-0.189196000	-3.501774000
7	-7.262685000	0.959200000	-2.793483000
1	-8.192218000	1.340824000	-2.691750000
1	-4.526817000	3.781192000	-0.329605000
6	-4.692373000	2.931198000	-0.981345000
6	-3.492725000	2.157925000	-1.416208000
6	-3.751358000	0.911961000	-2.170524000
6	-5.037955000	0.633080000	-2.617575000
1	-2.914495000	0.258090000	-2.387618000
1	-2.761901000	2.020764000	-0.609932000
1	-6.805811000	3.199623000	-1.082274000
6	-5.947932000	2.614700000	-1.402743000
6	-6.121925000	1.482406000	-2.245903000
7	-2.558461000	3.161662000	-2.335296000
8	-2.427663000	4.310941000	-1.933816000

^{2}TS2$_{C6}$:

26	0.080385000	0.266728000	0.697535000
7	1.591698000	-0.065895000	-0.593033000
7	-0.238896000	-1.713341000	0.834121000
7	-1.228439000	0.557707000	2.201711000
7	0.614449000	2.202850000	0.783670000
6	0.470215000	-2.714431000	0.206528000
6	-0.056919000	-4.001303000	0.591076000
6	-1.121102000	-3.768384000	1.403980000
6	-1.235024000	-2.338379000	1.550376000
6	-2.195709000	-1.715336000	2.356748000
6	-2.170713000	-0.346520000	2.646084000
6	-3.109386000	0.313559000	3.519247000
6	-2.709457000	1.608863000	3.625589000

6	-1.540307000	1.760904000	2.794729000
6	-0.877077000	2.978935000	2.603554000
6	0.136274000	3.157506000	1.654752000
6	0.796936000	4.416512000	1.410434000
6	1.630565000	4.230217000	0.352683000
6	1.510000000	2.848288000	-0.040773000
6	2.247112000	2.270031000	-1.081484000
6	2.264037000	0.892368000	-1.322413000
6	3.057748000	0.262266000	-2.348190000
6	2.887355000	-1.079452000	-2.213102000
6	1.965972000	-1.281023000	-1.121264000
6	1.509280000	-2.540597000	-0.715159000
8	-1.032306000	0.491341000	-0.465184000
8	-2.789275000	5.369308000	-4.594351000
6	-1.327561000	4.159717000	3.406733000
6	-1.118648000	4.201436000	4.794160000
6	-1.983097000	5.240684000	2.791364000
6	-1.551457000	5.294349000	5.548718000
1	-0.609507000	3.374253000	5.281053000
6	-2.418285000	6.332454000	3.547221000
1	-2.150370000	5.222889000	1.717929000
6	-2.204064000	6.361826000	4.928365000
1	-1.376058000	5.310906000	6.620859000
1	-2.922098000	7.160241000	3.055427000
1	-2.541671000	7.211563000	5.515004000
6	-3.270370000	-2.563100000	2.962431000
6	-3.329043000	-2.778340000	4.349249000
6	-4.241159000	-3.166823000	2.146274000
6	-4.333580000	-3.572865000	4.905221000
1	-2.578284000	-2.326320000	4.991441000
6	-5.247479000	-3.958752000	2.702605000
1	-4.208037000	-3.007175000	1.072030000
6	-5.296688000	-4.163985000	4.083670000
1	-4.360356000	-3.732380000	5.979692000
1	-5.993672000	-4.412888000	2.056405000
1	-6.079129000	-4.781154000	4.516462000
6	2.130575000	-3.752283000	-1.337583000
6	3.472099000	-4.075593000	-1.075882000
6	1.393934000	-4.582649000	-2.198203000
6	4.059524000	-5.202724000	-1.653785000
1	4.052944000	-3.441807000	-0.411361000
6	1.982265000	-5.707944000	-2.778666000
1	0.358415000	-4.338164000	-2.417762000
6	3.316277000	-6.022164000	-2.506964000
1	5.096997000	-5.440576000	-1.435239000
1	1.398520000	-6.335951000	-3.446098000
1	3.773625000	-6.898448000	-2.957972000
6	3.090529000	3.164041000	-1.938555000
6	4.491818000	3.132173000	-1.847655000
6	2.493445000	4.055277000	-2.844938000
6	5.276666000	3.970735000	-2.641713000
1	4.965613000	2.451590000	-1.145487000
6	3.279853000	4.890680000	-3.641355000
1	1.412160000	4.090073000	-2.942792000
6	4.672617000	4.852357000	-3.541692000
1	6.359238000	3.935894000	-2.554426000
1	2.799698000	5.568569000	-4.341772000
1	5.283166000	5.503908000	-4.160803000
1	3.668010000	0.785674000	-3.069125000
1	3.326029000	-1.867746000	-2.806631000
1	0.337272000	-4.954115000	0.270878000
1	-1.761989000	-4.493128000	1.883836000
1	-3.955464000	-0.160859000	3.993710000
1	-3.166805000	2.398582000	4.202795000
1	0.634153000	5.322560000	1.974953000
1	2.286304000	4.950913000	-0.113193000
8	1.613842000	-0.038157000	2.321872000
6	1.490979000	-0.997066000	3.403460000
6	2.879255000	0.666743000	2.409652000
6	2.605869000	-0.639003000	4.384921000
1	0.485506000	-0.909310000	3.818977000
6	3.697577000	-0.101414000	3.447280000
1	3.326802000	0.684498000	1.414389000
1	2.680315000	1.695755000	2.729602000
1	4.237181000	-0.930275000	2.974617000
1	4.426955000	0.538687000	3.951705000
1	2.927103000	-1.501298000	4.976152000
1	2.273614000	0.145726000	5.074448000
1	1.619966000	-2.004617000	2.991918000
1	-5.765953000	3.392774000	2.799414000
7	-5.746021000	4.411548000	2.806063000
1	-4.770400000	4.690108000	2.878630000
1	-5.846721000	5.884793000	1.335705000
1	-6.954572000	4.528632000	-0.428315000
6	-6.378025000	4.961302000	1.595276000
6	-6.381989000	4.028660000	0.360023000
6	-5.004368000	3.669989000	-0.115332000
6	-7.814904000	5.400444000	1.951091000
8	-8.058566000	5.403289000	3.265513000
1	-7.203195000	5.061738000	3.659918000
8	-8.642184000	5.735318000	1.126235000
1	-6.935274000	3.115457000	0.614999000
1	-4.721081000	1.566777000	0.595685000
6	-4.354615000	2.455885000	0.100487000
7	-3.092754000	2.489549000	-0.424127000
1	-2.398790000	1.735471000	-0.382849000
1	-0.869785000	6.122575000	-2.171848000
6	-1.811968000	5.573013000	-2.182081000
6	-3.016564000	6.370726000	-1.914158000
6	-4.106563000	5.842495000	-1.285795000
6	-4.079280000	4.493705000	-0.812982000
1	-4.988998000	6.456558000	-1.124178000
1	-3.027966000	7.399499000	-2.260474000
1	-0.827132000	3.664474000	-1.662458000
6	-1.742280000	4.240378000	-1.587321000
6	-2.878802000	3.731079000	-0.993998000
7	-1.759330000	5.275658000	-3.946378000
8	-0.673542000	4.907337000	-4.384495000

^{2}IM3$_{C6}$:

26	0.070893000	0.259990000	0.692090000
7	1.597348000	-0.065280000	-0.583849000
7	-0.270959000	-1.719714000	0.789033000
7	-1.258243000	0.537625000	2.182663000
7	0.624230000	2.189526000	0.821268000
6	0.430208000	-2.715343000	0.143982000
6	-0.109282000	-4.004493000	0.502552000
6	-1.171903000	-3.777647000	1.319045000
6	-1.274563000	-2.349616000	1.490745000
6	-2.236555000	-1.733216000	2.300394000
6	-2.209273000	-0.367929000	2.605260000
6	-3.158557000	0.286274000	3.471320000
6	-2.758055000	1.579860000	3.593979000
6	-1.575830000	1.735965000	2.782748000

6	-0.902359000	2.952025000	2.618478000
6	0.134604000	3.134636000	1.696411000
6	0.817948000	4.388794000	1.494140000
6	1.680728000	4.209766000	0.458915000
6	1.551642000	2.837664000	0.034772000
6	2.306112000	2.269931000	-0.999612000
6	2.298749000	0.898770000	-1.277533000
6	3.090476000	0.281160000	-2.312501000
6	2.889607000	-1.059796000	-2.218674000
6	1.953784000	-1.272734000	-1.141690000
6	1.474394000	-2.534376000	-0.770231000
8	-1.021658000	0.516692000	-0.482735000
8	-2.564777000	5.478735000	-4.540341000
6	-1.361439000	4.127004000	3.425242000
6	-1.184905000	4.151201000	4.817602000
6	-1.990844000	5.221797000	2.807033000
6	-1.624293000	5.240049000	5.574217000
1	-0.695409000	3.313677000	5.306932000
6	-2.432421000	6.309707000	3.564843000
1	-2.132524000	5.218099000	1.729753000
6	-2.250867000	6.321305000	4.950953000
1	-1.474078000	5.242778000	6.650295000
1	-2.915366000	7.148496000	3.070724000
1	-2.593325000	7.168032000	5.539119000
6	-3.317810000	-2.583771000	2.890241000
6	-3.384898000	-2.812460000	4.274540000
6	-4.286139000	-3.176117000	2.062885000
6	-4.394796000	-3.609323000	4.817207000
1	-2.636387000	-2.368912000	4.925199000
6	-5.297847000	-3.970417000	2.605922000
1	-4.246853000	-3.005800000	0.990493000
6	-5.355162000	-4.189309000	3.984580000
1	-4.427952000	-3.779319000	5.889892000
1	-6.041998000	-4.415679000	1.951245000
1	-6.141841000	-4.808326000	4.406931000
6	2.079325000	-3.740131000	-1.419811000
6	3.413934000	-4.092443000	-1.160301000
6	1.333069000	-4.536056000	-2.304328000
6	3.985337000	-5.214298000	-1.763990000
1	4.001971000	-3.485441000	-0.477349000
6	1.905491000	-5.655857000	-2.910738000
1	0.302727000	-4.268921000	-2.521891000
6	3.232739000	-5.999172000	-2.641160000
1	5.017590000	-5.475045000	-1.546845000
1	1.314656000	-6.256913000	-3.596498000
1	3.677639000	-6.871234000	-3.112356000
6	3.194638000	3.165412000	-1.807237000
6	4.592459000	3.065440000	-1.707990000
6	2.647701000	4.127100000	-2.672505000
6	5.422025000	3.905222000	-2.453398000
1	5.028305000	2.330568000	-1.036696000
6	3.478735000	4.964077000	-3.420355000
1	1.570063000	4.216466000	-2.774683000
6	4.867347000	4.857210000	-3.312653000
1	6.501004000	3.816833000	-2.359656000
1	3.036588000	5.697003000	-4.089678000
1	5.512749000	5.510027000	-3.893917000
1	3.718636000	0.811391000	-3.012669000
1	3.317350000	-1.839887000	-2.830712000
1	0.276917000	-4.954415000	0.164502000
1	-1.819748000	-4.505606000	1.784420000
1	-4.012289000	-0.190552000	3.929374000
1	-3.222020000	2.365684000	4.171181000
1	0.651567000	5.286324000	2.071043000
1	2.360609000	4.929455000	0.027632000
8	1.578705000	-0.088886000	2.334827000
6	1.432840000	-1.066306000	3.396798000
6	2.848962000	0.602588000	2.452590000
6	2.537273000	-0.736462000	4.399730000
1	0.422660000	-0.977091000	3.800485000
6	3.646334000	-0.191359000	3.487067000
1	3.310243000	0.634178000	1.463997000
1	2.654958000	1.627493000	2.788395000
1	4.185591000	-1.016107000	3.006849000
1	4.373967000	0.433111000	4.013147000
1	2.842989000	-1.612328000	4.979125000
1	2.202341000	0.038307000	5.099140000
1	1.558434000	-2.067260000	2.968398000
1	-5.764198000	3.430906000	2.770829000
7	-5.741946000	4.449500000	2.786746000
1	-4.766644000	4.724900000	2.874361000
1	-5.814280000	5.930063000	1.320804000
1	-6.925907000	4.588460000	-0.454818000
6	-6.357031000	5.011107000	1.572583000
6	-6.359325000	4.082860000	0.334257000
6	-4.981511000	3.718561000	-0.137041000
6	-7.792769000	5.463120000	1.917223000
8	-8.050699000	5.456001000	3.228840000
1	-7.202646000	5.101919000	3.628630000
8	-8.607285000	5.815008000	1.086653000
1	-6.918590000	3.171689000	0.583668000
1	-4.705862000	1.614963000	0.579444000
6	-4.337332000	2.501884000	0.082183000
7	-3.074454000	2.531224000	-0.445911000
1	-2.383208000	1.775681000	-0.401907000
1	-0.849258000	6.195528000	-2.019383000
6	-1.764767000	5.626754000	-2.217179000
6	-3.008083000	6.410908000	-1.963563000
6	-4.084619000	5.884002000	-1.323924000
6	-4.055390000	4.535994000	-0.837609000
1	-4.969300000	6.496249000	-1.166474000
1	-3.026319000	7.435541000	-2.321807000
1	-0.807633000	3.685273000	-1.700862000
6	-1.719893000	4.265091000	-1.620772000
6	-2.855991000	3.770845000	-1.019485000
7	-1.579811000	5.419906000	-3.817565000
8	-0.441583000	5.151606000	-4.197747000

^{4}TS2$_{C6}$:

26	0.506448000	-0.172452000	0.420315000
7	2.145222000	-0.434504000	-0.722666000
7	0.449236000	-2.148435000	0.795186000
7	-0.943399000	0.104647000	1.797917000
7	0.762473000	1.819194000	0.289814000
6	1.330210000	-3.104321000	0.338919000
6	0.963085000	-4.398012000	0.862698000
6	-0.171633000	-4.224478000	1.590414000
6	-0.493773000	-2.819215000	1.540760000
6	-1.586103000	-2.249310000	2.207272000
6	-1.779509000	-0.866537000	2.305825000
6	-2.873196000	-0.250662000	3.017396000
6	-2.673543000	1.092857000	2.965010000
6	-1.471096000	1.311749000	2.198271000
6	-0.968605000	2.581802000	1.891064000

6	0.087369000	2.790990000	0.995891000
6	0.589737000	4.094912000	0.636234000
6	1.529845000	3.906610000	-0.328087000
6	1.630375000	2.484400000	-0.546548000
6	2.524797000	1.899307000	-1.451950000
6	2.742376000	0.519049000	-1.519778000
6	3.687418000	-0.107526000	-2.411698000
6	3.682380000	-1.436019000	-2.124819000
6	2.714500000	-1.637515000	-1.073458000
6	2.397572000	-2.893623000	-0.542024000
8	-0.527872000	-0.251235000	-0.823688000
8	-2.039638000	0.425435000	-4.253963000
6	-1.626693000	3.773191000	2.515774000
6	-1.520012000	4.002098000	3.897347000
6	-2.366519000	4.679604000	1.738392000
6	-2.131434000	5.110949000	4.485915000
1	-0.948301000	3.309556000	4.509114000
6	-2.980108000	5.786778000	2.327798000
1	-2.466534000	4.508107000	0.669954000
6	-2.863179000	6.006936000	3.702606000
1	-2.033133000	5.275197000	5.555566000
1	-3.552078000	6.475746000	1.711978000
1	-3.339562000	6.869607000	4.160242000
6	-2.564321000	-3.164377000	2.875107000
6	-2.689636000	-3.191572000	4.273998000
6	-3.372759000	-4.022687000	2.111494000
6	-3.599952000	-4.050870000	4.892089000
1	-2.063490000	-2.540518000	4.877713000
6	-4.284960000	-4.880356000	2.729303000
1	-3.287340000	-4.010259000	1.028382000
6	-4.401385000	-4.897066000	4.121484000
1	-3.679184000	-4.061498000	5.975776000
1	-4.905864000	-5.533236000	2.121869000
1	-5.110434000	-5.565289000	4.602353000
6	3.214312000	-4.070751000	-0.976978000
6	4.564929000	-4.175252000	-0.605927000
6	2.654635000	-5.086189000	-1.769909000
6	5.333862000	-5.267814000	-1.011648000
1	5.009966000	-3.396839000	0.007807000
6	3.424238000	-6.177104000	-2.178543000
1	1.613923000	-5.012917000	-2.073024000
6	4.765728000	-6.271918000	-1.799629000
1	6.375743000	-5.334199000	-0.710257000
1	2.975796000	-6.950259000	-2.796493000
1	5.364180000	-7.121350000	-2.117201000
6	3.300861000	2.800941000	-2.360514000
6	4.691602000	2.943013000	-2.225454000
6	2.641076000	3.532700000	-3.361995000
6	5.405564000	3.795540000	-3.069875000
1	5.211774000	2.388558000	-1.449162000
6	3.356771000	4.382872000	-4.207443000
1	1.567467000	3.419829000	-3.480762000
6	4.739991000	4.517861000	-4.063552000
1	6.480499000	3.897792000	-2.947769000
1	2.832529000	4.937386000	-4.981146000
1	5.295547000	5.180894000	-4.721128000
1	4.277036000	0.408991000	-3.154402000
1	4.263430000	-2.218186000	-2.590412000
1	1.505422000	-5.315267000	0.688172000
1	-0.733636000	-4.970591000	2.132405000
1	-3.680970000	-0.783132000	3.497156000
1	-3.288660000	1.872496000	3.389472000
1	0.259262000	5.028227000	1.067088000
1	2.122002000	4.654751000	-0.833838000
8	1.950140000	-0.063713000	2.168710000
6	1.854853000	-0.872048000	3.367883000
6	3.104907000	0.810771000	2.237297000
6	2.820725000	-0.229730000	4.362429000
1	0.813140000	-0.871004000	3.693742000
6	3.916827000	0.316169000	3.434608000
1	3.634797000	0.748212000	1.284855000
1	2.753232000	1.838763000	2.381502000
1	4.596181000	-0.489247000	3.132114000
1	4.511999000	1.114313000	3.887417000
1	3.192564000	-0.946998000	5.099789000
1	2.329893000	0.591282000	4.898057000
1	2.149452000	-1.899213000	3.122449000
1	-8.157707000	5.866630000	-1.609840000
7	-7.363174000	6.221950000	-1.079137000
1	-7.070151000	5.477863000	-0.451992000
1	-5.333395000	6.511671000	-1.422101000
1	-5.387804000	6.306367000	-3.912635000
6	-6.271455000	6.625369000	-1.979466000
6	-6.160993000	5.829681000	-3.301228000
6	-5.856369000	4.374138000	-3.093009000
6	-6.402104000	8.138571000	-2.254130000
8	-7.239360000	8.760518000	-1.416418000
1	-7.602184000	8.020706000	-0.850861000
8	-5.787928000	8.723835000	-3.123529000
1	-7.104422000	5.938365000	-3.851816000
1	-7.835519000	3.361617000	-3.348750000
6	-6.776852000	3.332808000	-3.129751000
7	-6.154210000	2.143782000	-2.847569000
1	-6.600041000	1.237949000	-2.850168000
1	-1.790076000	1.475393000	-1.511910000
6	-2.440488000	2.005631000	-2.211087000
6	-2.258117000	3.465669000	-2.257233000
6	-3.288358000	4.309671000	-2.557896000
6	-4.599869000	3.784860000	-2.775181000
1	-3.115566000	5.381414000	-2.613202000
1	-1.261128000	3.853230000	-2.078279000
1	-3.982687000	0.431738000	-2.159337000
6	-3.797985000	1.490711000	-2.301537000
6	-4.805560000	2.373653000	-2.630942000
7	-1.540877000	1.359046000	-3.645960000
8	-0.445633000	1.853227000	-3.879343000

^{4}IM3$_{C6}$:

26	0.514498000	-0.156488000	0.382603000
7	2.176753000	-0.435645000	-0.722324000
7	0.439407000	-2.129557000	0.770845000
7	-0.964339000	0.138672000	1.724899000
7	0.782762000	1.833067000	0.241919000
6	1.322857000	-3.093793000	0.337360000
6	0.938185000	-4.381747000	0.862498000
6	-0.208128000	-4.196457000	1.568808000
6	-0.521065000	-2.789784000	1.503566000
6	-1.622737000	-2.209305000	2.144882000
6	-1.813233000	-0.825019000	2.225818000
6	-2.919692000	-0.199079000	2.908212000
6	-2.716090000	1.143353000	2.844903000
6	-1.497230000	1.351231000	2.101365000
6	-0.984325000	2.616778000	1.792766000
6	0.093560000	2.813912000	0.921364000

6	0.608810000	4.112754000	0.561520000
6	1.572300000	3.912105000	-0.376741000
6	1.673275000	2.487573000	-0.579044000
6	2.585997000	1.891231000	-1.458221000
6	2.797804000	0.509508000	-1.511267000
6	3.759162000	-0.127956000	-2.377620000
6	3.738622000	-1.454821000	-2.084103000
6	2.745817000	-1.644309000	-1.054054000
6	2.408951000	-2.895288000	-0.523213000
8	-0.492275000	-0.239706000	-0.883808000
8	-1.975464000	0.444273000	-4.298997000
6	-1.653955000	3.816172000	2.389243000
6	-1.579743000	4.059828000	3.770398000
6	-2.373571000	4.715002000	1.584592000
6	-2.203598000	5.175616000	4.332237000
1	-1.023946000	3.373182000	4.403121000
6	-2.999607000	5.829091000	2.147277000
1	-2.448077000	4.531579000	0.516052000
6	-2.915374000	6.063816000	3.522083000
1	-2.130662000	5.351320000	5.402094000
1	-3.555663000	6.512221000	1.510566000
1	-3.401464000	6.931831000	3.958942000
6	-2.615856000	-3.113940000	2.805017000
6	-2.764469000	-3.125945000	4.201845000
6	-3.414937000	-3.977094000	2.037080000
6	-3.688047000	-3.975463000	4.813710000
1	-2.146125000	-2.470624000	4.808970000
6	-4.340432000	-4.824995000	2.648626000
1	-3.311691000	-3.976283000	0.955450000
6	-4.479781000	-4.826836000	4.038798000
1	-3.785224000	-3.974429000	5.895989000
1	-4.953724000	-5.481907000	2.037822000
1	-5.199106000	-5.487503000	4.514816000
6	3.225833000	-4.080626000	-0.935256000
6	4.566422000	-4.195349000	-0.532380000
6	2.675877000	-5.094137000	-1.737319000
6	5.334972000	-5.296142000	-0.916016000
1	5.003767000	-3.418520000	0.088843000
6	3.445179000	-6.193272000	-2.123927000
1	1.643083000	-5.013118000	-2.064607000
6	4.776545000	-6.298316000	-1.713344000
1	6.368924000	-5.370428000	-0.590165000
1	3.004486000	-6.964905000	-2.749306000
1	5.374752000	-7.154164000	-2.013692000
6	3.386253000	2.781523000	-2.357130000
6	4.773366000	2.923165000	-2.189038000
6	2.753195000	3.501692000	-3.383872000
6	5.509803000	3.763744000	-3.026137000
1	5.272932000	2.377595000	-1.393165000
6	3.491260000	4.339864000	-4.222031000
1	1.682465000	3.389950000	-3.527581000
6	4.870742000	4.474282000	-4.045384000
1	6.581552000	3.865815000	-2.878540000
1	2.987475000	4.885462000	-5.015407000
1	5.443894000	5.127834000	-4.697316000
1	4.369465000	0.380660000	-3.109014000
1	4.325067000	-2.243263000	-2.532042000
1	1.477872000	-5.303404000	0.703611000
1	-0.784289000	-4.935468000	2.105601000
1	-3.738308000	-0.724612000	3.377110000
1	-3.337965000	1.928801000	3.248254000
1	0.270589000	5.051202000	0.974868000
1	2.179206000	4.653396000	-0.875070000
8	1.917477000	-0.037077000	2.162772000
6	1.797781000	-0.843715000	3.360876000
6	3.090376000	0.812903000	2.239387000
6	2.761935000	-0.214693000	4.365222000
1	0.752603000	-0.827558000	3.675095000
6	3.878317000	0.308857000	3.448861000
1	3.630194000	0.732975000	1.293933000
1	2.758537000	1.848890000	2.372789000
1	4.547308000	-0.509305000	3.157703000
1	4.481760000	1.098252000	3.906034000
1	3.112406000	-0.935840000	5.109219000
1	2.278789000	0.616447000	4.892108000
1	2.080412000	-1.875172000	3.119543000
1	-8.118009000	5.707436000	-1.292521000
7	-7.302874000	6.042484000	-0.780077000
1	-6.975453000	5.269091000	-0.207673000
1	-5.293554000	6.375239000	-1.196216000
1	-5.454719000	6.292264000	-3.688800000
6	-6.256302000	6.502973000	-1.706693000
6	-6.193869000	5.774186000	-3.069139000
6	-5.861132000	4.314671000	-2.949109000
6	-6.415575000	8.025860000	-1.900572000
8	-7.220342000	8.595684000	-0.996403000
1	-7.548548000	7.824553000	-0.451909000
8	-5.847858000	8.660748000	-2.766751000
1	-7.161481000	5.895727000	-3.573212000
1	-7.842141000	3.287098000	-3.134197000
6	-6.771903000	3.263978000	-2.981681000
7	-6.116000000	2.070909000	-2.799079000
1	-6.549507000	1.159550000	-2.821495000
1	-1.744251000	1.469763000	-1.603295000
6	-2.342427000	1.947057000	-2.391015000
6	-2.201493000	3.436923000	-2.386826000
6	-3.262343000	4.264915000	-2.577583000
6	-4.581970000	3.729454000	-2.741538000
1	-3.110494000	5.341513000	-2.585816000
1	-1.203558000	3.835459000	-2.244611000
1	-3.890882000	0.354412000	-2.350819000
6	-3.727045000	1.421498000	-2.445654000
6	-4.757937000	2.309264000	-2.656876000
7	-1.496027000	1.368877000	-3.657603000
8	-0.388948000	1.858392000	-3.856322000

^{2}TS4:

26	0.495516000	0.371891000	-0.072232000
7	2.012672000	0.240271000	-1.386813000
7	0.251191000	-1.610903000	-0.146254000
7	-0.824217000	0.462214000	1.448073000
7	0.910599000	2.335498000	0.174001000
6	1.021214000	-2.519649000	-0.844087000
6	0.566150000	-3.859707000	-0.569337000
6	-0.509865000	-3.754043000	0.255489000
6	-0.704214000	-2.350424000	0.519043000
6	-1.694487000	-1.851299000	1.373602000
6	-1.730709000	-0.516823000	1.794837000
6	-2.702002000	0.017104000	2.717030000
6	-2.356472000	1.311462000	2.950982000
6	-1.190674000	1.590301000	2.148626000
6	-0.586459000	2.851850000	2.076064000
6	0.398356000	3.176885000	1.135207000
6	0.990544000	4.487673000	1.005169000

6	1.821752000	4.442143000	-0.068998000
6	1.768254000	3.095822000	-0.586115000
6	2.541538000	2.645934000	-1.664247000
6	2.633963000	1.296077000	-2.022463000
6	3.459700000	0.802519000	-3.097084000
6	3.358899000	-0.553325000	-3.085842000
6	2.448195000	-0.899667000	-2.022847000
6	2.052539000	-2.212099000	-1.736953000
8	-0.635373000	0.729102000	-1.213795000
8	-0.895940000	-1.091258000	-3.314311000
6	-1.060034000	3.914230000	3.018754000
6	-0.814421000	3.799472000	4.396915000
6	-1.762339000	5.037551000	2.552119000
6	-1.253627000	4.784051000	5.284095000
1	-0.270660000	2.935987000	4.770354000
6	-2.204575000	6.020537000	3.439558000
1	-1.968429000	5.133803000	1.489738000
6	-1.950303000	5.897559000	4.807942000
1	-1.049266000	4.681218000	6.346383000
1	-2.751339000	6.879875000	3.061081000
1	-2.293637000	6.663182000	5.498190000
6	-2.735772000	-2.799978000	1.878001000
6	-2.809189000	-3.148056000	3.236734000
6	-3.661048000	-3.368154000	0.986416000
6	-3.783134000	-4.038844000	3.692268000
1	-2.093422000	-2.724047000	3.935554000
6	-4.636429000	-4.256758000	1.442565000
1	-3.615242000	-3.101773000	-0.065927000
6	-4.700245000	-4.594855000	2.796779000
1	-3.821665000	-4.301109000	4.746057000
1	-5.347427000	-4.682625000	0.739758000
1	-5.458453000	-5.287506000	3.151604000
6	2.727069000	-3.329284000	-2.470333000
6	4.076380000	-3.631213000	-2.225167000
6	2.029971000	-4.086880000	-3.425855000
6	4.710855000	-4.668040000	-2.912348000
1	4.626439000	-3.051946000	-1.488513000
6	2.665323000	-5.121219000	-4.115544000
1	0.989254000	-3.853554000	-3.632895000
6	4.007068000	-5.415692000	-3.859774000
1	5.754068000	-4.891415000	-2.706072000
1	2.112625000	-5.693397000	-4.855742000
1	4.501006000	-6.221105000	-4.396333000
6	3.340831000	3.653768000	-2.431269000
6	4.744077000	3.656898000	-2.365446000
6	2.697448000	4.620836000	-3.222212000
6	5.488774000	4.602338000	-3.072953000
1	5.250892000	2.918722000	-1.749821000
6	3.445904000	5.563203000	-3.931680000
1	1.612369000	4.627455000	-3.291596000
6	4.841113000	5.558493000	-3.859355000
1	6.573396000	4.593265000	-3.006081000
1	2.935121000	6.301234000	-4.544556000
1	5.419827000	6.294358000	-4.411106000
1	4.041295000	1.419353000	-3.765875000
1	3.837012000	-1.260318000	-3.747636000
1	1.013285000	-4.759885000	-0.964148000
1	-1.108196000	-4.550938000	0.671848000
1	-3.533177000	-0.533029000	3.132528000
1	-2.854784000	2.026114000	3.589206000
1	0.788093000	5.327982000	1.652353000
1	2.436073000	5.235222000	-0.468779000
8	2.034998000	0.009440000	1.496645000
6	1.952292000	-1.029442000	2.507168000
6	3.233142000	0.805850000	1.682452000
6	3.036695000	-0.684917000	3.527985000
1	0.940367000	-1.024937000	2.916110000
6	4.096271000	0.003869000	2.654692000
1	3.688583000	0.960596000	0.702903000
1	2.945741000	1.777249000	2.100738000
1	4.690644000	-0.742258000	2.114472000
1	4.779335000	0.642049000	3.222461000
1	3.410535000	-1.572331000	4.046564000
1	2.648780000	0.013741000	4.278314000
1	2.137696000	-1.995332000	2.023948000
1	-3.637244000	1.306746000	-3.414803000
7	-3.001473000	1.833761000	-4.011585000
1	-3.438701000	1.897258000	-4.928280000
1	-3.394413000	3.939656000	-3.901264000
1	-2.689160000	4.178756000	-1.551879000
6	-2.758432000	3.170196000	-3.447456000
6	-2.977193000	3.183226000	-1.908746000
6	-4.381788000	2.851292000	-1.499863000
6	-1.298028000	3.560320000	-3.731160000
8	-0.549636000	2.553939000	-4.189438000
1	-1.189862000	1.785519000	-4.236145000
8	-0.851952000	4.675145000	-3.528034000
1	-2.281270000	2.463646000	-1.461591000
1	-4.237753000	0.772904000	-0.718027000
6	-4.809631000	1.658989000	-0.958831000
7	-6.167674000	1.707312000	-0.719373000
1	-6.712317000	0.960315000	-0.314948000
1	-9.138510000	5.195475000	-1.477828000
6	-8.142850000	4.761096000	-1.505726000
6	-7.066219000	5.526601000	-2.003718000
6	-5.777994000	5.005352000	-2.055223000
6	-5.552417000	3.691800000	-1.602570000
1	-4.957203000	5.607488000	-2.436766000
1	-7.250465000	6.539815000	-2.350635000
1	-8.780056000	2.872720000	-0.660330000
6	-7.952627000	3.461368000	-1.047071000
6	-6.654046000	2.940188000	-1.101190000
7	-1.511989000	-0.784449000	-2.327499000
8	-2.655467000	-1.002637000	-2.010139000

^{2}P2:

26	0.669086000	0.519709000	0.268720000
7	2.181939000	0.263938000	-0.997155000
7	0.120412000	-1.374595000	0.002983000
7	-0.790762000	0.760234000	1.630817000
7	1.288392000	2.389594000	0.635635000
6	0.824203000	-2.358862000	-0.659094000
6	0.123840000	-3.613588000	-0.552915000
6	-1.031828000	-3.368473000	0.121655000
6	-1.024742000	-1.971309000	0.479496000
6	-2.000366000	-1.375395000	1.289783000
6	-1.847650000	-0.098712000	1.846575000
6	-2.748466000	0.472303000	2.817205000
6	-2.202408000	1.654193000	3.221536000
6	-0.996951000	1.845909000	2.454807000
6	-0.207134000	3.001057000	2.513279000
6	0.838564000	3.247404000	1.616554000
6	1.525608000	4.510513000	1.514500000
6	2.360265000	4.423342000	0.443975000

6	2.211728000	3.096536000	-0.101594000
6	2.967818000	2.605754000	-1.174472000
6	2.957345000	1.257982000	-1.555258000
6	3.833394000	0.689902000	-2.550157000
6	3.618610000	-0.653614000	-2.550454000
6	2.575157000	-0.914627000	-1.592460000
6	2.004057000	-2.176313000	-1.388549000
8	-0.508023000	1.287633000	-1.012245000
8	-0.256097000	-0.176037000	-2.667430000
6	-0.539598000	4.056697000	3.522835000
6	0.317357000	4.284977000	4.611163000
6	-1.697245000	4.841880000	3.398812000
6	0.021565000	5.269564000	5.556202000
1	1.216161000	3.683446000	4.716667000
6	-1.992567000	5.826591000	4.343869000
1	-2.363227000	4.681815000	2.555354000
6	-1.134752000	6.042485000	5.425400000
1	0.693673000	5.430198000	6.394735000
1	-2.890812000	6.427474000	4.231270000
1	-1.365192000	6.808950000	6.160142000
6	-3.222026000	-2.173969000	1.624432000
6	-3.441579000	-2.660612000	2.923553000
6	-4.168337000	-2.463914000	0.627980000
6	-4.581105000	-3.411133000	3.219756000
1	-2.710210000	-2.456636000	3.700692000
6	-5.308703000	-3.212887000	0.924755000
1	-4.009243000	-2.094288000	-0.381300000
6	-5.518708000	-3.687896000	2.221611000
1	-4.732675000	-3.783222000	4.229306000
1	-6.032958000	-3.422917000	0.142515000
1	-6.405588000	-4.271476000	2.452402000
6	2.642639000	-3.356666000	-2.051091000
6	3.902850000	-3.808391000	-1.626652000
6	2.010596000	-4.023775000	-3.113370000
6	4.511868000	-4.903883000	-2.241946000
1	4.402427000	-3.299889000	-0.806517000
6	2.621055000	-5.117350000	-3.730403000
1	1.042053000	-3.675767000	-3.461159000
6	3.872297000	-5.561662000	-3.295452000
1	5.484715000	-5.243070000	-1.896700000
1	2.120253000	-5.618381000	-4.554290000
1	4.346355000	-6.413129000	-3.775788000
6	3.869543000	3.557783000	-1.897347000
6	5.266165000	3.465497000	-1.781699000
6	3.325679000	4.574575000	-2.699011000
6	6.097251000	4.364204000	-2.453356000
1	5.699848000	2.690304000	-1.155994000
6	4.157006000	5.472091000	-3.371984000
1	2.246676000	4.655796000	-2.797785000
6	5.545020000	5.369524000	-3.251074000
1	7.175576000	4.280637000	-2.348991000
1	3.718977000	6.249414000	-3.992023000
1	6.191790000	6.068684000	-3.773841000
1	4.528993000	1.250232000	-3.156925000
1	4.097725000	-1.401865000	-3.164339000
1	0.469338000	-4.554361000	-0.954709000
1	-1.807937000	-4.071336000	0.386240000
1	-3.660062000	0.010594000	3.166658000
1	-2.585373000	2.341566000	3.961269000
1	1.367636000	5.356486000	2.166932000
1	3.028493000	5.179862000	0.059982000
8	1.946824000	-0.168852000	1.808791000
6	1.605974000	-1.228252000	2.752467000
6	3.173560000	0.503970000	2.211074000
6	2.606761000	-1.075876000	3.898152000
1	0.566364000	-1.095138000	3.054135000
6	3.826768000	-0.457530000	3.198046000
1	3.757619000	0.692065000	1.309365000
1	2.912739000	1.457714000	2.680853000
1	4.396461000	-1.226751000	2.664492000
1	4.502863000	0.059093000	3.884974000
1	2.822901000	-2.034099000	4.378473000
1	2.216788000	-0.390591000	4.659080000
1	1.713920000	-2.184333000	2.231992000
1	-3.376341000	1.188593000	-3.621942000
7	-4.359339000	1.053584000	-3.868324000
1	-4.778355000	0.500178000	-3.126089000
1	-6.104729000	2.187478000	-3.777269000
1	-4.997471000	4.419593000	-3.442547000
6	-5.044842000	2.348712000	-4.012339000
6	-4.511992000	3.492566000	-3.117820000
6	-4.741089000	3.256609000	-1.652698000
6	-5.017106000	2.742265000	-5.503968000
8	-4.663332000	1.734344000	-6.309700000
1	-4.461642000	0.989790000	-5.669210000
8	-5.314357000	3.844115000	-5.923228000
1	-3.439576000	3.612746000	-3.314581000
1	-2.808090000	2.449718000	-0.904931000
6	-3.835428000	2.750239000	-0.749358000
7	-4.415633000	2.650708000	0.500699000
1	-3.957166000	2.278602000	1.322353000
1	-8.742340000	3.738939000	1.795746000
6	-7.956018000	3.660680000	1.049661000
6	-8.217718000	4.060750000	-0.278694000
6	-7.236702000	3.974132000	-1.260944000
6	-5.964888000	3.477334000	-0.918211000
1	-7.450776000	4.288543000	-2.279659000
1	-9.202659000	4.442395000	-0.534554000
1	-6.505238000	2.864642000	2.445160000
6	-6.707981000	3.169996000	1.422066000
6	-5.722879000	3.083433000	0.430547000
7	-0.715391000	0.881581000	-2.259867000
8	-1.403544000	1.656922000	-2.939694000

[4]TS4:

26	0.515038000	0.433727000	-0.065847000
7	2.040077000	0.292622000	-1.374461000
7	0.274429000	-1.561772000	-0.127971000
7	-0.800385000	0.519333000	1.457871000
7	0.966098000	2.372863000	0.211136000
6	1.024589000	-2.466836000	-0.845070000
6	0.534667000	-3.803715000	-0.609390000
6	-0.548358000	-3.692065000	0.204953000
6	-0.709868000	-2.289392000	0.501699000
6	-1.697011000	-1.784037000	1.357780000
6	-1.713963000	-0.455505000	1.797785000
6	-2.671314000	0.075514000	2.737659000
6	-2.308238000	1.361291000	2.989393000
6	-1.146363000	1.638688000	2.179757000
6	-0.525373000	2.892690000	2.119249000
6	0.459739000	3.213706000	1.177766000
6	1.054304000	4.522721000	1.047439000
6	1.875750000	4.479979000	-0.034648000
6	1.818640000	3.135819000	-0.554620000

6	2.583708000	2.691429000	-1.640008000
6	2.674987000	1.342854000	-2.001704000
6	3.513401000	0.845685000	-3.065515000
6	3.406579000	-0.509327000	-3.053748000
6	2.478337000	-0.850965000	-2.002475000
6	2.067771000	-2.160841000	-1.726983000
8	-0.604711000	0.722019000	-1.199970000
8	-1.403219000	-1.789609000	-3.585301000
6	-0.980649000	3.950463000	3.076429000
6	-0.721739000	3.820233000	4.450745000
6	-1.678910000	5.083802000	2.628480000
6	-1.143981000	4.799244000	5.352244000
1	-0.181205000	2.948749000	4.810043000
6	-2.103766000	6.061608000	3.530099000
1	-1.894915000	5.192447000	1.569285000
6	-1.836478000	5.923026000	4.894488000
1	-0.929632000	4.684055000	6.411306000
1	-2.647281000	6.929104000	3.165765000
1	-2.166472000	6.684447000	5.595816000
6	-2.753097000	-2.723667000	1.850551000
6	-2.814927000	-3.103884000	3.201205000
6	-3.701648000	-3.251476000	0.958964000
6	-3.800144000	-3.986148000	3.648962000
1	-2.081483000	-2.710802000	3.899797000
6	-4.688337000	-4.131842000	1.407195000
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