

Synthetic Access to a Phosphorescent Non-Palindromic Pincer Complex of Palladium by a Double Oxidative Addition – Comproportionation Sequence†

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S 1. Reaction of pre-ligand 5 with $[\text{Pd}(\text{PPh}_3)_4]$ forming $[(\text{C}^{\wedge}\text{C}^{\wedge}\text{N})\text{PdPPPh}_3]$ (3)

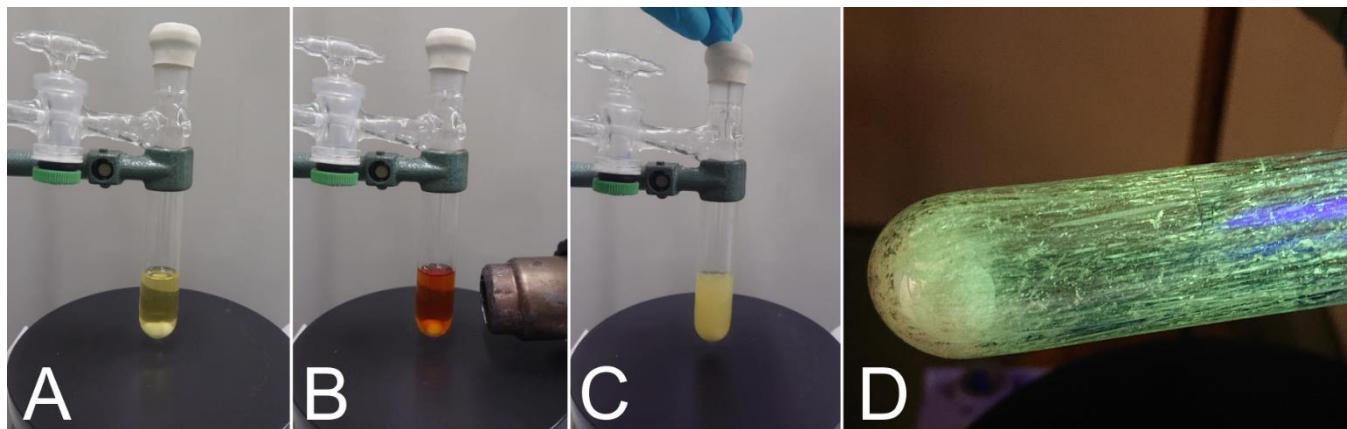
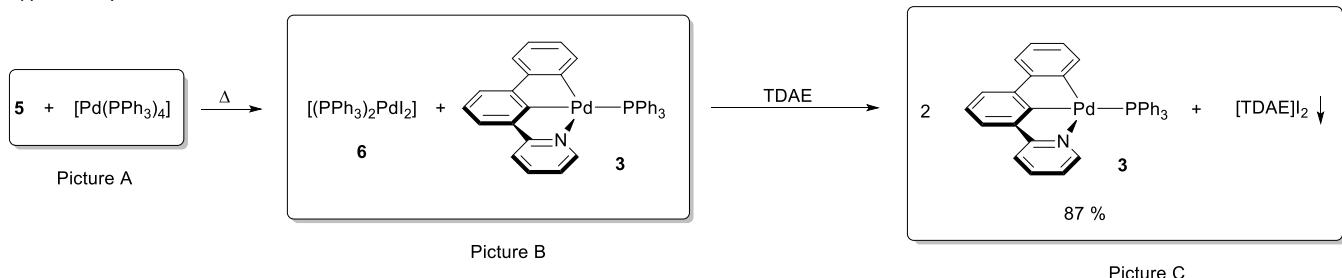
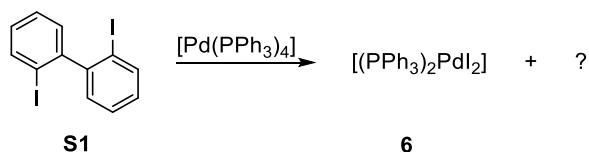


Figure S 1 Color change during synthesis of **3**. A: **5** and $[\text{Pd}(\text{PPh}_3)_4]$ in toluene. B: Oxidative addition and formation of red $[(\text{PPh}_3)_2\text{PdI}_2]$ (**6**) upon heating to $100\text{ }^\circ\text{C}$. C: Addition of TDAE and reduction of **6**, colour change from red to yellow and precipitation of insoluble $[\text{TDAE}]I_2$. D: Green luminescence of **3** under UV irradiation ($\lambda_{\text{exc}} = 364\text{ nm}$). Use of a heatgun (picture B) for heating was only done for ease of taking pictures; in general, reactions were heated with an oil bath. Please refer to the video attached to the supplementary documents.



Scheme S 1 The reaction of preligand **5** with $[\text{Pd}(\text{PPh}_3)_4]$ is accompanied by colour changes due to the different intermediates/products formed.

S 2. Reaction of 2,2'-diiodobiphenyl (**S1**) with $[\text{Pd}(\text{PPh}_3)_4]$



Scheme S 2 Reaction of **S1** with $[\text{Pd}(\text{PPh}_3)_4]$ leading to the formation of diiodide **6** and a mixture of unidentified products.

S 3. Reaction of preligand 5 with $[(\text{py})_4\text{NiCl}_2]$

Motivated by the possibility to synthesize palladium complex **3** using $[(\text{PPh}_3)_2\text{PdCl}_2]$ and preligand **5** in the presence of two equivalents TDAE, we reacted $[(\text{py})_4\text{NiCl}_2]$ ($\text{py} = \text{pyridine}$) with **5** in THF. TDAE served to generate $\text{Ni}(0)$ species *in situ* as it is known from Ni-catalysed reductive couplings.¹ After warming to $70\text{ }^\circ\text{C}$ for 12 h, the cyan coloured suspension became dark red and clear. We were able to isolate single crystals suitable for X-ray diffraction analysis from this reaction showing the formation of the anticipated $[(\text{C}^{\wedge}\text{C}^{\wedge}\text{N})\text{Ni}(\text{II})]$ complex **S2** (Figure S 2). The $\text{Ni}(\text{II})$ centre is coordinated in a distorted square-planar manner with a pyridine molecule closing the fourth coordination site. The latter is distorted by 64.6° with respect to the pincer plane. The $\text{Ni}-\text{N}$ bond is of similar length as the $\text{Ni}-\text{N}$ bonds of bis(phenylpyridine)nickel(II).² However, the latter exhibits a distorted tetrahedral coordination environment.

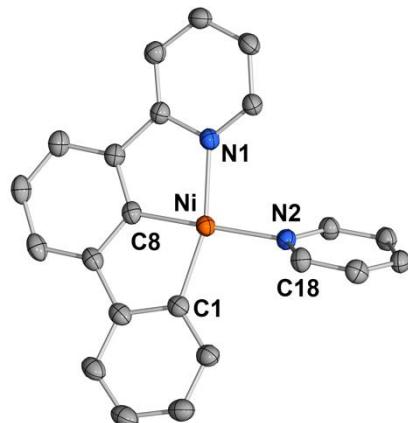


Figure S 2 Molecular structure of **S2**. Thermal ellipsoids are drawn at the 30 % probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (pm) and angles (°): Ni–N1 198.1(2), Ni–C8 184.1(3), Ni–C1 193.8(3), Ni–N2 195.8(2), N1–Ni–C8 82.6(1), C8–Ni–C1 82.0(1), C1–Ni–N2–C18 64.6(2).

Unfortunately, until now the isolation of pure bulk samples of **S2** on a preparative scale failed. During the synthesis many unidentified side products formed, which we could not remove by washing or filtration. We had to manually pick from many red coloured, crystalline fragments and to identify complex **S2** by determination of the unit cell; a procedure not suitable for isolation of bulk samples. In addition, the NMR spectra of manually chosen single crystals of **S2** at room temperature in C_6D_6 showed signs of fast decomposition and/or many unidentified side products. We tried to record mass spectra of **S2** but were only able to detect the mass of the pincer ligand ($C_{17}H_{13}N$ m/z = 231.3). Palindromic $[(C^N^NC)Ni(II)]$ complexes were investigated theoretically in view of their potential for aliphatic C–H bond activations³ underlining their possible reactivity and, associated therewith, challenges regarding preparation and handling. Thus, we could show that $[(C^C^N)Ni(II)]$ complexes are accessible, however, a way to prepare pure bulk samples remains elusive and is currently searched for in our group.

S 4. Additional photophysical details and TD-DFT calculations

Table S 1 Optical properties of **3** in the solid state and in solution^a at 293 K.

Complex	Solv.	λ_{abs} nm	ϵ $10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$	λ_{em} nm	Φ_p ^b	τ_p ^c μs	k_p ^d 10^5 s^{-1}	k_{nr} ^e 10^5 s^{-1}
3	THF	303, 351, 380	1.35, 0.68, 0.41	--	--	--	--	--
3	CH_2Cl_2	307, 330, 401	0.84, 0.72, 0.06	--	--	--	--	--
3	Solid	--	--	487, 524, 561	0.10	0.4	2.50	22.50
3	THF (77 K)	--	--	481, 519, 558	-- ^f	370	--	--

^a Recorded in dry, degassed solvents. S: Solid state. ^b Absolute quantum yields, determined by means of an integrating sphere, error ± 0.02 . ^c Phosphorescence lifetime.

^d Rate constant phosphorescence, $k_p = \Phi_p / \tau_p$. ^e Rate constant radiationless relaxation, $k_{nr} = (1 - \Phi_p) / \tau_p$. ^f Quantum yields could not be detected in frozen solution.

Complex **3** exhibits intensive absorption bands at wavelengths < 300 nm with extinctions (ϵ) ranging from 10^3 to $10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$ which are rooted in metal-perturbed IL transitions ($\pi \rightarrow \pi^*$).⁴⁻⁶

Structured bands between 330 nm and 380 nm with band distances of approximately 1300 cm^{-1} indicate skeletal vibrations of the pincer backbone.^{4, 5, 7, 8} The blueshift of these bands in CH_2Cl_2 compared to THF indicates a charge-transfer, thus the bands are assigned to $\pi \rightarrow \pi^*$ $^1\text{IL}/\text{MLCT}$ transitions. The band at about 400 nm can be assigned to MLCT transitions with IL character.^{5, 9} We calculated the first five vertical transitions of **3** and the hypothetical palindromic congener $[(C^N^NC)PdPPPh_3]$ on the RIJK-PBEO-D3(BJ)/def2-TZVP level of theory with structures optimized on the RI-TPSS-D3(BJ)/def2-TZVP level. The results are given in Table S 2. In addition, we calculated the phosphorescent $S_0 \leftarrow T_1$ transitions of these complexes on the spin-flip TDA/RI-PWLDA/def2-TZVP level of theory using the S_0 optimized and T_1 optimized structures.

Table S 2 By means of TDDFT (RIJK-PBEO-D3(BJ)/def2-TZVP) calculated singlet vertical excitation energies (λ_{vee}) of **3** and its palindromic congener $[(C^N^C)Pd(II)PPh_3]$ at the respective S_0 geometry as well as spin-flip TDA/RI-PWLDA/def2-TZVP calculations of the phosphorescence transition $S_0 \leftarrow T_1$ at the respective minimum structure of the electronic ground state S_0 ($T_1\{S_0\}$) and the T_1 state ($T_1\{T_0\}$). VEE: vertical excitation energy, f_{0n} : oscillator strength of transition $0 \leftarrow n$.

L_n	$\frac{\lambda_{vee}}{\text{nm}}$		$\frac{E_{vee}}{\text{eV}}$		f_{0n}	
	(C ^N C ^N C)	(C ^N N ^C)	(C ^N C ^N C)	(C ^N N ^C)	(C ^N C ^N C)	(C ^N N ^C)
S_1	405	399	3.06	3.11	0.046	0.004
S_2	374	378	3.31	3.28	0.005	0.002
S_3	349	341	3.56	3.63	0.038	0.016
S_4	344	332	3.60	3.73	0.014	0.022
S_5	341	323	3.64	3.84	0.006	0.079
$T_1\{S_0\}$	431	481	-2.88 ^c	-2.58	--	--
$T_1\{T_1\}$	512	1305	-2.42 ^c	-0.95	--	--

^a Based on significant orbital contributions (> 10 %). ^c: phenyl-centred orbital (C^NC^NC); c^c: biphenyl-centred orbital (C^NC^NC); n: pyridine centred orbital; p: PPh₃ centred orbital; d_{jk}: Pd centred d orbital. ^b HOMO-LUMO transition. ^c Experimental phosphorescence energy in the solid state: 2.55 eV.

Non-relaxed difference densities give an illustrative picture of the electronic transitions responsible for the absorption bands of the investigated complexes.¹⁰ They are based on weighing orbital contributions of calculated transitions according to their coefficients. We show the non-relaxed difference densities for the first five transitions of $[(C^N^C)PdPPh_3]$ (**3**) and its palindromic congener $[(C^N^C)PdPPh_3]$ in Figure S 3. The difference densities of **3** confirm the assignments of bands based on the experimental absorption spectra.

For both complexes the first transition $S_0 \leftarrow S_1$ is mainly of $\pi-\pi^*$ character with small metal contributions. The transition energy is slightly lower for the (C^NC^NC) complex **3** standing in line with a higher lying HOMO of the biphenyl unit compared to the HOMO of the two separated phenyl groups of the (C^NN^C) pincer. The other transitions are shifted to higher energies in the palindromic case as well, however, a direct comparison is possible in limited form only due to the symmetry differences of the palindromic and non-palindromic system. Furthermore, the ordering of the transitions of similar kind is interchanged between the two complexes. Symmetry properties are responsible for the notably different oscillator strengths found for the transitions of the (C^NC^NC) and (C^NN^C) system as well (*vide infra*).

The transition densities indicate the metal orbital's contribution to be slightly higher for the palindromic $[(C^N^C)PdPPh_3]$ complex compared to non-palindromic **3**. This stands in line with a weaker ligand field splitting in the palindromic case which enables more pronounced metal's orbitals admixture to the lower lying electronic transitions.

The most striking difference between the palindromic and non-palindromic complex is found for the phosphorescent $S_0 \leftarrow T_1$ transition. At the S_0 geometry, the phosphorescence energy of the two investigated complexes differs by only 0.3 eV with the non-palindromic system at higher energies. However, at the optimized T_1 structure the transition energy of the palindromic (C^NN^C) complex is notably red-shifted by 1.63 eV to the infra-red indicating a high probability for non-radiative relaxation. The respective transition of non-palindromic **3** is only red-shifted by 0.46 eV. $[(C^N^C)PdPPh_3]$ experiences strong structural distortions upon relaxation to T_1 : The palladium atom is notably bent out of the pincer plane (Figure S 4 left). On the contrary, the structure of non-palindromic complex **3** is negligibly affected in the T_1 state (Figure S 4 right).

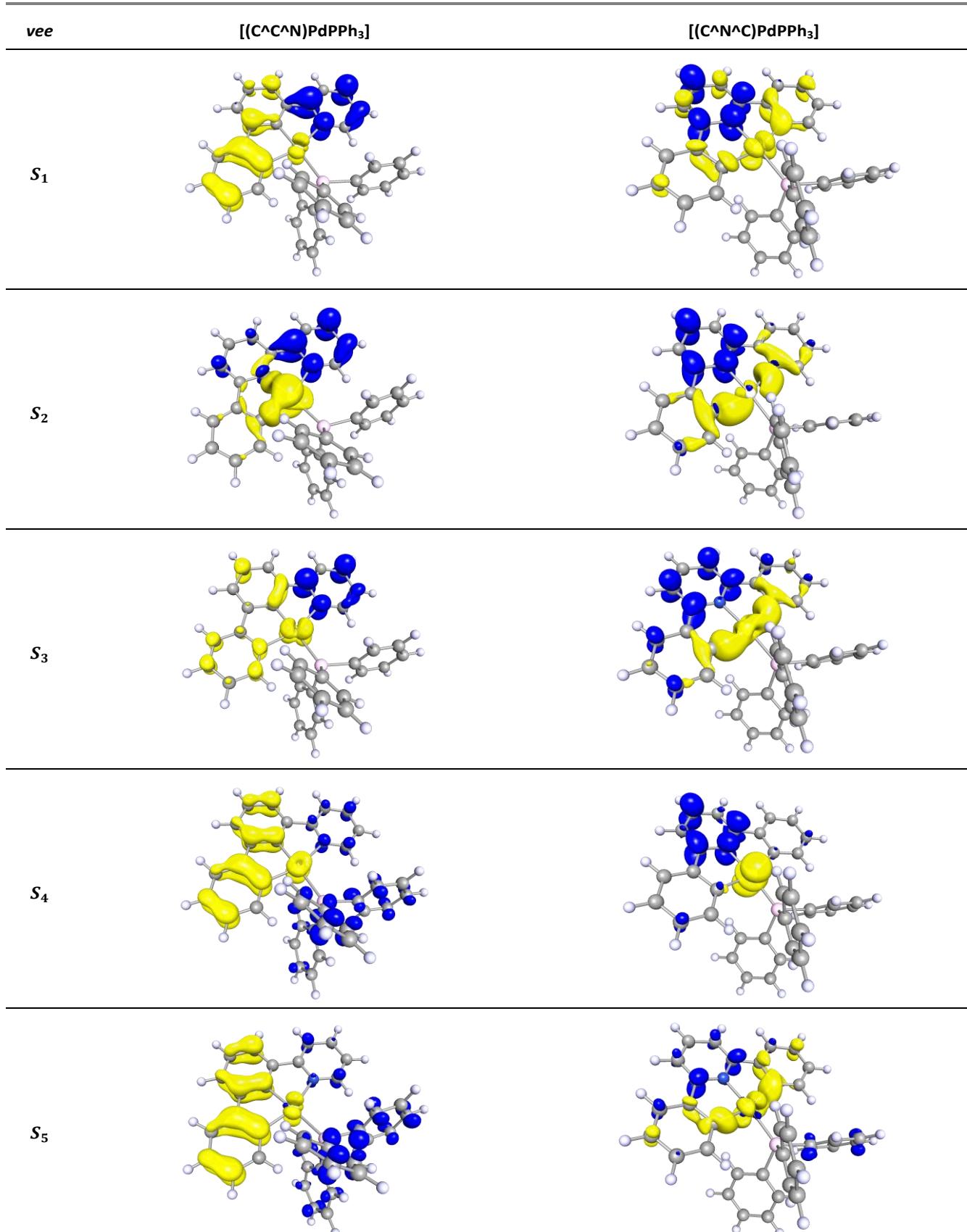


Figure S 3 Non-relaxed difference densities of the first five electronic singlet transitions of **3** (left column) and its palindromic analogue (right column). Areas of decreasing density are coloured yellow; areas of increasing density are coloured blue. The densities are plotted with isovalues of 0.002 a.u. (blue) and -0.002 a.u. (yellow), respectively.

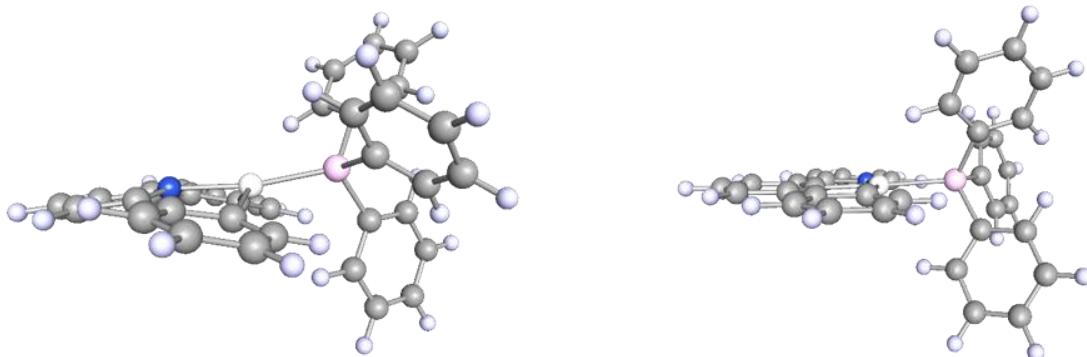


Figure S 4 Structural distortion of $[(C^N^C)PdPPPh_3]$ (left) and $[(C^C^N)PdPPPh_3]$ (right) upon relaxation in the T_1 state.

The different structural relaxation in the T_1 state is rooted in different metal's orbitals contribution (Figure S 5). The phosphorescent transition at the respective S_0 structure, $S_0 \leftarrow T_1\{S_0\}$, is comparable between both complexes. The transitions are of $\pi^*-\pi$ character. At the S_0 structure, the donor orbital 153_α is, in both cases, mainly pyridine centred without metal contribution. Therefore, the highest lying metal orbital $d_{x^2-y^2}$, which is anti-bonding in an (approximately) square-planar coordination environment, is not populated neither in the palindromic nor in the non-palindromic case. However, in the non-palindromic case, population of 153_α increases the bond strength between lateral pyridine and central phenyl group. The latter is reflected in a slightly shorter bond between pyridine and central phenyl (146.1 pm at S_0 , 142.2 pm at T_1). Upon structural relaxation in T_1 the orbital character does not significantly change for the non-palindromic (C^C^N) system in contrast to the palindromic congener. The latter shows increasing metal character. Thus, after relaxation the T_1 state of $[(C^N^C)PdPPPh_3]$ may approximately be seen as metal-centred d-d state.

The acceptor orbital 152_β exhibits notable metal character. For the (C^C^N) system the palladium orbital d_{yz} involved is rotated with respect to the C-Pd and C-N axes. Therefore, the latter orbital exhibits low anti-bonding character between pincer moiety and palladium atom in contrast to the respective orbital of the palindromic (C^N^C) complex which points onto the lateral phenyl

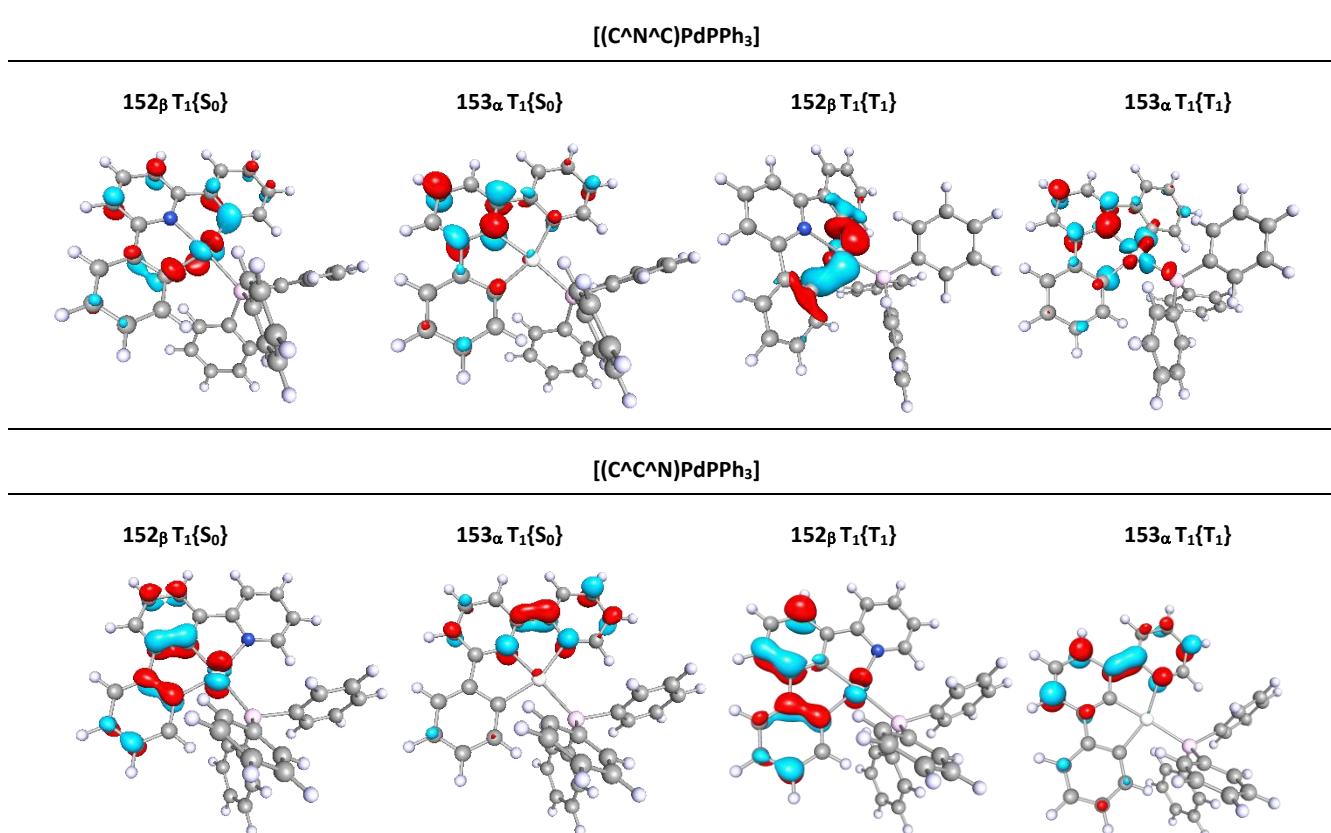


Figure S 5 Spin orbitals (isovalue: 0.06 a.u.) of the phosphorescence transition $S_0 \leftarrow T_1$ of $[(C^C^N)Pd(PPh_3)]$ (3) and palindromic $[(C^N^C)PdPPPh_3]$ calculated by Spin-Flip-TDDFT (RI-PWLDA/def2-TZVP) at the respective S_0 and T_1 optimized structure. Orbital contributions (square of orbital coefficients) in all cases > 99 %. The donor orbital 153_α is depopulated upon $S_0 \leftarrow T_1$ transition, the acceptor orbital 152_β populated.

donors. Upon relaxation in T_1 , the metal character of 152β increases for the (C^N^C) system further supporting the assignment of the T_1 state to be of d-d character. However, the T_1 state of the palindromic complex remains a $\pi^*-\pi$ state with only small metal contribution to the acceptor orbital 152β .

In summary, our calculations support the assumption that the palindromic $[(C^N^C)PdPPPh_3]$ complex is non-radiative due to structural distortions in the excited state which are rooted in the population of a metal-centred d-d state upon excitation. The non-palindromic (C^C^N) system shows much lower metal contributions in the excited state and, thus, is less prone to structural distortions and non-radiative relaxations. These findings nicely fit to the considerations of Ballhausen *et al.*¹¹ already described in 1965.

S 5. Ligand field and symmetry considerations of the non-palindromic (C^C^N) pincer

Stronger ligand field splitting is held responsible for the outstanding photophysics of (C^C^N) complexes compared to the palindromic (C^N^C) analogues.^{8, 12} Our TD-DFT calculations point into the same direction because, for the non-palindromic $[(C^C^N)PdPPPh_3]$ (**3**), they show less metal orbitals' contributions to the excited state T_1 compared to the palindromic (C^N^C) analogue. However, these calculations do not directly link the exchange of the pyridine donor's position to the different behaviour of the complexes and the postulated stronger ligand field splitting of the (C^C^N) pincer.

We want to propose a simple picture to understand the stronger ligand field splitting of the non-palindromic (C^C^N) pincer based on a very simplified orbital picture. In addition, we discuss the mutual *trans*-influence of the pincer's lateral donors on the ligand field and finally want to point out some symmetry properties of the (C^N^C) and (C^C^N) system playing a role for photophysical properties. The aim of these proposals is not a final and comprehensive explanation but to motivate a fundamental discussion about the electronic influences of the (C^N^C) and (C^C^N) pincer.

Ligand-field

Figure S 6 visualizes the ligand-field of a square-planar metal complex coordinated by three σ -donors, two strong phenyl rings and one weak pyridine.¹³ Possible π -donating or -accepting properties are neglected. The herein discussed pincer ligands do not yield coordination environments with perpendicular donor sites but show distorted structures with angles of about 160° between metal and lateral donors.^{8, 14} Thus, on the one hand, overlap of lateral ligand σ -orbitals and the $d_{x^2-y^2}$ orbital of the central metal is reduced. On the other hand, the overlap with the d_{xy} orbital is increased compared to an exactly orthogonal ligand arrangement. The σ -donor orbital of the central pyridine ring of the (C^N^C) pincer directly points onto the $d_{x^2-y^2}$ orbital and points in between the lobes of the d_{xy} orbital. Considering the non-palindromic (C^C^N) pincer, the central pyridine ring is replaced by a phenyl ring, which is a stronger σ -donor. Thus, the $d_{x^2-y^2}$ orbital is energetically destabilized. On the contrary, at one lateral position the stronger σ -donating phenyl ligand is replaced by the weaker pyridine donor resulting in an energetically lowered d_{xy} orbital. This interpretation stands in line with our TDDFT calculations showing no admixture of the $d_{x^2-y^2}$ orbital to the T_1 state of $[(C^C^N)PdPPPh_3]$, but the one of the palindromic (C^N^C) system (Figure S 5).

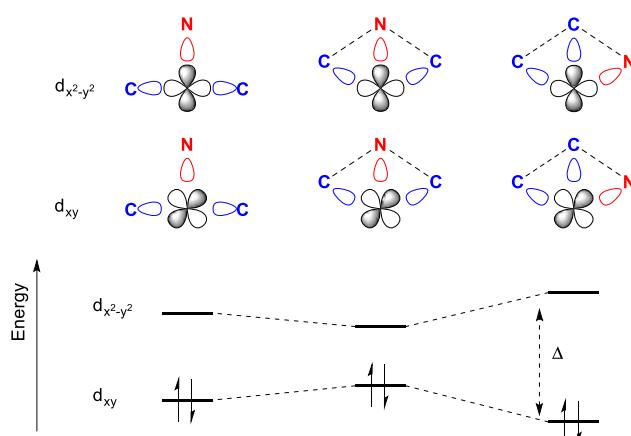


Figure S 6 Schematic ligand field splitting Δ of palindromic (C^N^C) pincer (middle) and non-palindromic (C^C^N) ligand (right) compared to a hypothetical orthogonal coordination environment. The stronger phenyl donors are coloured in blue.

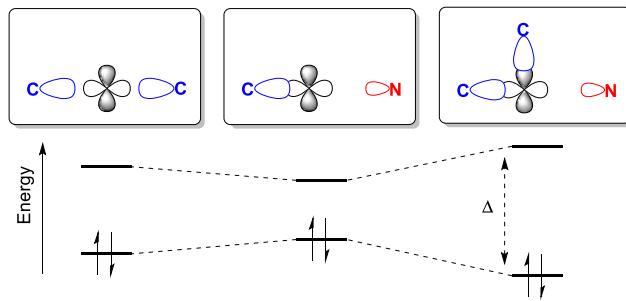


Figure S 7 The *trans* influence of the pincers lateral donors have an impact on the central metal's ligand field splitting.

trans-Influence

The lateral donors of pincer ligands compete for the central metal's orbitals (Figure S 7). In case of two identical lateral donors (Figure S 7, left) the overlap with the metal orbitals is equally distributed resulting in equally bonding and antibonding molecular orbitals. However, in case of different lateral donors, the ligand with stronger *trans* influence will usurp the weaker donor, thus, resulting in stronger bonding and anti-bonding interactions (Figure S 7, middle). In a linear coordination environment replacement of one strong donor (phenyl) by a weaker donor (pyridine) would result in a smaller ligand field splitting; but in case of the non-palindromic pincer, only the lateral phenyl donor is replaced and thus intensively interacts with the central metals orbitals from the central position (Figure S 7, right).

Of course, this is only a qualitative picture and the magnitude of different influences may only be speculated.

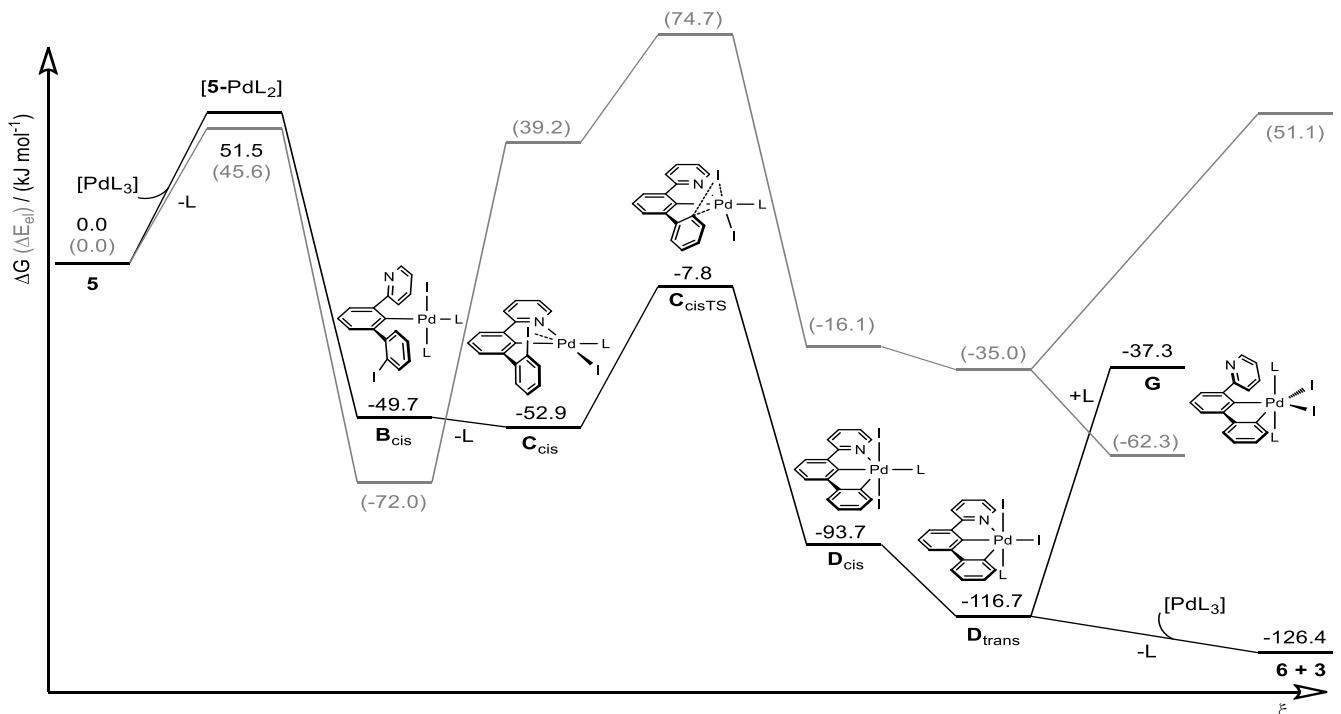
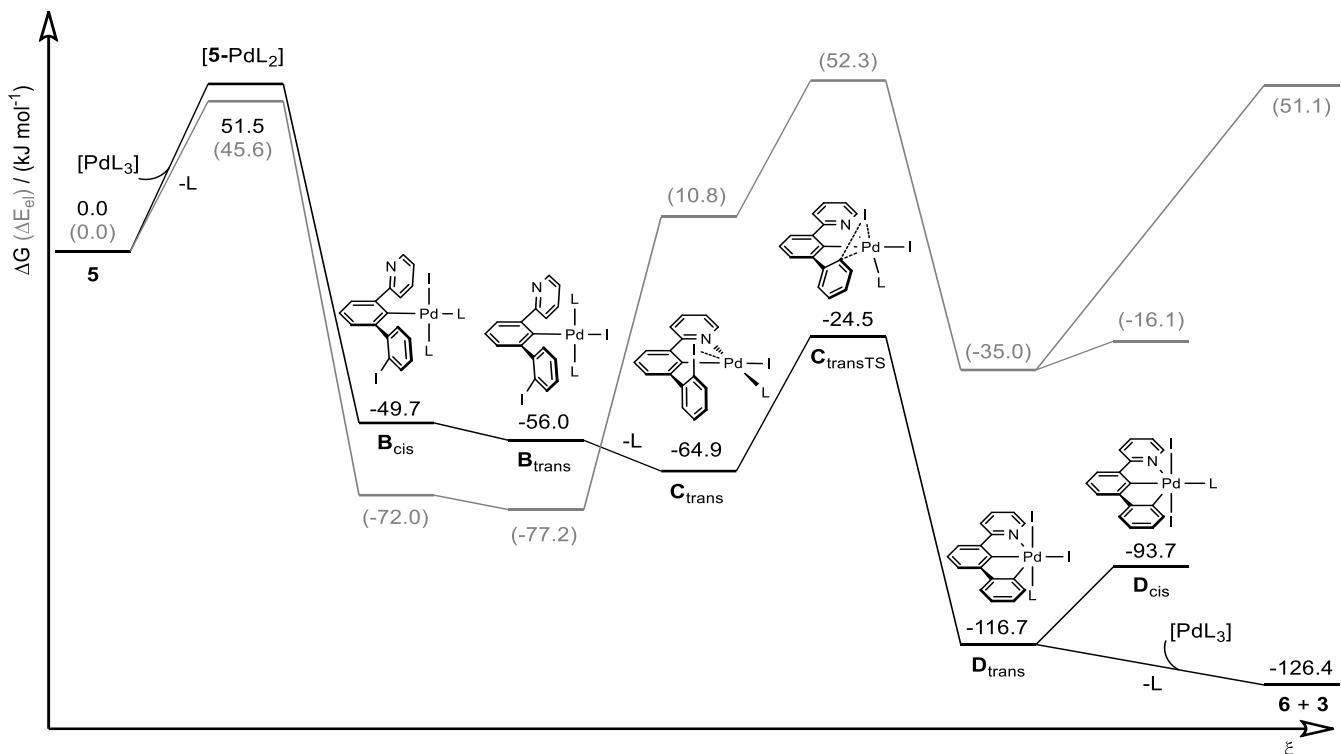
Symmetry and Group theory

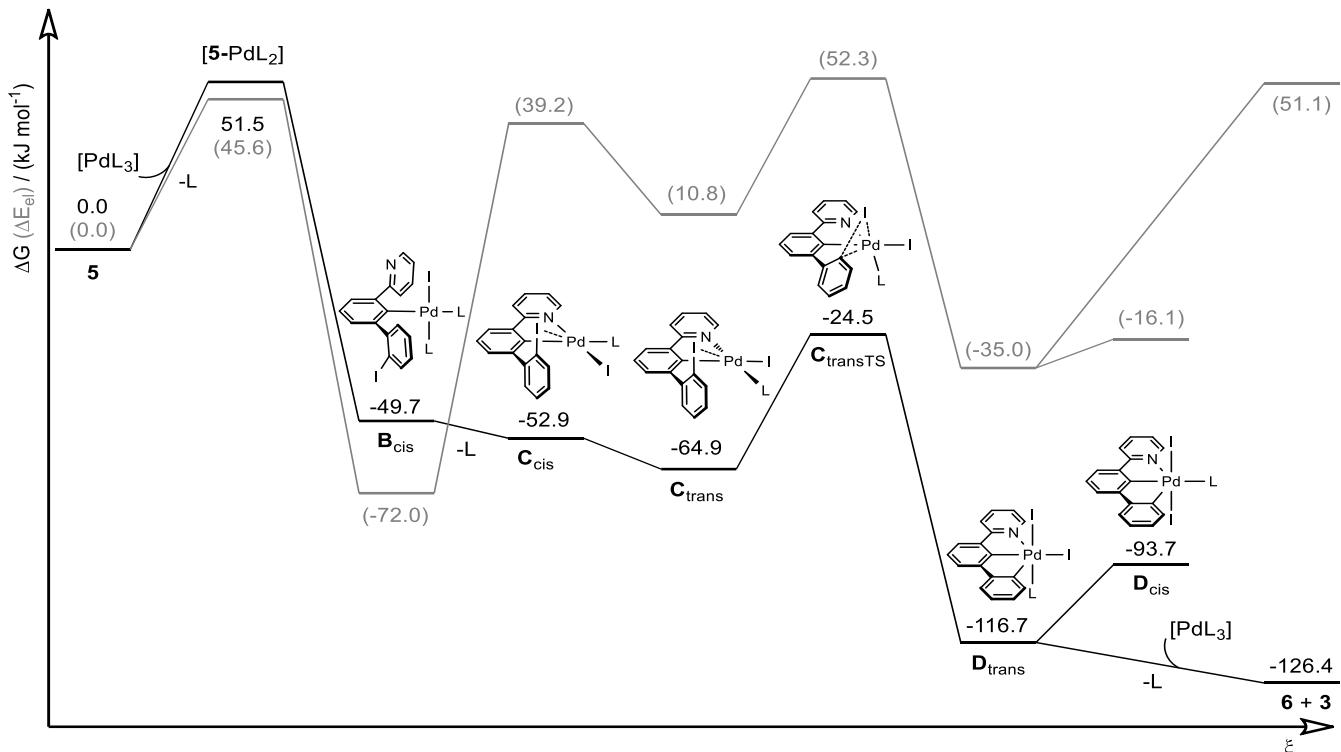
The palindromic (C^N^C) pincer complexes discussed herein belong to the C_{2v} point group whereas the non-palindromic (C^C^N) congener is of C_s symmetry. This affects transition dipole moments and thereby transition intensities. The first absorption as well as the emissive transition of the complexes discussed in this study are mainly of $\pi-\pi^*$ character localized in the pincer ligand (cf. Figure S 3). Thus, the first transition $S_0 \leftarrow S_1$ is of B_1 symmetry for the C_{2v} symmetric (C^N^C) ligand and of A' symmetry for the C_s symmetric (C^C^N). Both transitions are dipole allowed but the A' transition in two directions in contrast to B_1 transitions which are allowed in one direction only. Thus, oscillator strengths of $\pi-\pi^*$ absorptions of the non-palindromic (C^C^N) complex are expected to be higher compared to the (C^N^C) analogue as it is found by our TD-DFT calculations (Table S 2). Same arguments are applicable to the emissive transition: If the latter is symmetry forbidden it will not be observed and the photo-excited system will exhibit long excited state lifetimes and take non-radiative relaxation pathways. Allowed transitions, however, are readily observed and may lead to intense luminescence. The emissive transition of the non-palindromic (C^C^N) pincer is of A' symmetry and therefore shows a higher intensity as the B_1 symmetric transition of the (C^N^C) congener (Figure S 5).

S 6. Alternative pathways of double oxidative addition

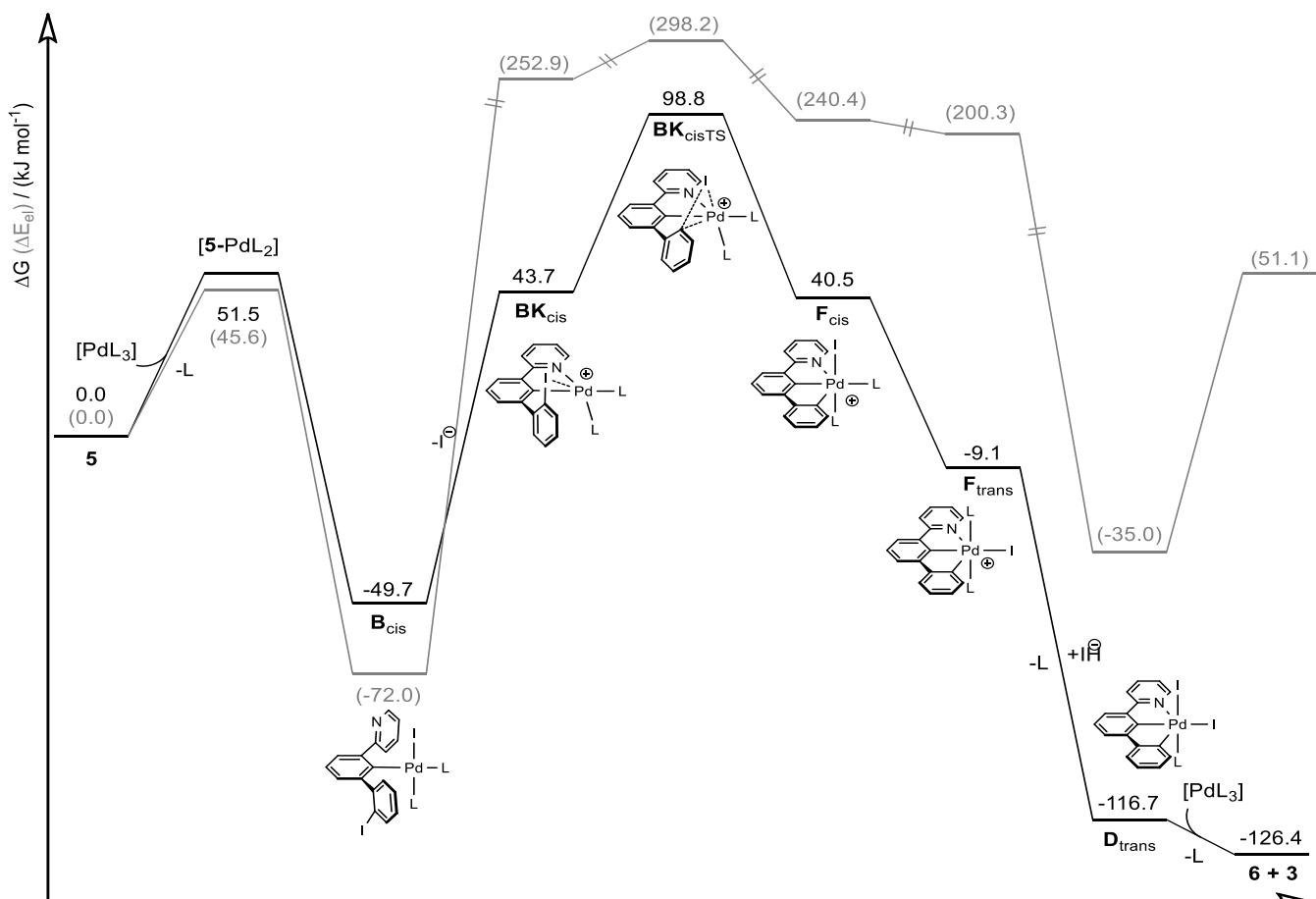
In the main text we presented the lowest energy pathways of the double oxidative addition - comproportionation sequence. Here, further pathways are shown involving higher energy intermediates and/or cationic intermediates. The latter may be stabilized in more polar solvents than toluene

All calculations were performed on the RI-TPPS-(D3BJ)/def2-TZVP level of theory with inclusion of solvent effects by means of the SMD model (*vide infra*). Thermochemical properties were calculated at 298.15 K and 0.1 MPa. Please note, that we have not determined the transition state of the first oxidative addition, since the oxidative addition of aryl iodides to Pd^0 is known to readily happen.¹⁵



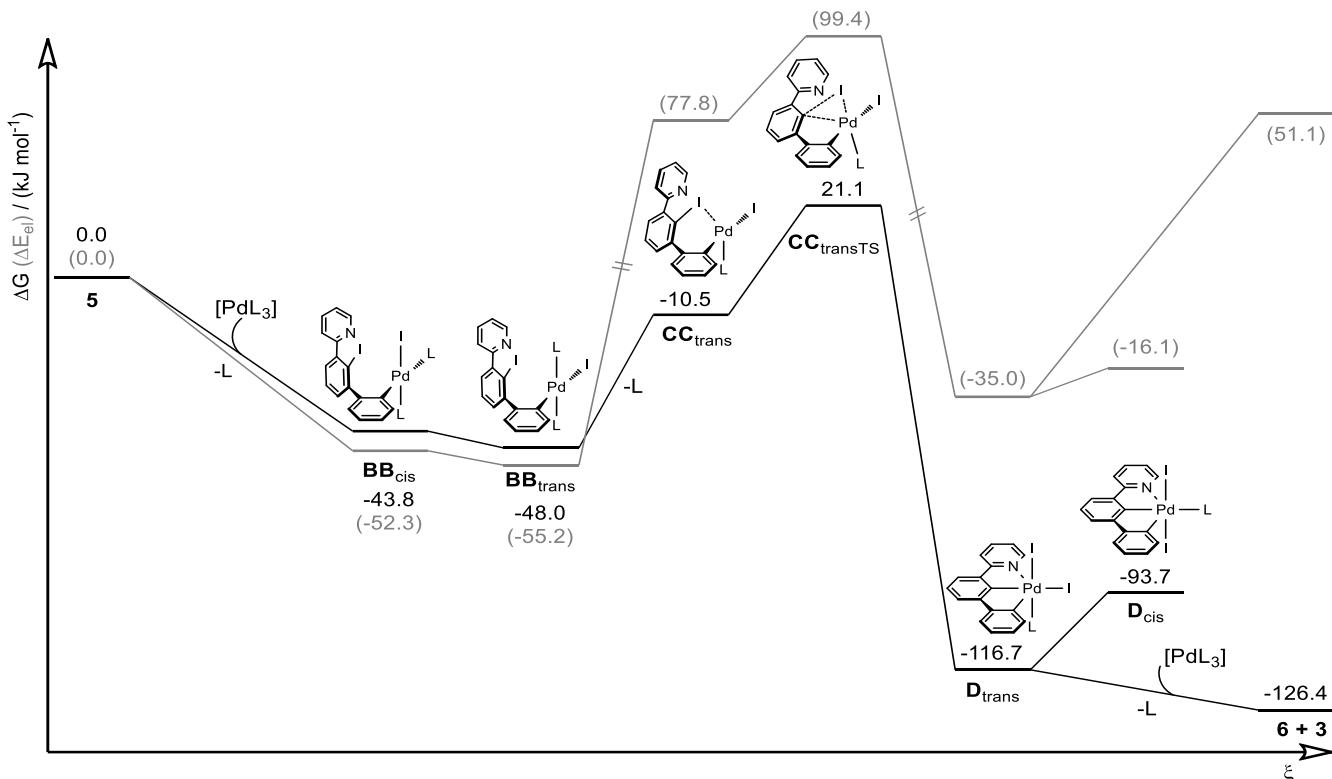


Scheme S 5 Gibbs free energies ΔG (black) and electronic energies E_{el} (grey) of a possible mechanism of formation of **3** starting with oxidative addition into the central iodophenyl group of **5**, ($C\equiv N$) cyclometallation to form **C_{cis}** and cis-trans isomerization of the latter to give **C_{trans}**. The following steps are the same as shown in Scheme S 3.

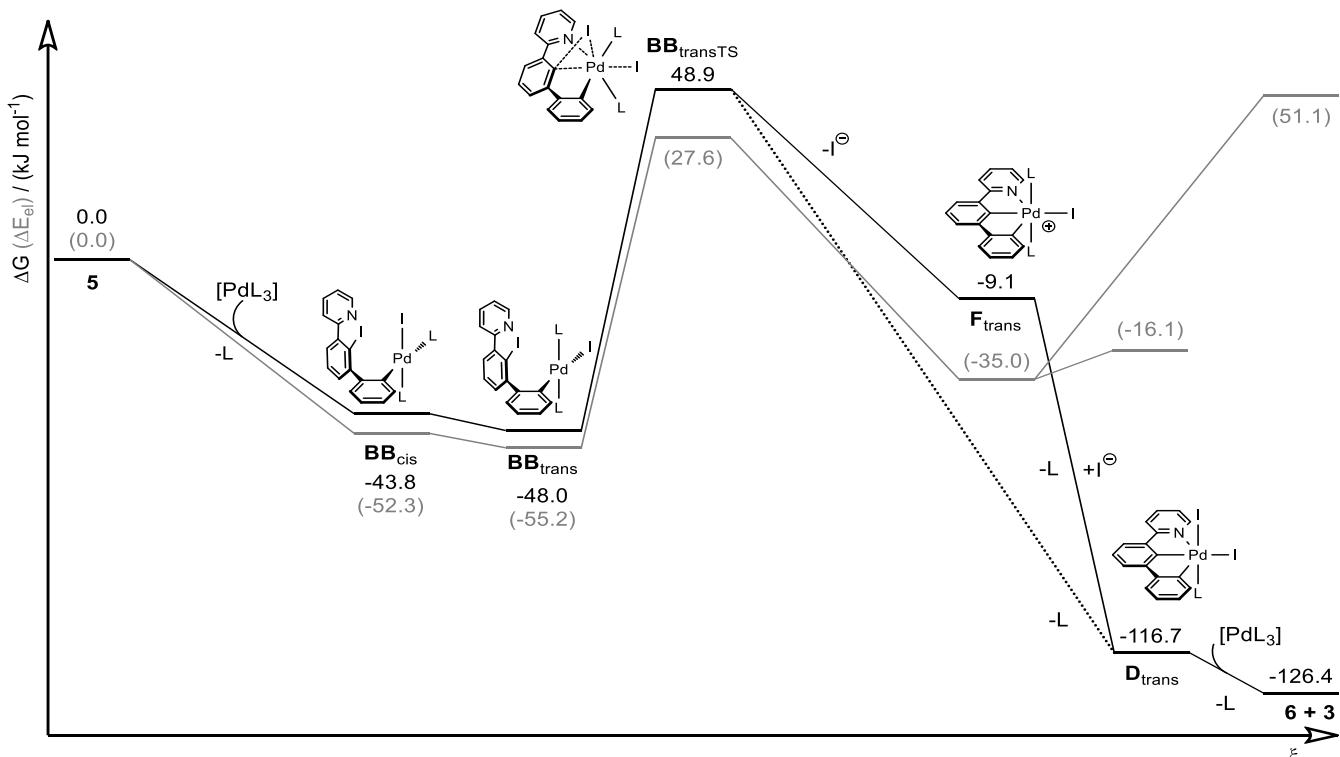


Scheme S 6 Gibbs free energies ΔG (black) and electronic energies E_{el} (grey) of a possible mechanism of formation of **3** starting with oxidative addition into the central iodophenyl group of **5** and direct second oxidative addition without *cis-trans* isomerization of **B_{cis}**. If the latter does not lose a PPh_3 ligand, the second iodophenyl group may oxidatively add, however, only with prior loss of the iodide ligand forming the cationic Pd(II) species **BK_{cis}**. The transition state **BK_{cisTS}** leading to formation of the cationic Pd(IV) species **F_{cis}** is

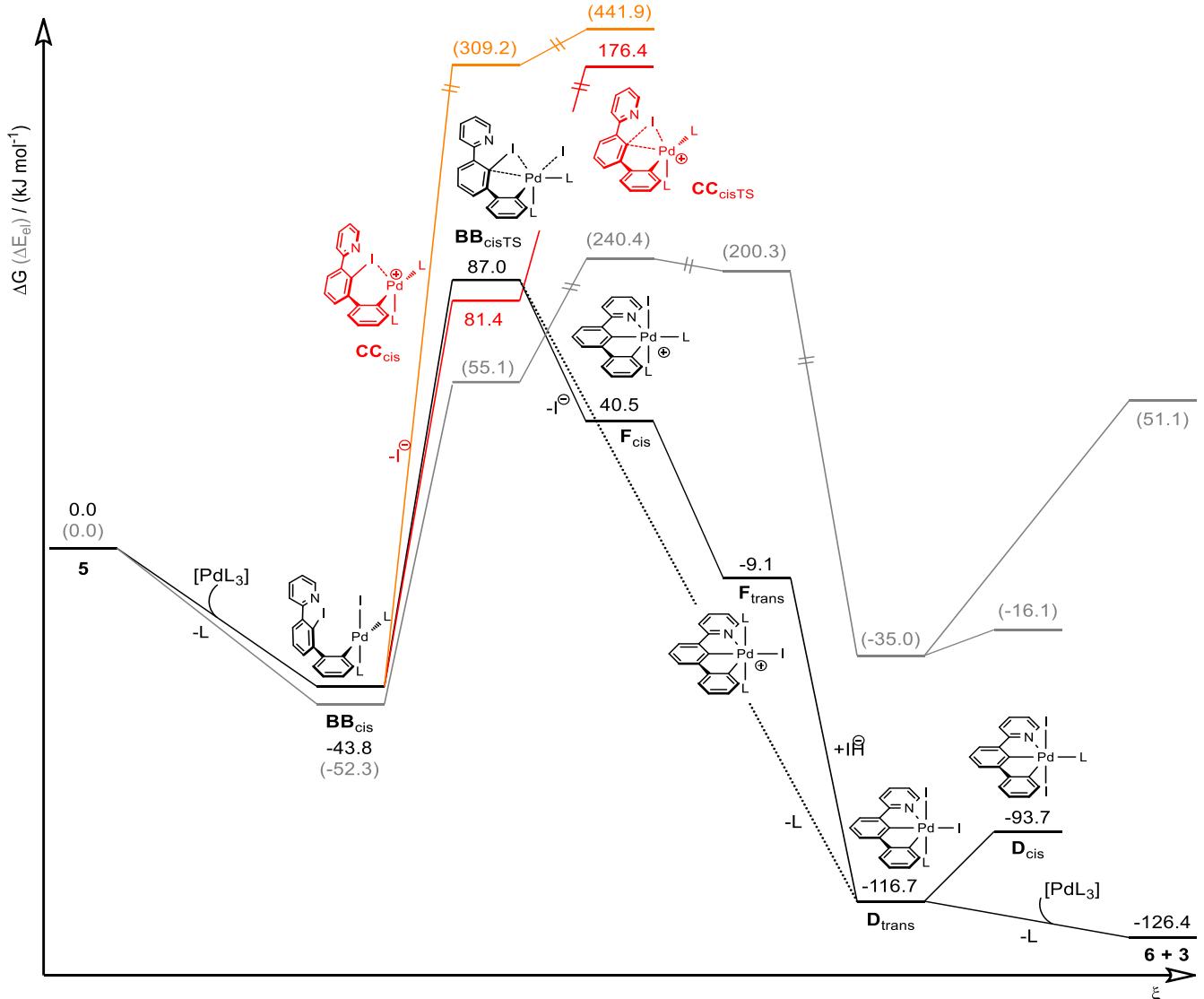
notably higher in energy than the transition state passed during the mechanism with dissociation of a neutral ligand (Scheme S 3) making the latter pathway much more likely. This may be different in more polar solvents.



Scheme S 7 Gibbs free energies ΔG (black) and electronic energies E_{el} (grey) of the overall minimum energy pathway for the formation of **3** starting with oxidative addition into the lateral iodophenyl group of **5** (see also main text, black pathway).



Scheme S 8 Gibbs free energies ΔG (black) and electronic energies E_{el} (grey) of a possible mechanism of formation of **3** starting with oxidative addition into the lateral iodophenyl group of **5** and different transition state for the second oxidative addition into the central iodophenyl group of **BB_{trans}**. The transition state **BB_{transTS}** is 27.8 kJ/mol higher in energy than **CC_{transTS}** (Scheme S 7). **BB_{transTS}** shows a notable elongation of the bond between the palladium atom and iodide atom in trans position ($d_{TS}(Pd-I) = 292$ pm, $d_{BBtrans}(Pd-I) = 271$ pm) as well as between the palladium atom and the phosphine arranged on the same side as the adding phenyliodide ($d_{TS}(Pd-P) = 256$ pm, $d_{BBtrans}(Pd-P) = 237$ pm). However, the imaginary frequency characterizing this transition states suggests loss of the iodide of the central phenyl group during oxidative addition which corresponds to formation of the cationic Pd(IV) species **F_{trans}**. The latter may lose one PPh_3 ligand and upon reassociation of I^- form the final Pd(IV) product **D_{trans}**.



Scheme S 9 Gibbs free energies ΔG (black) and electronic energies ΔE_{el} (grey) of a possible mechanism of formation of **3** starting with oxidative addition into the lateral iodophenyl group of **5** and direct second oxidative addition without *cis-trans* isomerization of **BB_{cis}**. The transition state **BB_{cisTS}** is notably higher in energy than transition states discussed so far. It may, on the one hand, upon loss of one ligand L directly form the Pd(IV) species **D_{trans}**. On the other hand, the transition state **BB_{cisTS}** shows a notably elongation of the bond between palladium atom and iodide in trans position ($d_{TS} = 291$ pm; $d_{BBcis} = 265$ pm) and leads upon loss of this iodide to the cationic Pd(IV) species **F_{cis}**. The latter, after isomerization (**F_{trans}**) yields upon ligation of I⁻ **D_{trans}**. In principle, **BB_{cis}** may lose the iodide ligand forming the cationic Pd(II) species **CC_{cis}** (red and orange pathway). However, the barrier of oxidative addition into the second iodophenyl group is calculated to be far too high making a pathway involving cationic Pd(II) species very unlikely. In summary, a mechanism involving Pd(IV) species formation after *cis-trans* isomerization of **BB_{cis}** (Scheme S 7) without cationic intermediates seems to be most likely. This may be different in more polar solvents.

S 7. Quantum chemical details

All quantum chemical calculations except for solvent effects (*vide infra*) were performed with the TURBOMOLE¹⁶ program package (version 7.4). Fine integration grids (m4) and SCF convergence criteria of 10^{-8} a.u., density convergence $\leq 10^{-7}$, cartesian gradient $\leq 10^{-4}$ were used. The Turbomole module AFORCE¹⁷ (analytically frequency calculations) was used.

Thermochemistry

Structure optimizations in the gas phase were done on the RI¹⁸-TPSS¹⁹-D3²⁰(BJ)²¹/def2-TZVP²² level of theory. We've chosen the meta-GGA functional TPSS since it showed good overall performance in calculating structures of transition metal complexes²³ and yields reliable thermochemical results.²⁴

All optimized structures were checked for minima (no imaginary frequencies) or transition states (one imaginary frequency according to the bond-forming and -breaking processes connecting the respective minima). Thermal Gibbs free energy contributions $\Delta G_{thermal}$ with inclusion of zero point energies (ZPE) were calculated with the TURBOMOLE module FREEH based on assumptions of statistical thermodynamics of an ideal gas and added to the total gas-phase electronic energies ΔE_{gas}

$$\Delta G_{gas} = \Delta E_{gas} + \Delta G_{thermal}.$$

For Gibbs free energies in solution ΔG_{sol} , we added free energies of solvation ΔG_{solv} (solvent: toluene) to the gas phase free energies²⁵

$$\Delta G_{sol} = \Delta E_{gas} + \Delta G_{thermal} + \Delta G_{solv}.$$

The latter were obtained by means of single point calculations on the same level of theory as mentioned above with the gas phase optimized structures including the SMD²⁶ solvation model as implemented in ORCA 4.1.2²⁷ where electrostatic contributions are calculated using the C-PCM model.²⁸ This relies on the assumption that thermal contributions to the Gibbs free energy in the gas and solution phase are sufficiently similar.²⁹ The solvation free energy was then obtained by taking the difference of electronic energies obtained in the gas phase E_{gas} and in solution E_{sol} ³⁰

$$\Delta G_{solv} = \Delta E_{gas} - \Delta E_{sol},$$

where ΔE_{sol} contains the electronic energy of the system corrected for electrostatic effects in solution and contributions which account for changes in Gibbs free energy due to non-electrostatic effects which enter by parametrization of the solvation model.³¹

We note that both single point energies were calculated with ORCA to avoid errors arising from inconsistencies due to slightly different method implementations of ORCA and TURBOMOLE.

Photophysical Properties

TDDFT calculations for investigation of photophysical properties were done with TURBOMOLE 7.4 on the RI-PBE0-D3(BJ)/def2-TZVP³² level of theory neglecting solvent effects with structures optimized on the RI-TPSS-D3(BJ) /def2-TZVP level of theory. The PBE0 functional was shown to give reliable results for the calculation of vertical and adiabatic transitions³³ and was successfully applied for the calculation of photophysical properties of some [(C^NN)Pt(II)]-acetylides.³⁴

Unrelaxed different densities were calculated with the TURBOMOLE module PANAMA.¹⁰

Structures of T₁ states were optimized on the RI-TPSS-D3(BJ) /def2-TZVP level of theory by using an unrestricted Kohn Sham³⁵ triplet wave function as pseudo ground state. Phosphorescence energies were then obtained as negative excitation energies by spin-flip TDDFT³⁶ calculations in the Tamm-Danoff approximation³⁷ on the PWLDA³⁸/def2-TZVP level of theory. This procedure was shown to give meaningful phosphorescence energies of some platinum complexes far more reliable than TDDFT calculations using a singlet reference state.³⁹

Molecular orbitals and densities were visualized using the TmoleX program suite.⁴⁰

S 8. Experimental details

Synthetic and workup procedures

Manipulations were performed under a dry and oxygen-free argon or nitrogen atmosphere using standard Schlenk techniques.⁴¹ THF, toluene and *n*-hexane were freshly distilled under argon or nitrogen from sodium/benzophenone. Acetonitrile was distilled under argon or nitrogen from CaH₂. CH₂Cl₂ and *n*-pentane was purchased pre-dried and de-oxygenated and further purified by passing through alumina columns of an Innovative Technology® Solvent Purification System.

For NMR measurements of air- or moisture sensitive compounds C₆D₆ was vacuum transferred from potassium/benzophenone, CD₂Cl₂ from CaH₂ into thoroughly dried glassware equipped with Young Teflon valves.

Air sensitive compounds were stored and weighed in glove boxes (Braun MB150 G-I and Unilab system). Transfer of liquids and solutions was done by use of PP disposable syringes equipped with steel cannula which were purged with inert gas three times prior to use.

Analytics and instrumentation

NMR Spectroscopy. If not stated otherwise, solution NMR spectra were recorded at 300 K using Bruker Avance Instruments operating at ¹H Larmor frequencies of 300 or 400 MHz; chemical shifts are given in parts per million (ppm) relative to TMS for ¹³C and ¹H, to H₃PO₄ for ³¹P. ¹H spectra are referenced to residual ¹H solvent signals of the deuterated solvents, ¹³C spectra to the respective solvent ¹³C signal as internal standard.⁴²

Coupling constants J are given in Hertz (Hz) as positive values regardless of their real individual signs. The multiplicity of the signals is indicated as s, d, t, q, m, dd, dt, td, or ddd for singlets, doublets, triplets, quartetts, multiplets, doublets of doublets, doublets of triplets, triplets of doublets or doublet of doublets of doublets, respectively. The abbreviation br is given for broadened signals, brm for broadened multiplets. Other couplings than H-H (J) couplings are indicated by an index (_{J_{nucleus1-nucleus2}}).

The assignments were confirmed, as necessary, with the use of 2D NMR correlation experiments (COSY = Correlated Spectroscopy; NOESY = Nuclear Overhauser Enhancement Spectroscopy; HSQC = Heteronuclear Single Quantum Coherence; HMBC = Heteronuclear Multiple Quantum Correllation; HMQC = Heteronuclear Multiple Quantum Correlation Transfer).

The multiplicity of ¹³C-NMR-signals was determined by the use of DEPT 90- and DEPT 135-spectra (DEPT = Distortionless Enhancement by Polarization Transfer): DEPT: + = primary CH or tertiary CH₃ (positive DEPT-signal), - = secondary CH₂ (negative DEPT-signal), C_q = quaternary C-atoms (no DEPT-signal).⁴³ The spectra were analysed according to first order.

NMR samples were prepared in oven-dried 5 mm NMR tubes. Air or moisture sensitive compounds were prepared inside a glovebox using screw cap or Young valve NMR tubes or by vacuum transfer of the solvent to the samples and melting off the NMR tube.

Unless otherwise stated, standard Bruker software routines (TOPSPIN⁴⁴) were used for the 1D and 2D NMR measurements.

IR Spectroscopy. IR spectra were recorded on a Bruker Alpha FT-IR spectrometer using the ATR technique (attenuated total reflection) on bulk material, and the data are quoted in wavenumbers (cm⁻¹). The intensities of the absorption bands are indicated as follows: vs = very strong (0 – 10 % transmission (T)), s = strong (11 – 30 % T), m = medium (31 – 70 % T), w = weak (71 – 90 % T), vw = very weak (91 – 100 % T).

Mass Spectrometry. Mass spectra were recorded using a Varian MAT 3830 (70 eV) with Electron Ionization (EI).

Air or moisture sensitive samples were melted off in glass capillaries under argon (EI).

If detectable, the positive molecular ion peak [M]⁺ or the protonated molecular ion peak [M+H]⁺ as well as characteristic fragment peaks ([M-fragment]⁺ and [fragment]⁺) are given. For ESI-MS, if detectable, the negative molecular ion peak [M]⁻ is given. Intensities are given relative to the base peak (100 %).

Elemental Analysis. Elemental analyses were done by the institutional technical laboratories of the Karlsruhe Institute of Technology (KIT).

Melting Points. Melting points were measured with a Thermo Fischer Scientific digital melting point apparatus of the IA9300 series and are not corrected. Pure samples of the compounds were added to a capillary tube under argon which was then sealed from air by fusemelting the glass end.

UV/Vis Spectroscopy. UV/Vis spectra were recorded on a Lambda 750 Spectrometer (Perkin Elmer).

Photoluminescence Spectroscopy. Photoluminescence spectra were recorded on a Horiba Jobin Yvon Spex Fluorolog 3 (Horiba Jobin Yvon, Bensheim, Germany). It was equipped with a 450 W Xe lamp, double grating monochromators for excitation and emission, integrating sphere and photomultiplier detector (excitation source and detector in orthogonal arrangement).

Slit widths for excitation and detection were adjusted individually for each sample.

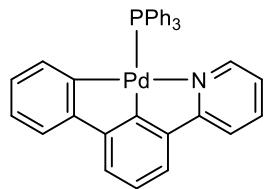
Absolute quantum yields were determined as average of three independent measurements by means of an integrating sphere (error ± 2 %).

Photoluminescence spectra in frozen solution at 77 K were acquired by using a small optical dewar. The sample solution was sealed in a quartz tube of 3 mm diameter under oxygen-free conditions, placed into the dewar and quickly cooled to 77 K before the measurement by addition of liquid nitrogen. The solution was of 50 µmol/L concentration. At this concentration absorbance of the sample at the excitation wavelengths (337 nm) was below 0.05.

If not stated otherwise, OriginPro 2019b⁴⁵ was used for data evaluation.

S 9. Experimental procedures

$[(C^NC^N)Pd(II)PPh_3]$ (3)



2-(2,2'-Diiodo-[1,1'-biphenyl]-3-yl)pyridine (**5**) (138 mg, 0.29 mmol, 1.10 eq.) and $[Pd(PPh_3)_4]$ (300 mg, 0.26 mmol, 1.00 eq.) were dissolved in toluene (5 ml) and heated to 100 °C for 2 h. The mixture turned dark red and TDAE (104 mg, 121 μ l, 0.52 mmol, 2.00 eq.) was added on which the solution changed to yellow. Heating was continued for 2 h. The mixture was filtered, and the residue extracted with hot toluene (2 x 10 ml). The combined filtrates were evaporated in vacuo to yield a sticky orange solid. *n*-Hexane (10 ml) was added and the mixture sonicated for 15 min inside an ultrasonic bath. The supernatant *n*-hexane extract was taken off and the dried residue washed with MeCN (5 ml) to remove orange coloured impurities. After drying in vacuo, 134 mg (86 %) of a yellow solid were obtained. Crystals suitable for X-ray diffraction analysis were obtained upon layering a concentrated solution in benzene with *n*-hexane.

M.p. = 291 °C (Z). **1H-NMR** (300 MHz, CD_2Cl_2): δ = 7.90 – 7.80 (m, 6 H), 7.71 (ddd, J = 8.1, 1.7, 0.8 Hz, 1 H), 7.64 (ddd, J = 8.1, 7.2, 1.7 Hz, 1 H), 7.53 – 7.36 (m, 9 H), 7.31 (t, J = 8.8 Hz, 2 H), 7.27 (dd, J = 7.5, 1.6 Hz, 1 H), 7.09 (t, J = 7.6 Hz, 1 H), 6.89 (ddd, J = 5.5, 1.7, 0.9 Hz, 1 H), 6.84 (td, J = 7.4, 1.3 Hz, 1 H), 6.63 – 6.54 (m, 2 H), 6.33 (td, J = 7.4, 1.5 Hz, 1 H). **13C-NMR** (101 MHz, CD_2Cl_2): δ = 184.3 (d, J_{C-P} = 96.4 Hz, C_q), 166.9 (d, J_{C-P} = 6.1 Hz, C_q), 160.7 (d, J_{C-P} = 9.3 Hz, C_q), 159.9 (d, J_{C-P} = 4.9 Hz, C_q), 155.8 (C_q), 151.7 (CH), 144.4 (C_q), 141.6 (d, J_{C-P} = 9.1 Hz, CH), 138.6 (CH), 135.7 (d, J_{C-P} = 14.1 Hz, 6 CH), 134.0 (d, J_{C-P} = 29.6 Hz, 3 C_q), 130.9 (d, J_{C-P} = 1.7 Hz, 3 CH), 129.2 (d, J_{C-P} = 9.3 Hz, 6 CH), 125.8 (CH), 125.4 (CH), 124.5 (CH), 122.1 (CH), 120.8 (d, J_{C-P} = 4.2 Hz, CH), 120.5 (d, J_{C-P} = 4.8 Hz, CH), 120.2 (CH), 119.0 (CH). **31P NMR** (121 MHz, CD_2Cl_2): δ = 24.0. **IR (ATR)**: $\tilde{\nu}/cm^{-1}$ = 3046 (vw), 2169 (vw), 2073 (vw), 2034 (vw), 2004 (vw), 1989 (vw), 1909 (vw), 1600 (w), 1575 (vw), 1480 (w), 1455 (vw), 1430 (m), 1390 (vw), 1310 (vw), 1283 (vw), 1262 (vw), 1247 (vw), 1236 (vw), 1185 (vw), 1155 (w), 1129 (vw), 1091 (w), 1038 (vw), 1027 (vw), 1012 (vw), 997 (w), 957 (vw), 930 (vw), 883 (vw), 853 (vw), 820 (vw), 774 (vw), 750 (vs), 739 (vs), 692 (vs), 637 (w), 622 (w), 526 (vs), 505 (vs), 489 (s), 476 (m), 459 (w), 427 (m), 396 (vw), 383 (vw). **UV/Vis (THF)**: λ_{max}/nm ($\epsilon/[dm^3mol^{-1}cm^{-1}]$) = 303 (13500), 351 (6800), 380 (4100). **Luminescence** (solid): λ_{ex} = 417 nm, λ_{em} = 487 nm. **MS (EI, 70 eV)**, m/z (%): 334.0 (21 %) [$M-PPh_3]^+$, 231.1 (93 %) [$(CH^NCH^N)]^+$. **Elemental analysis** calculated (%) for $C_{35}H_{26}NPPd$: C 70.30, H 4.38, N 2.34, found: C 70.76, H 4.554, N 2.15.

S 10. NMR spectra

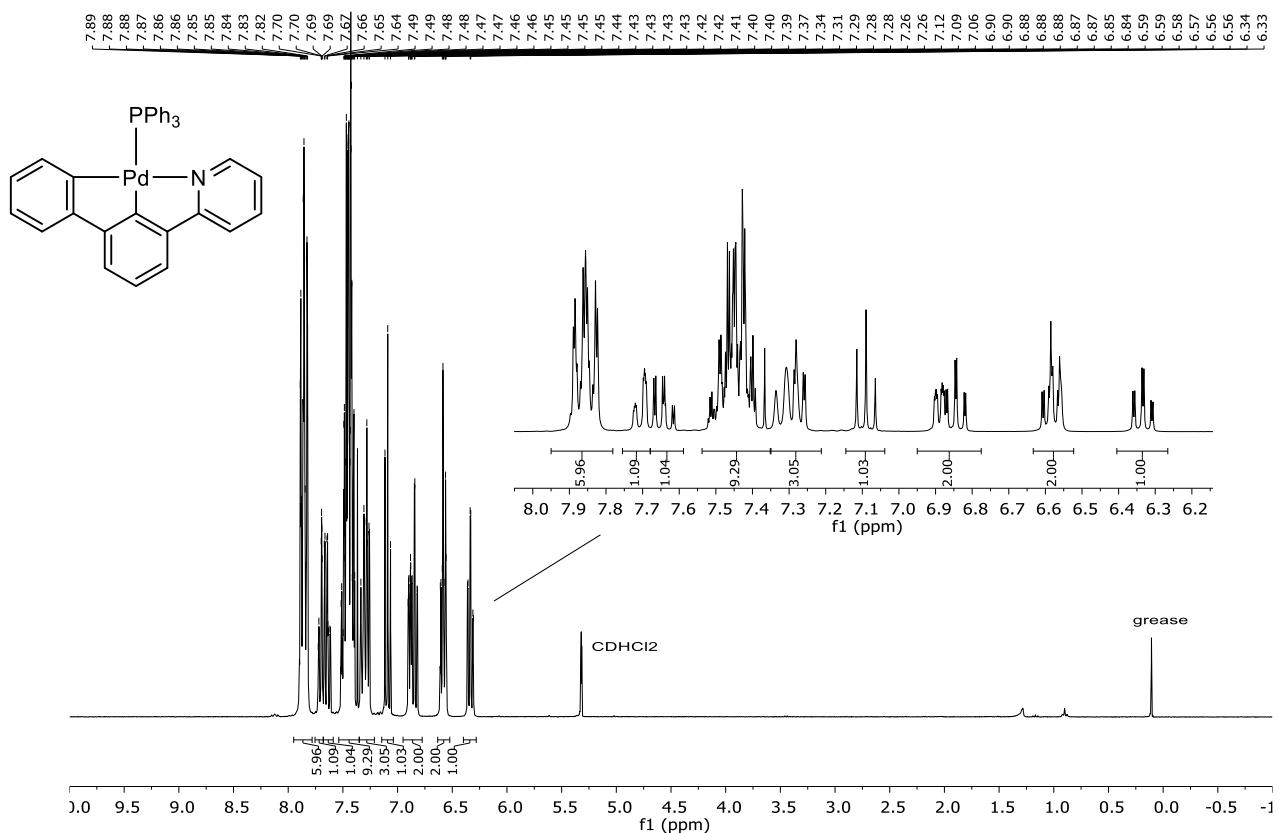


Figure S 8 ^1H NMR (300 MHz, CD_2Cl_2) of **3**.

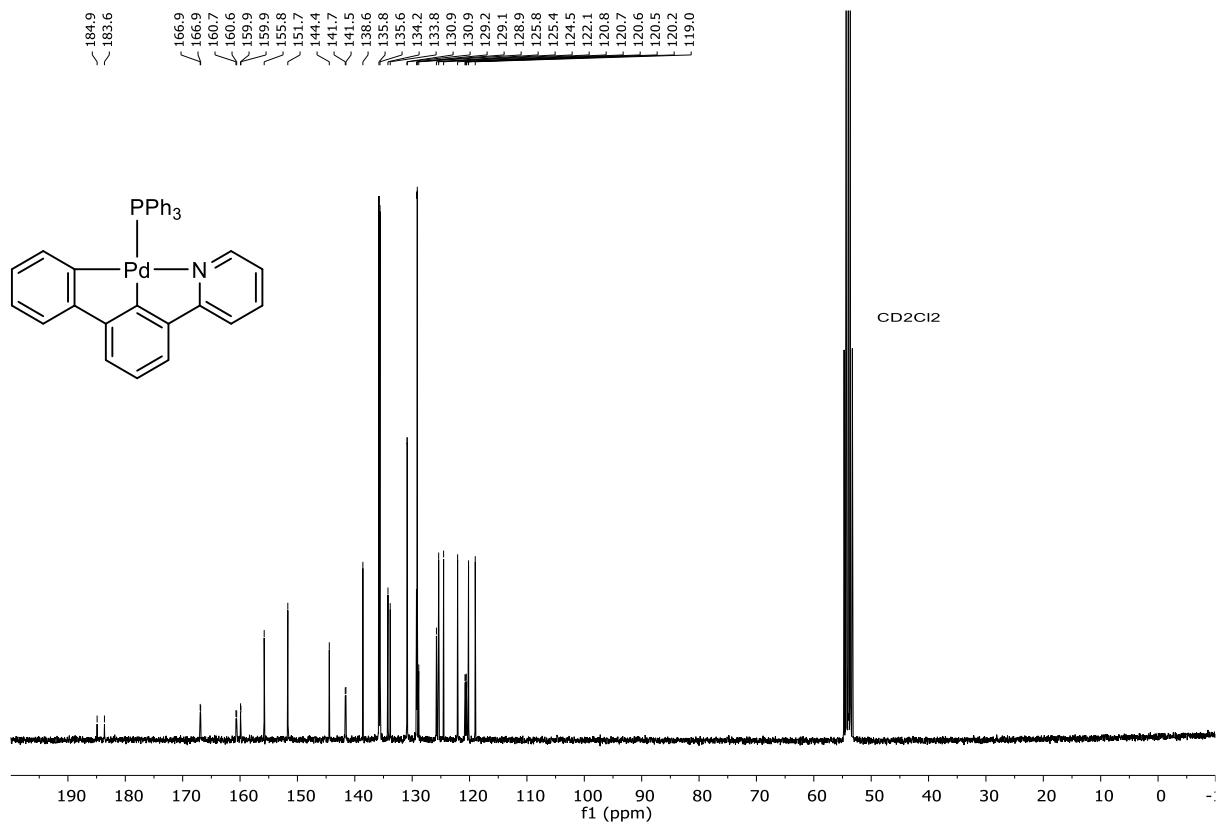


Figure S 9 ^{13}C NMR (75 MHz, CD_2Cl_2) of 3.

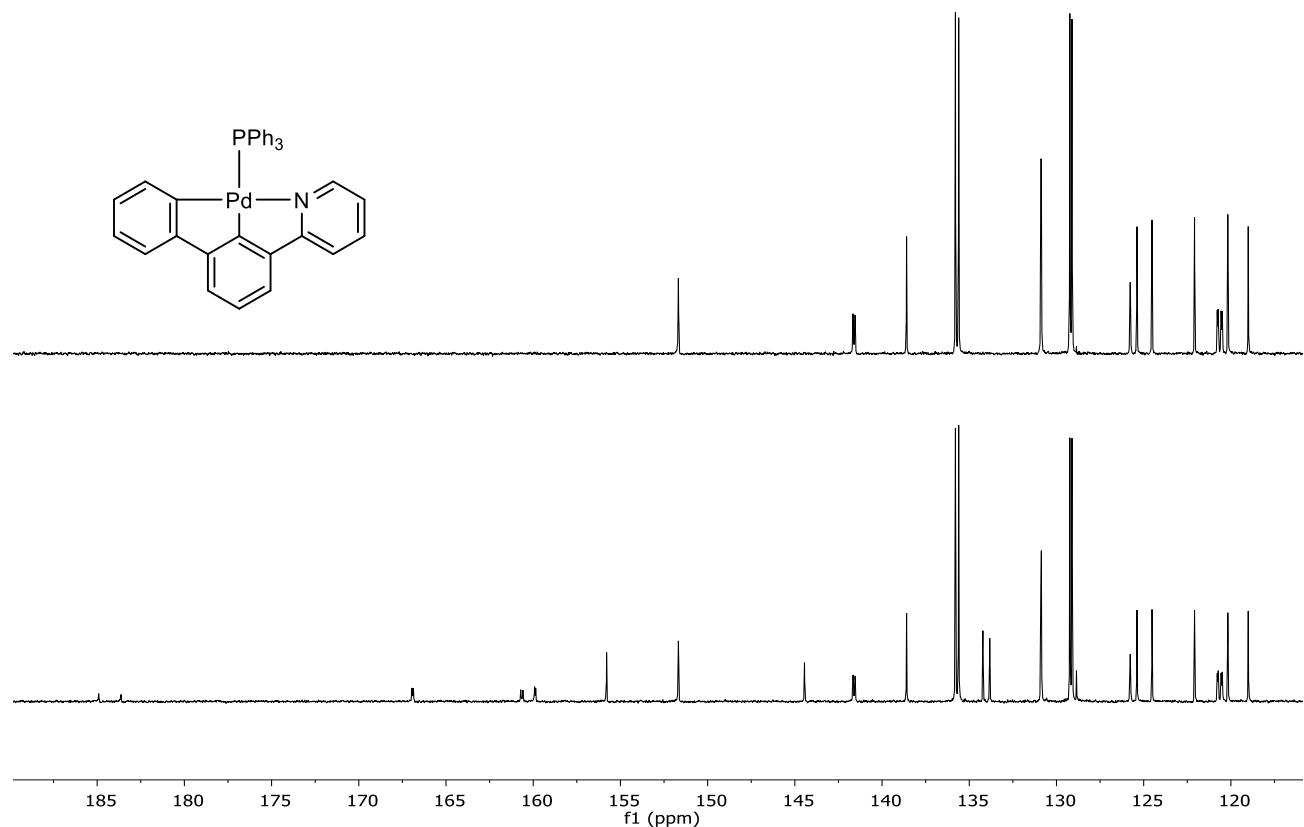


Figure S 10 ${}^{13}\text{C}$ NMR (bottom) and dept135 (top) spectrum of **3**.

S 11. Crystallographic details

In order to avoid degradation, single crystals were mounted in perfluoropolyalkylether-oil on top of the edge of an open Mark tube and then brought into the cold nitrogen stream of a low-temperature device (Oxford Cryosystems Cryostream unit) so that the oil solidified. Diffraction data were measured using a Stoe IPDS II diffractometer (graphite-monochromated MoK α (0.71073 Å) radiation). The structures were solved by dual-space direct methods with SHELXT,⁴⁶ followed by full-matrix least-squares refinement using SHELXL-2014/7.⁴⁷ All non-hydrogen atoms were refined anisotropically, with organic hydrogen atoms placed in calculated positions using a riding model. Absorption corrections were applied for all compounds (multi-scan). Crystallographic data, data collection, and refinement details are summarized in the following tables. Crystallographic data (excluding structure factors) for the structures in this paper have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained from <https://www.ccdc.cam.ac.uk/structures/>.

Compound	3	S2
Empirical Formula	C ₃₅ H ₂₆ NPPd	C ₂₂ H ₁₆ N ₂ Ni
<i>M</i>	597.94	367.08
Temperature / K	200.0	200
Crystal system	monoclinic	monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> / Å	22.264(6)	9.282(5)
<i>b</i> / Å	9.403(2)	12.710(7)
<i>c</i> / Å	26.426(7)	14.038(7)
α / °	90.00	90.00
β / °	102.18(2)	90.89(4)
γ / °	90.00	90.00
<i>V</i> / Å ³	5407.7(21)	1655.9(15)
<i>Z</i>	8	4
ρ_{calc} g/cm ³	1.469	1.472
μ / mm ⁻¹	0.771	1.177
Crystal size / mm ³	1 × 0.5 × 0.2	0.3 × 0.183 × 0.1
Radiation	Mo K α (λ = 0.71073)	Mo K α (λ = 0.71073)
2 θ_{\min} / °	3.154	4.324
2 θ_{\max} / °	51.998	58.404
Reflections collected	25049	11940
Independent Reflections	10623 ($R_{\text{int}} = 0.0508$)	4459 ($R_{\text{int}} = 0.0311$)
Data/restraints/parameters	10623/0/686	4459/0/227
GooF on F ²	1.054	1.024
<i>R</i> 1 [$I \geq 2\sigma(I)$]	0.0505	0.0406
<i>wR</i> 2 [$I \geq 2\sigma(I)$]	0.1430	0.1008
<i>R</i> 1 (all data)	0.0571	0.0719
<i>wR</i> 2 (all data)	0.1482	0.1119
Largest diff. peak/holes /e · Å ³	1.26 / -1.40	0.40 / -0.47
Diffractometer	Stoe IPDS II	Stoe IPDS II
CCDC number	1986490	1986487

S 12. Coordinates of quantum chemical calculations

Given in TURBOMOLE coord format.

5 @ RI-TPSS-D3(BJ)/def2-TZVP

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-2.15866949775163  1.30660893911060  -0.02317551579336 c
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1.52443955007649  2.27182454856621  -3.68689259471970 c
-0.68798085584663 3.69187697031041  -3.65645784028750 c
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[Pd(PPh₃)₃] @ RI-TPSS-D3(BJ)/def2-TZVP

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-1.28586428194001	3.95132241139998	5.86510452510905 h
-5.09595220923556	0.76417708581102	-0.96886111080528 c
-5.88058515776706	3.26257600854103	-0.54837668271876 c
-6.60731150306126	4.79051272291282	-2.56880529086582 c
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-5.44087193181860	-0.21784762495962	4.41191801911448 c
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-7.89635472479509	1.02975796113879	8.94049036886270 c
-5.33498981801365	0.40071418924602	8.95936541719685 c
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-2.10792017615821	-0.65340252449217	6.68669458836128 h
-4.98120376087863	-4.30935381156966	1.03654183677747 c

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-4.37237420372797 -8.82032726326808 1.64813551598081 c
-3.54475530113980 -6.33775264129640 1.94979385099849 c
-8.40829274518410 -3.25869883020959 -0.91303030981908 h
-9.85711245289829 -7.66290403328872 -1.50204919992666 h
-7.28190162829454 -11.23678324956046 0.12316072286453 h
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\$end

PPh₃ @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

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4.56957414651800 -0.63987977431143 6.09742194566142 c
6.62153249512916 -0.15136002052154 4.51150527875263 c
6.20110692239675 0.76049314515410 2.07405737824488 c
3.74214800461675 1.16700720873764 1.21197481959309 c
0.52162883303938 -0.56272996030508 6.49606686261937 h
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8.53722797614638 -0.46865296204690 5.17803848948778 h
7.79056111234910 1.14972651857483 0.83312868785482 h
3.42892501823491 1.86433230698821 -0.69226103373425 h
-1.26877952522029 2.83595188814127 -1.17130223737178 c
-1.26057806909658 1.64842274647095 -3.53819049839781 c
-0.97269001881696 3.06558116060475 -5.74353962401699 c
-0.67367363360450 5.68148634579944 -5.61319151772483 c
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-1.47859444313440 -0.38868117508975 -3.65330113890473 h
-0.97369336954005 2.12011717868924 -7.56666982693424 h
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-1.03219208321335 6.41701517748671 0.76221085377512 h
-2.51382207843041 -2.02919823508846 0.76097921138028 c
-5.08121480280678 -2.47856096804374 0.26341286511348 c
-5.89376746973569 -4.83363320640716 -0.58766918300806 c
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-6.44319856914557 -0.96487704873487 0.54375245488659 h
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\$end

[5-Pd(PPh₃)₂] @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

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3.33118558626010 5.91903329050716 -3.18124419735061 c
1.88208980092723 7.91830448973496 -2.27957187044150 c
1.54832013833509 8.22089045590569 0.30587409500992 c
1.36788709071375 -1.20341354290896 -0.97405073970798 pd
3.58549066321027 5.64996120870170 -5.19894154238128 h
1.00396144299621 9.22178753805534 -3.59678307414991 h
0.42499793803582 9.77464766608971 1.03652345034606 h
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5.21477324272845 -0.29819836097251 -2.27433968735615 n
6.60858514865686 -2.16787898144887 -3.31227219987488 c
8.74563665033724 -1.73005620537081 -4.76897556046460 c

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0.08659876218359	5.78734343318591	8.67807119154205 c
0.56626213961896	5.38922543156348	6.12371825915273 c
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0.92232955804452	8.08282544157760	11.94622378819276 h
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-1.59915541535700	0.25335311450969	-3.67569377498345 p
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-4.28521547798527	-6.12687924859240	4.53949742507037 h
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-3.88348076816255	-2.39662256289206	-7.80029688862259 c
-5.48852682834903	-4.23808213440597	-8.79887618025213 c
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-5.12053241686067	-3.63123429556104	-3.58448308567465 c
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B_{cis} @ RI-TPSS-D3(BJ)/def2-TZVP

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7.99126182185772  7.17707070195935 -2.65534070100002 c
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4.72904275080360  9.49676400411295 -3.30238207092933 h
-5.60429887627113  3.59077014213426 -2.94288342533568 c
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7.14712048006056  -8.04374518719733 -2.88035324424925 c

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4.58174505539028	-0.43999371910774	0.30178887597559 h
-1.03239922294523	4.83565505488014	3.08391680031513 c
-2.75616738920575	5.18328033703534	5.06039011394701 c
-3.09036583774471	7.57361260804050	6.12297919242137 c
-1.73316833583930	9.63474194250980	5.20577440611319 c
-0.03773691768069	9.30284004183283	3.20997379022426 c
0.32021257196489	6.91893821748943	2.16284547081625 c
-3.83247712707205	3.59362814116247	5.77771385449371 h
-4.43524358850002	7.82065049268824	7.65395680778211 h
-2.00493452059555	11.49620266057132	6.02783642263815 h
1.01446542214580	10.90297250848625	2.47082352320224 h
1.66944993319790	6.66343768402920	0.64469446007907 h

\$end

B_{trans} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord		
-2.97035290775676	3.55352185057853	-0.13501053967836 c
-0.47841139945308	2.62566209733567	0.15026721157127 c
1.51119859032646	4.41721621663828	0.45341453816634 c
0.97376625060698	7.01254931841216	0.56011277559659 c
-1.47045483771051	7.89818959946250	0.21668061272643 c
-3.40831504068112	6.17635625245211	-0.17798061298349 c
0.66271681612232	-1.08335007995117	0.23653169955253 pd
2.48789010162063	8.35096978173362	0.91278760571158 h
-1.86393639562874	9.91220122857541	0.24685949685374 h
-5.30619486846580	6.85683546401493	-0.55202512826335 h
4.19478369973511	3.61634012178954	0.51654247277967 c
4.66961899195747	1.17270383623543	1.05687197576614 n

7.03583444923535	0.29218601746411	1.01785040011876 c
9.11013172825477	1.81611508565930	0.48189549904205 c
8.66284974902227	4.35588951138659	-0.06142833944562 c
6.19750142283798	5.26209512943217	-0.06304135945696 c
7.23119245203600	-1.71540663905583	1.42035667249932 h
11.00329318903905	1.02929123560276	0.45339894561454 h
10.21812180570824	5.61149622739678	-0.53062284365591 h
5.82904125331229	7.21420341888870	-0.56664842081346 h
-5.22338874281214	1.93115087166251	-0.61283206640663 c
-7.60842223282694	2.24399741633945	0.52865901189934 c
-9.70318161936007	0.80725274410703	-0.18944237340805 c
-9.47714956039922	-1.00985839360960	-2.07935214624126 c
-7.13888919401164	-1.39263276231665	-3.22635468954599 c
-5.07990296016340	0.06043322889688	-2.48955616558007 c
-11.49721145612272	1.09126897349678	0.75874441417136 h
-11.11840358544953	-2.11425209345885	-2.62840723653760 h
-6.91162406877252	-2.79040769360461	-4.71187924635341 h
-3.28164713001082	-0.18350895022507	-3.42190279958221 h
1.46348485966234	-1.20916554361979	-4.13695678342195 p
-8.32215359983634	4.77383236157628	3.57154247552919 i
2.56866356969188	-5.81525403359949	0.58733641130222 i
-0.53932587833452	-0.99226569090542	4.51769536759447 p
0.26170924188239	2.05725285876674	5.90023495087012 c
2.81069541877372	2.64424665119766	6.34807806585431 c
3.50173106384704	5.05059956067344	7.15997247086881 c
1.66777901048446	6.91384464709693	7.50306067040679 c
-0.86253312860655	6.35480596306773	7.02354391839550 c
-1.56153050078645	3.94391362940369	6.23147561918470 c
4.25944357115382	1.23883151231659	5.99978836393899 h
5.48266282234878	5.47484901303543	7.49331177714772 h
2.21234532994417	8.79630273951842	8.11575024876763 h
-2.30402040241616	7.80099870415648	7.23496540239658 h
-3.52802962672709	3.55323259577801	5.81389790570892 h
0.65072536624069	-3.32525250128344	6.80696208695434 c
-0.12083528296510	-5.84137696103883	6.46368177496394 c
0.58820612090691	-7.70268242051360	8.17935912553927 c
2.08685998706097	-7.08893927060527	10.26135506154246 c
2.84154740295109	-4.59346029436251	10.62852696234635 c
2.12175243893692	-2.71771978297327	8.91815821647830 c
-1.29585645067374	-6.33362867182242	4.85921935267564 h
-0.02393315405398	-9.63881294281109	7.87991395263855 h
2.64694212449575	-8.54499587167625	11.59611260729836 h
3.98063956579618	-4.08645944707310	12.26009813605415 h
2.67755982813634	-0.77963975203696	9.27316138096118 h
-3.90482811688199	-1.53367649403361	5.03565280743626 c
-5.21491318058790	-2.92172933354105	3.20779734421147 c
-7.68428084011599	-3.71691853968062	3.66524949379241 c
-8.86953792527541	-3.09318501541352	5.93314630296677 c
-7.56948303010876	-1.70497704399901	7.76454331528648 c
-5.08611075895999	-0.95466838017361	7.33621162222744 c
-4.26749138700811	-3.36604589632691	1.44029254505797 h
-8.68401176489096	-4.79797652803861	2.23738846609680 h
-10.80293556032850	-3.68968055130536	6.28206404776217 h
-8.48808582223997	-1.22531154999214	9.53659354918694 h
-4.05611908609885	0.06198533493144	8.79096446771488 h
0.01796355849328	1.19261894281430	-6.20648612385037 c
0.29815669398089	3.77336626448025	-5.65634568233403 c
-0.87777364648164	5.60313928664829	-7.13745508690209 c
-2.37664669886235	4.89272019668182	-9.18577441884238 c
-2.67647353798540	2.33635120297761	-9.74656538322232 c
-1.48992108336447	0.50075662334748	-8.27509586593325 c
1.40089667779932	4.36422839142029	-4.03875038913078 h
-0.64065731186302	7.58538407138532	-6.66070969077489 h
-3.31404635970821	6.31901260068548	-10.32650332644818 h
-3.84593329524364	1.75680826073501	-11.33147986526821 h
-1.76229898933689	-1.47833536124527	-8.72813099612127 h
4.83542660461576	-1.00320960740927	-4.92748770943490 c
6.37231907509286	-3.13149755408700	-4.53914371579336 c
8.95222694317243	-3.01949314857273	-5.04624248462171 c
10.04156861167491	-0.78568410300793	-5.92874140404738 c

8.52660672945498 1.33443996607525 -6.31242574373504 c
 5.93902879380183 1.22787036768390 -5.82368437533632 c
 5.53832329237721 -4.86171105787076 -3.82088386293173 h
 10.1112092742690 -4.68719441910981 -4.74384742022239 h
 12.05567126493979 -0.70051713983715 -6.31906452914826 h
 9.35150434070236 3.08310818954019 -7.00331195592402 h
 4.78585757252345 2.88525358842379 -6.16716968974969 h
 0.43627709723745 -4.13366934605214 -5.65258471658008 c
 1.55027392464728 -5.01340910955671 -7.88639526045414 c
 0.61724786052687 -7.17857535330036 -9.06457713014932 c
 -1.44826700619262 -8.45794709089964 -8.03858250767034 c
 -2.56962194202073 -7.58095077837487 -5.81745520979559 c
 -1.61896000519849 -5.43989686314093 -4.61870283138885 c
 3.14661578795767 -4.01074289307592 -8.69652160620565 h
 1.50376129751360 -7.86362839713668 -10.78491845249382 h
 -2.17006952625946 -10.14557719037001 -8.95847198393984 h
 -4.15750114561465 -8.58885935886699 -4.99466690727233 h
 -2.41986323141376 -4.78354125101671 -2.84646252213128 h

\$end

C_{trans} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
 -2.14452430854607 4.31027176801263 -1.39776404336971 c
 0.37253837018884 3.67092227748964 -1.95863312455076 c
 2.22613427093526 5.60779718934446 -1.92408770839947 c
 1.63193904920321 8.02665707342481 -1.01597506895441 c
 -0.81737528538245 8.57511900788529 -0.24265237391405 c
 -2.69713671866010 6.75144104380697 -0.50617139517840 c
 1.71760051125979 0.29650561838116 -3.05369887928716 pd
 3.06448622910703 9.49702049967896 -0.96680663677354 h
 -1.28816499468922 10.44460871771681 0.45973658573368 h
 -4.64699496526318 7.22548439820423 -0.06807370016748 h
 4.66579805091172 5.01291129324452 -3.07675613255270 c
 4.75368529846310 2.72342156060637 -4.26021915519047 n
 6.84625852775759 2.02468333524149 -5.51532515792969 c
 8.97499496021508 3.55464116172691 -5.65315737787352 c
 8.93789813196436 5.88392512361571 -4.41737167025345 c
 6.77186113774253 6.61414550813916 -3.12687231666065 c
 6.76304254783567 0.16703458063237 -6.38635440555795 h
 10.61999253800053 2.91832555753172 -6.69775375810039 h
 10.57890287341875 7.11608047062835 -4.45824971656922 h
 6.70486761809888 8.41466173820615 -2.15035683982098 h
 -4.32206816494325 2.58915967497266 -1.79240467749551 c
 -4.823633395041432 1.33281032739837 -4.08220771846649 c
 -7.06813954125606 0.00135104724426 -4.47167106008018 c
 -8.85414373624700 -0.15333188506023 -2.54124435165825 c
 -8.37601120879709 1.00661197069034 -0.22308631711428 c
 -6.15147841567895 2.36306396227053 0.12392927079743 c
 -7.40366457723721 -0.92237367013405 -6.26994534361731 h
 -10.59241491276415 -1.20011311365142 -2.85083650351357 h
 -9.72657971173759 0.85436297840158 1.31418483208084 h
 -5.76596211369326 3.25693644475784 1.93049581425389 h
 0.39061836986495 -1.99483381658196 0.29488978609536 p
 -2.24516190268891 1.39550005625684 -7.13712201605057 i
 3.55197902379751 -3.99874467691270 -5.13885066332197 i
 -1.30780774817946 -0.43757953083987 2.89201713259080 c
 -3.33938158638015 -1.54919032992095 4.17374435242401 c
 -4.46081238649361 -0.31650805102358 6.21599800900661 c
 -3.56501603968457 2.03414803557911 7.00373350220465 c
 -1.51535411056842 3.13586072178141 5.75826490000949 c
 -0.39065467945209 1.90602702016895 3.72245424331027 c
 -4.05323754212437 -3.37439459095064 3.57436633646232 h
 -6.03920726016193 -1.19854899980591 7.18921305552747 h
 -4.44920455423199 2.99822317680462 8.58619750410108 h
 -0.79514606384655 4.95981808565478 6.36449054153736 h
 1.20340091554364 2.76602905132159 2.76014626705805 h
 3.15077091843436 -3.10072089750705 2.08148031490563 c
 2.79008586024618 -4.52070633988445 4.29079415159427 c

4.85820064178826 -5.30229349050443 5.71707037466039 c
 7.30364541681360 -4.64714282436962 4.96767822175630 c
 7.66976682933653 -3.21554453627097 2.78653057328316 c
 5.60115599028917 -2.44858603485382 1.34348306929779 c
 0.88959910036459 -5.01045641929904 4.89292257211780 h
 4.56268177001061 -6.41385637931015 7.41773636308406 h
 8.91588321886545 -5.25248234991167 6.08575770589154 h
 9.56721217066168 -2.70401106841624 2.19308957568074 h
 5.86738137906742 -1.36386127629853 -0.37752062246876 h
 -1.44403665351685 -4.83449817043088 -0.33501719041122 c
 -3.99084611184960 -4.57583075491151 -1.00888404853008 c
 -5.41508823428672 -6.68918912539266 -1.66158228753232 c
 -4.30220768251781 -9.08118873843219 -1.66520297039107 c
 -1.76032911001959 -9.34502527776291 -1.01736350787899 c
 -0.32807341009974 -7.23375852648780 -0.36066894543286 c
 -4.85605647678470 -2.71941033940413 -1.02279024999980 h
 -7.38939210747739 -6.46134045121859 -2.17729777209824 h
 -5.40783125647476 -10.73105859068002 -2.18538489922490 h
 -0.87721531180316 -11.19779072109745 -1.04398227160096 h
 1.65797111376612 -7.44118949949527 0.09893782252633 h

\$end

C_{transTS} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

0.12800004671118	4.06397002306900	-3.72708740469283 c
1.92986551587954	3.08152148341138	-2.04773310016936 c
3.15069424259610	4.62847670886273	-0.27292264045020 c
2.43459959578814	7.17920960639152	-0.10707934065000 c
0.59866761350563	8.15369355985847	-1.72503590768361 c
-0.53412182806712	6.62200424422482	-3.54909649055979 c
2.88961108837253	-0.56680026289536	-2.31577946244548 pd
3.34715314445852	8.42272054098531	1.24873513453494 h
0.08314482114352	10.13591637179980	-1.59622883681573 h
-1.90446832178942	7.41886555154567	-4.85683627419090 h
5.18533228927096	3.48485600554930	1.22260521525169 c
5.97276626321301	1.19140512915410	0.37438905562396 n
7.88522498236351	0.00504352271844	1.52894365574537 c
9.12103428927490	1.01843479277257	3.61693972793659 c
8.29798502716414	3.34690499146331	4.54635234016918 c
6.31841033826171	4.58846211792947	3.34632945031060 c
8.39778665481163	-1.81844631002912	0.72705039913864 h
10.67660324991343	0.00626933994163	4.48918106623819 h
9.19123480110340	4.18414333581246	6.19402328479868 h
5.63684701378511	6.38889181920362	4.05136141510881 h
-0.94693697646872	2.24882187653377	-5.52465750255983 c
0.57169425709002	0.19069999241965	-6.32000773057691 c
-0.42009186092574	-1.78110345196568	-7.76304984115498 c
-2.96925826536277	-1.72171031579530	-8.43183184504928 c
-4.50186582842778	0.29908893006830	-7.70991820127574 c
-3.48969184769756	2.24956576757204	-6.25489242458705 c
0.78618360799499	-3.32878047485722	-8.35354900016800 h
-3.74824825852442	-3.26994132125954	-9.53143835602554 h
-6.48509370787411	0.33085065350729	-8.23229108745126 h
-4.69837662557294	3.77257142164263	-5.58799832567143 h
-0.33808609204868	-1.64856477675175	0.39086105402861 p
4.76224234922103	0.85254810987705	-6.94163799691256 i
4.59191349976493	-5.39932562628505	-2.74752848797785 i
-1.45883034522407	1.02934117791201	2.25572550943220 c
-0.50050879103108	1.44709720761278	4.68813341432346 c
-1.13274282828534	3.63707244214622	6.01181355122947 c
-2.72928590643470	5.42975625612533	4.92820612448308 c
-3.69489626061168	5.02390156212058	2.50628000030214 c
-3.06155312560020	2.84721502658140	1.17548469804941 c
0.74421226416866	0.06187970717498	5.54680904408349 h
-0.37492726933793	3.93367262646900	7.89691535578814 h
-3.21860943046248	7.13593563448198	5.95951984549530 h
-4.92672934780601	6.41781581696042	1.63929109325588 h
-3.79323539884817	2.56160104015885	-0.71754867193538 h

0.46492829887057 -3.95759094023251 2.82911651288493 c
 2.94685578783009 -4.08737874462431 3.73117010991592 c
 3.56155308758422 -5.72930478693464 5.69412851239537 c
 1.70705277903416 -7.28093713520343 6.74605302593194 c
 -0.76520485540570 -7.17843798783730 5.83372001036615 c
 -1.39186299411430 -5.51735605750899 3.88682114242104 c
 4.38991110070013 -2.92640476229648 2.85951784192758 h
 5.49607161044878 -5.82233276137414 6.37428059550580 h
 2.19055355659358 -8.58273596411508 8.25811395418553 h
 -2.21047347287613 -8.39812109673088 6.63258312479966 h
 -3.31549409284797 -5.44977040324393 3.17781295507216 h
 -3.13418076066220 -3.00161899744578 -1.09662307167290 c
 -5.60618843186766 -2.40343889587271 -0.34983149741257 c
 -7.65563654633467 -3.62601972813330 -1.46415894554399 c
 -7.25682703370033 -5.47679067575629 -3.30083043990748 c
 -4.79960644450564 -6.09992162011063 -4.02240510616672 c
 -2.74430515882168 -4.85672490235981 -2.94679600426194 c
 -5.92897491814987 -1.00377106619818 1.11315612741672 h
 -9.56442632329319 -3.14503526063457 -0.88021522060667 h
 -8.85774202080900 -6.43524106648986 -4.15778659445835 h
 -4.47525489632676 -7.54531313152682 -5.44358645914529 h
 -0.82439691080166 -5.33130586958895 -3.50504207997065 h

\$end

D_{trans} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
 -0.10550027775074 4.15729303100250 -3.66822085423901 c
 1.76340172299112 3.24202506207488 -2.04295079452450 c
 2.97010857845298 4.69822637147014 -0.20894496345530 c
 2.21621057121725 7.23675553612759 0.03043833909221 c
 0.35911756364901 8.20341208482266 -1.56997058461305 c
 -0.79307428839860 6.70315596081020 -3.41837197978553 c
 2.73314316467377 -0.36528618112310 -2.37550283232993 pd
 3.08030894499041 8.45908255739695 1.43546234808101 h
 -0.19612805123675 10.17048958483048 -1.38400410729427 h
 -2.21771301212267 7.52388226323992 -4.65034405840134 h
 5.01379693158880 3.45714965220168 1.17689296825671 c
 5.41724983872927 0.98971718945385 0.54189157073181 n
 7.42307996123525 -0.25244813343282 1.46262773808363 c
 9.08749387947645 0.84676469346736 3.16778457952011 c
 8.64104672722368 3.33125679933854 3.93470098068255 c
 6.60690553005190 4.64476899277156 2.92380887479521 c
 7.65633107782032 -2.17197176784109 0.76461754342694 h
 10.69183365067104 -0.22145754157584 3.86454675750108 h
 9.89350526258797 4.24707398914715 5.27817190910688 h
 6.26285284498961 6.59788730075401 3.44012415217628 h
 -1.04504346674961 2.24330656143584 -5.42617606589940 c
 0.13591556780876 -0.15157566264505 -5.23092750607705 c
 -0.44512868448905 -2.07693410378923 -6.90924913974951 c
 -2.30441969621082 -1.67302763461538 -8.74615672971448 c
 -3.54996063414795 0.64634797372361 -8.90991933672114 c
 -2.91197452864064 2.60334366445488 -7.26993951674834 c
 0.54941142333884 -3.86629913120260 -6.80973134958341 h
 -2.76561880128809 -3.18413884015884 -10.05842180310044 h
 -4.99453976886507 0.93829385806619 -10.33879814562030 h
 -3.84523945823697 4.42707761275612 -7.43194793675462 h
 -0.46734439887252 -1.66447094537310 0.50207243721215 p
 6.07293699085896 1.18858559895883 -5.84161510626247 i
 4.35582806715145 -5.33262382267059 -2.65885238078224 i
 -1.47661045252108 1.03051579646353 2.39022106499797 c
 -0.50953783675621 1.37003852821666 4.83168688767523 c
 -1.07531756944039 3.55409552624184 6.19345958096879 c
 -2.61309721894190 5.41398918464154 5.13853883791050 c
 -3.58255973992471 5.08761976616257 2.70677082630324 c
 -3.01174865256182 2.92009574282233 1.33329906852562 c
 0.68352977230195 -0.07193694123724 5.66890206866855 h
 -0.31408545139764 3.79225059287337 8.08498274856123 h
 -3.05118031799492 7.11511431889859 6.20047830070464 h

-4.76376345443632 6.53638382830034 1.86140629187861 h
 -3.73330030405165 2.70609341012389 -0.57114501567599 h
 0.34602385902206 -4.02168169121854 2.88787466020214 c
 2.80362315548992 -4.18821394159929 3.84557497210235 c
 3.36845268955705 -5.88606286967791 5.77411375417519 c
 1.48536429419759 -7.45560518994620 6.74520834639712 c
 -0.96580518521580 -7.30969634190978 5.78685081051101 c
 -1.54231833182078 -5.59697566257511 3.86940074963411 c
 4.27209950477391 -3.00964626196078 3.05456565342047 h
 5.28759649653442 -6.00536536751846 6.49180855014931 h
 1.93016968667298 -8.79973697741046 8.23151567999651 h
 -2.43772080739989 -8.53550777555526 6.52441100785354 h
 -3.45119996557079 -5.49945591737924 3.12867796068859 h
 -3.28886716746520 -3.00112334191197 -0.94096334587367 c
 -5.73824866399530 -2.16783764029892 -0.38571186425011 c
 -7.81887147874324 -3.38020105167046 -1.45841957808897 c
 -7.47201704076008 -5.43914710409434 -3.06543609977298 c
 -5.03380671895954 -6.29820946341664 -3.58896208549397 c
 -2.94913244849576 -5.08621192330441 -2.54215404989326 c
 -6.03326125804917 -0.60442858584780 0.90479704031601 h
 -9.71180264670207 -2.71754527951433 -1.02085544066309 h
 -9.09654195666717 -6.37903642034342 -3.89723063158658 h
 -4.74840656092657 -7.90990081681865 -4.82719189067349 h
 -1.04645146224893 -5.75833270341292 -2.92956986667908 h

\$end

D_{cis} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

-0.62292174643197	7.64998816822226	-0.12259980971429 c
1.39740550282597	5.96316534256423	0.03743748541011 c
3.92843009347494	6.66380380905428	-0.06525038180409 c
4.46784299399922	9.25387270484178	-0.34039281533473 c
2.49199181812907	10.98886328843654	-0.50483987333400 c
-0.03560946100346	10.21823620137630	-0.39610351009768 c
0.53995997285321	2.30321767921091	0.23869631810447 pd
6.40909767150095	9.91636929938644	-0.43338108190870 h
2.92507480130512	12.98306443094190	-0.72158219246760 h
-1.53127600605048	11.61994554089069	-0.52759477500079 h
5.77059960046003	4.61887690603417	0.14827318520682 c
4.77090859852691	2.24672325531361	0.36133810437854 n
6.31570203377303	0.27121347210684	0.70312874477779 c
8.92932723394346	0.50590241797260	0.78056939875772 c
9.98306153716985	2.90489905111909	0.50466543279710 c
8.39218643800383	4.96814687400948	0.20069262099486 c
5.41421635400914	-1.55219266519031	0.91545788345370 h
10.09064475167386	-1.16089581952430	1.05030848482087 h
12.01839144348187	3.16596685035929	0.54641286785121 h
9.15868483485614	6.85993403727467	0.01963417437772 h
-3.09238282453180	6.42938441757845	0.08142282657158 c
-3.03094187779480	3.77122883350114	0.39242350040873 c
-5.23220717794750	2.43593327057510	0.88383530902044 c
-7.55444386554760	3.70389948947845	0.91304700942144 c
-7.65569314926204	6.30471752032606	0.49405954355609 c
-5.43487121494256	7.66293910710016	0.10436356575526 c
-5.18382317531303	0.42495981717544	1.27911534479517 h
-9.27467138574539	2.64493448046244	1.28342113055857 h
-9.46176989803845	7.27986818550020	0.51502896177505 h
-5.50987167970097	9.69968513026548	-0.15466691148989 h
-0.66065731648925	-2.29006056468296	-0.01728557593642 p
0.53388028603904	2.83015268924472	5.23354683205733 i
0.73326152528557	2.56729454572235	-4.83871836101655 i
-2.75509121924940	-3.26339487234068	-2.59540386594690 c
-2.79519385565729	-5.80999938151222	-3.33667624492350 c
-4.44126235874368	-6.61977706637348	-5.22322667470022 c
-6.06578714335985	-4.89582135767088	-6.38733410332645 c
-6.02995585445887	-2.36369161670234	-5.66171844903518 c
-4.37640217295616	-1.54414105634282	-3.77981091374636 c
-1.53354717570281	-7.15507126708630	-2.43651265086731 h

-4.45260055119703 -8.59400735932096 -5.78598292512158 h
 -7.34535410751460 -5.52646763185098 -7.86395771824028 h
 -7.27169059004052 -1.00744893429822 -6.57325800753159 h
 -4.33207499962520 0.43227465642461 -3.25203974351768 h
 -2.18914671698443 -3.65207843293449 2.75997216741250 c
 -4.66008783677811 -4.60420715148355 2.64677556283185 c
 -5.83480623699916 -5.52348383032052 4.81870800105531 c
 -4.55524866994058 -5.51920538645784 7.12306292037182 c
 -2.09977887043726 -4.56933873584911 7.25395218299751 c
 -0.92973031186921 -3.61772755177140 5.09634418316500 c
 -5.66346738524515 -4.63174582167868 0.85887662100319 h
 -7.75129866361299 -6.24990428722482 4.70263387626375 h
 -5.47166744694867 -6.24047996600517 8.81237577845971 h
 -1.09931988951952 -4.53243638471643 9.04564497754851 h
 0.95190391902593 -2.81957656039920 5.23445024326493 h
 2.08114748513239 -4.32357451833699 -0.61451971867804 c
 3.34531552059071 -3.97698183479970 -2.92469904559805 c
 5.50443258608573 -5.37138923275048 -3.47905370806027 c
 6.43982491852892 -7.12333224789104 -1.73921519690969 c
 5.18295743264193 -7.48871277066755 0.54729943860196 c
 3.00741365548984 -6.10338136778885 1.10864536526074 c
 2.64310973333589 -2.58521616182372 -4.26230148564957 h
 6.46431135739286 -5.07917396114331 -5.26983961814658 h
 8.13103500494728 -8.20429472349210 -2.17017246142334 h
 5.88197327400168 -8.86483935689790 1.90115453246603 h
 2.03056045715505 -6.42541159514083 2.88136324397392 h

\$end

6 @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
 -3.87700227031424 7.33927335598809 -2.77789722308191 i
 -2.11042177430466 2.66943055311021 -2.70535990559054 pd
 -0.47430258959341 -1.36333590756348 -3.15055680090689 p
 -3.59293766433399 2.14957676562657 -7.50396572626782 i
 -1.00149448125777 3.16631352385396 1.44688032042756 p
 -2.64274673414038 0.91014777734750 3.47547718700519 c
 -4.52753214269363 -0.59855873742638 2.39667671999715 c
 -5.89229423200359 -2.30255276269748 3.87171566174622 c
 -5.38446135100146 -2.50212580960908 6.44965234682647 c
 -3.55629960414832 -0.94992123345320 7.55706525535368 c
 -2.21272145469371 0.77169353032037 6.08859356009481 c
 -4.91046233660984 -0.42030574511485 0.38811075471427 h
 -7.33959382945615 -3.46777980546076 2.99985863935245 h
 -6.43505844245661 -3.83307579095735 7.60684953920783 h
 -3.19834203713024 -1.06283278793426 9.57536104697344 h
 -0.86946107274343 2.04069403304887 6.97899576908716 h
 -1.58861821692534 6.08808947830598 3.19583718811947 c
 0.33428871967291 7.81998124611537 3.72750515721504 c
 -0.21029921637592 10.03000139243225 5.05896421976284 c
 -2.66796426954014 10.52028188030832 5.86730100924585 c
 -4.59426291903902 8.79556195438640 5.33542853179022 c
 -4.06412091274960 6.59752578068359 3.99737081785286 c
 2.25317143208960 7.45263917312045 3.10790239681986 h
 1.29535792691817 11.36571188168485 5.46265689996035 h
 -3.08707573863298 12.24247735896281 6.90280007289801 h
 -6.51737193631948 9.17592774854407 5.94306814455675 h
 -5.57162394220651 5.27741158524171 3.55770958756345 h
 2.41605446817006 2.81772274901583 1.76219239729735 c
 3.85245838371965 3.96588748489375 -0.15023829318422 c
 6.48145287045707 3.97165780914967 -0.01921014720648 c
 7.69996096731578 2.81627161876734 2.01393746452196 c
 6.27946006851658 1.64800870186941 3.90195507462703 c
 3.64780630360490 1.65005610137092 3.78551418650562 c
 2.88140395766634 4.86388495581364 -1.72431512583478 h
 7.57325922612481 4.87218222343666 -1.50590441200473 h
 9.75017659286679 2.80876383253541 2.11643099724256 h
 7.22077304505237 0.70947473167222 5.46585255117522 h
 2.57092351337195 0.69777266297501 5.24358458657736 h

1.51427333546561 -1.57240401272531 -5.96871088142494 c
 2.98280445637544 0.53898746493301 -6.60127152593488 c
 4.64798391013330 0.43685517169457 -8.63398443447143 c
 4.83276056433982 -1.76312420247830 -10.07910122515859 c
 3.35009109041277 -3.85642525104979 -9.47540784532915 c
 1.70553605268476 -3.77224616583240 -7.41679640677280 c
 2.76384981921295 2.27287740656914 -5.52473230480733 h
 5.76695963320332 2.08832567662883 -9.11705827351103 h
 6.10736292679705 -1.83432439960827 -11.68656993374737 h
 3.46047091799873 -5.56033339067387 -10.61514907234343 h
 0.53948465396116 -5.40056459970143 -6.97932836068085 h
 1.67464731806332 -2.70651847795191 -0.76234190614258 c
 0.71027761522982 -3.88572249208947 1.40809358032445 c
 2.33120683473034 -4.93832389045951 3.19507562732956 c
 4.94131572907327 -4.83764274336354 2.83971031554619 c
 5.91684510424117 -3.66081429345316 0.69308741117257 c
 4.30096496859236 -2.59721419691099 -1.09306818460214 c
 -1.31277007001298 -4.02483116329359 1.68446484131100 h
 1.54395157403567 -5.85308086422574 4.85583146604328 h
 6.20609724195621 -5.67266263985356 4.22471498810598 h
 7.94586380471342 -3.56501057381588 0.40003282354973 h
 5.08623149758647 -1.70361143835668 -2.76102303537847 h
 -2.85412474035703 -3.86467848192672 -3.35966021794342 c
 -2.16869195384560 -6.41610708902981 -3.11181122792045 c
 -3.99991030358787 -8.30454823414173 -3.23658008734113 c
 -6.53575373678014 -7.66756019042339 -3.58454137125457 c
 -7.23245309114170 -5.13524946612069 -3.81223368299312 c
 -5.40303663886764 -3.24334679925647 -3.70591787391766 c
 -0.20786085649232 -6.92415208573040 -2.78868611577715 h
 -3.44451893686275 -10.27218975157974 -3.05131031634189 h
 -7.96256114288454 -9.14129038603101 -3.67213992944903 h
 -9.20154803064174 -4.62374334701426 -4.08385057435735 h
 -5.93582785420900 -1.27325840309188 -3.92353671622243 h

\$end

3 @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
 -0.50286563465856 1.29017971813758 1.73554818101124 pd
 0.67686880634867 -1.29281837213758 -1.69228540707654 p
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 -1.70949041359614 3.25809606306618 4.67761700964476 c
 -4.27320978447547 0.37941184456608 1.68083310509138 c
 3.95122610884035 -1.18804279363462 -2.82739003355028 c
 0.25150930052450 -4.68742583638441 -1.17370711336232 c
 -1.10039714845488 -0.50126724560824 -4.55833255675068 c
 2.59909920919604 4.68463177768845 5.03601495961807 c
 5.22514932313124 3.13763655374888 1.83533522525466 c
 0.02825500650221 4.71009342952981 6.04097148888474 c
 -4.26179999895449 3.11424358286619 5.37967237808508 c
 -5.72491488744353 1.49979141289351 3.66837814421548 c
 -5.57521048558095 -1.14521063673246 -0.04095767285226 c
 4.67073683729722 0.42514330075410 -4.80082239367294 c
 5.82847748645505 -2.54148200802274 -1.52695563450174 c
 -1.17745240745036 -5.47145504668190 0.91312744599600 c
 1.33485280569278 -6.51654576424135 -2.76183672926522 c
 -2.15312422850852 1.92658365938818 -4.67204750507363 c
 -1.43023003176073 -2.15569075920607 -6.59718558150318 c
 4.62881820385767 6.05109886880838 6.04461307444880 c
 5.38612721214890 1.96522373888228 0.16699667146809 h
 7.30018933425966 4.46418638552085 2.74914749679311 c
 -0.80283346630563 6.06100570775754 8.17947473931353 c
 -5.06850871865789 4.46482532646023 7.50674744209768 c
 -8.32277503479740 1.05720480785060 3.86758480845673 c
 -4.58253779374579 -2.0383843190557 -1.59924296462965 h
 -8.17849021015967 -1.58016731932519 0.16374833620070 c
 3.23838791871772 1.48193822347242 -5.82219841745792 h
 7.21110070338140 0.67858230971641 -5.46005277453014 c
 5.29754203581747 -3.78713890379107 0.01622984262897 h

8.36210185978080 -2.29217207869056 -2.19575792484785 c
 -1.98217658022317 -4.05238613538668 2.15877373125684 h
 -1.56084403854884 -8.03832895321899 1.37308820541357 c
 2.52094051466228 -5.93610714213019 -4.33334975698862 h
 0.94748427485879 -9.07844506641381 -2.29822498134135 c
 -1.95936413551459 3.16868345027523 -3.04474876603414 h
 -3.48672743506580 2.70102934937394 -6.80789273419730 c
 -0.66194488493361 -4.05536240391833 -6.51734016184081 h
 -2.78303831144495 -1.38539188676885 -8.72143011245721 c
 4.32685296395583 7.19997612053661 7.71495029267954 h
 6.99129767925678 5.94310218305310 4.90751213713623 c
 9.10060308243409 4.32441205276164 1.77958146256006 h
 0.49460452281276 7.20780477627059 9.28587046710626 h
 -3.33507820380198 5.92021428064076 8.88525252831274 c
 -7.03215275922002 4.40013027075777 8.11161244997485 h
 -9.39296868462658 1.92822498423533 5.39219128926544 h
 -9.55698250204356 -0.48338707947980 2.12060180278187 c
 -9.11753775387198 -2.77994464998520 -1.21577552745873 h
 7.74021711094211 1.93234400944491 -6.99741300506104 h
 9.06293215600927 -0.67622480183790 -4.16170912572242 c
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 -2.67614396803794 -8.62256392396329 2.99418991561486 h
 -0.51044511033519 -9.84288651126668 -0.23457456198356 c
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 -3.80417846599813 1.04553653681916 -8.83444608168143 c
 -3.04729317280683 -2.68633884992671 -10.28781325870865 h
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 -3.97976958696504 6.95922801913856 10.53475354024248 h
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 11.03924166435737 -0.48096279381916 -4.68096472266375 h
 -0.80666198133884 -11.84218211377778 0.12698002243510 h
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\$end

C_{cis} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
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 -1.63972797466246 5.25183941628658 -1.28048845222083 c
 -0.16236193671843 6.49119778424109 -3.13497219541697 c
 -0.59822688893350 9.03822998401719 -3.74438495047686 c
 -2.45994976749553 10.38639134224395 -2.48231429562421 c
 -3.84883248291101 9.21172028864333 -0.57581276850106 c
 -0.64465811661741 1.61254666551622 -0.67594300060412 pd
 0.54729218166752 9.97780759268212 -5.16640332211422 h
 -2.79652910282409 12.35978846493685 -2.93283279299021 h
 -5.24250275171427 10.28934317676444 0.48116030943168 h
 1.88682625490301 5.03727559245496 -4.26910962130046 c
 2.36913477814938 2.76449663504326 -3.13393299235441 n
 4.23801117150521 1.29656362989217 -4.03886888793705 c
 5.72600391941939 1.97736612088098 -6.08631706502058 c
 5.25206174087973 4.28604775641780 -7.27013453437741 c
 3.32609144733676 5.81143415964981 -6.35299769019379 c
 4.52723058116352 -0.49089972968246 -3.08328560336273 h
 7.20737947042513 0.71519303647959 -6.72929314925297 h
 6.35901434153468 4.87910341411756 -8.89321514528334 h
 2.89864505657585 7.59740419269292 -7.26185263295737 h
 -4.99477854333745 5.60332987495058 2.14819018683712 c
 -4.00160386248921 4.28170507659294 4.22072447639362 c
 -5.52349968306017 3.32204536209094 6.14361241021717 c
 -8.12974043954231 3.68990826086223 6.03890830396394 c
 -9.17743056086551 5.03491159425391 4.03088180102633 c
 -7.62523496133156 5.97560307382413 2.13196724238906 c
 -4.67899458039657 2.30702779631169 7.71187476370982 h
 -9.32163453420366 2.92822845356075 7.52609831579959 h
 -11.20666818396464 5.32016335792705 3.92340004139392 h
 -8.44654452253857 6.95334236711726 0.52570990119719 h
 0.67906890755523 -2.51632200714160 0.29256467013785 p

-0.06255280074646 3.62037690923119 4.55880038338467 i
 -5.38419220110656 0.08841261485086 -1.32695225445599 i
 -1.48629843706136 -4.59708849059023 1.98261159528563 c
 -1.70975668261475 -7.17023732100507 1.42079818809019 c
 -3.35276582540893 -8.68936995964454 2.81776110580932 c
 -4.77016373325885 -7.64757095988387 4.77966156544095 c
 -4.56015001262960 -5.07548328557251 5.33537951860027 c
 -2.94001606130044 -3.55145360616099 3.93458163118425 c
 -0.61915500314016 -7.98079268373518 -0.11698916448783 h
 -3.52878918791184 -10.68388661049927 2.36359951295069 h
 -6.05446308537058 -8.83079817985309 5.85942964355116 h
 -5.69139297289354 -4.24780925837822 6.83513722445006 h
 -2.81837893381142 -1.53935598134853 4.31566684678287 h
 3.49840569870413 -2.57091555946179 2.30940518592769 c
 4.07837594766227 -4.62999340263432 3.87133823065599 c
 6.23944776309656 -4.58871988365083 5.37883559659394 c
 7.84150683222334 -2.49352608658647 5.34507904390285 c
 7.26913758684399 -0.42834953924616 3.80785041847601 c
 5.10406185153685 -0.46271971872734 2.30750827320888 c
 2.81984847992553 -6.25036028935431 3.92551886597190 h
 6.66466440822378 -6.18973177346587 6.59184077565465 h
 9.51792486491427 -2.46169407130740 6.52960141589677 h
 8.49447459507195 1.21890327254498 3.79270973455555 h
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 1.60538558712939 -4.34475917264991 -2.48926320766158 c
 0.01202410581749 -4.20429764315139 -4.60657235397904 c
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 2.86751927234839 -6.90109014247443 -6.94439179016021 c
 4.46481066535829 -7.03128297880179 -4.85147127344988 c
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 -1.70249288111445 -3.07379978681586 -4.49810118919345 h
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 3.36022184270068 -7.88910816121194 -8.67547542102027 h
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C_{cisTS} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
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 4.61813910701532 7.95169292419526 0.48230081276339 c
 2.69085013988455 9.73514044046309 0.29933666731087 c
 0.16975620054111 8.97354337017000 0.13203076701163 c
 0.65237109107451 0.91885730742327 0.18778854194316 pd
 6.56195899380270 8.58751993127363 0.67088872983175 h
 3.15148468226461 11.73465474079495 0.32528754387716 h
 -1.32736874702545 10.37864555857046 0.05095856780651 h
 5.94259098660840 3.35242578339272 0.71986684739511 c
 4.98751637318853 0.98415104386736 1.04826066752916 n
 6.57606405462527 -0.96139862137632 1.35608026464841 c
 9.19014348801036 -0.69448588608815 1.33903662039291 c
 10.19408941594142 1.71434830719576 0.96721660332699 c
 8.56152942497352 3.74558609287874 0.65728065416032 c
 5.70863625697781 -2.80158713028535 1.60819188882689 h
 10.39088180940660 -2.33590362419090 1.59827162198796 h
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 9.30022669354527 5.63239509182043 0.34847412568835 h
 -3.00305605628619 5.36472372453161 -0.03621601961946 c
 -3.52739869760016 3.01026975375001 1.12000969031191 c
 -5.84733426401165 1.79251469631082 0.80756150905433 c
 -7.68251277222328 2.90200588596094 -0.72526968222199 c
 -7.22675113901185 5.23442617333236 -1.87129860736186 c
 -4.90686517608581 6.43510136530360 -1.52866213666552 c
 -6.21859283528631 0.01553554334314 1.75949202777719 h
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 -8.65994420807118 6.09925001508672 -3.05757244390808 h

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-4.49791403043503  8.18826590108626 -2.51697283292379 h
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-2.66047424766300 -4.52103070278808 -2.36292458076808 c
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3.40556774200133 -3.06975903281934 -3.99955518446331 h
7.14340134743515 -5.60477326629423 -5.23261085918279 h
8.33508923904759 -9.41842993146352 -2.74831176797486 h
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\$end

G @ RI-TPSS-D3(BJ)/def2-TZVP

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9.52291453727229  6.27095825824003 -5.89166274422603 h
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-3.23517280800765 -3.04870009406080 -0.95267797748296 c
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-3.18312785408101 -3.25753944056719  3.63453312787253 c
-4.96684548949257 -5.20358257123210  3.55935357634286 c
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-5.00435054496007 -5.02799069775486 -0.99446839099214 c
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 2.14795551851372 -5.48734148770763 5.93927754924147 c
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 -5.54919825976857 12.17395137848662 -2.07184108010593 h
 -5.46057311682796 8.64495638471247 0.95634639253394 h
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 -6.64370302141426 5.29445773680689 4.59137544801038 c
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 -9.65269797088111 -0.85980200316192 0.67791476830939 c
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BK_{cis} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

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9.07618986415409	1.62531060160914	-3.06724805876057 c
9.26811873009545	4.23312130445739	-3.40006230458487 c
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 -0.57879868500993 1.24181537012317 7.62305271481336 h
 2.97952396788611 1.61556865260916 10.61595454344034 h
 7.31733694576131 2.46733280380774 9.03838008306547 h
 8.07492633213797 2.93934425344109 4.42144935490075 h
 4.50909302701056 2.45051432147080 1.41304958215967 h
 -2.19592784232587 4.83784256045235 2.84878605429287 c
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 -1.61509553471017 9.38736456273622 2.85172321999019 c
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 -6.84286252198466 7.75799594953383 6.20782253224871 h
 -4.44162960252341 11.55685836281390 4.83172784310545 h
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\$end

BK_{cisTS} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

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2.95179728731368	0.71734774321547	-4.86850036305924 n
4.92229645464099	-0.84797175910346	-5.19700744501052 c
7.11907900955700	-0.14276004657386	-6.44932668666823 c
7.28118106432288	2.31246010679415	-7.39849632848404 c
5.25664170895683	3.94750783680843	-7.06325705128501 c
4.71108940802627	-2.73534842842545	-4.42569011647205 h
8.65010624194225	-1.48720411481074	-6.67185183244435 h
8.96679977150305	2.94424149834747	-8.3828357952865 h
5.35330209561877	5.86785524703515	-7.77065583757976 h
-5.26394406319595	3.65777632751587	-1.96124577530348 c
-5.17113354333329	0.98550055515049	-1.95424562036266 c
-6.93664643090559	-0.46881252995458	-0.64385496448183 c
-8.82029788790684	0.75315453723385	0.73634069561990 c
-8.94755228923148	3.39100952445981	0.79074278249004 c
-7.17236406587594	4.81636839192111	-0.53173602952527 c
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-10.20596657055165	-0.37989423223826	1.74060812560438 h
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-4.12381029604984	-1.02414316674496	-5.80832377216402 i
0.42989751308236	2.34717491333332	1.59421487875403 p
2.04662659056898	-4.76915977184284	1.68912064200555 c

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6.19640095005053	-3.89378403096467	3.44096162535634 c
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-0.16041040663871	-7.53863556043186	3.72247584352486 h
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7.96622787464328	-2.85917151790354	3.35815656673048 h
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0.93098384502270	-6.26392303179947	-3.33601716294249 c
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3.14843283500144	-11.02356989703573	-8.47678116567837 h
1.93855994655802	-6.64649951663969	-9.68146063589183 h
0.53573528727406	-3.62263347732486	-6.40488167396410 h
-3.14523060470750	-5.53457217446767	0.12814341424874 c
-4.09430757938432	-5.07465385241780	2.55938933366331 c
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-7.90450590652684	-7.37422284210286	1.52949876836457 c
-6.97816018226988	-7.81960189336642	-0.89972730432654 c
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-2.99429756764140	-3.98801660794856	3.90135490850879 h
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-8.09935486875636	-8.87963365145035	-2.25215532409804 h
-3.88710839993427	-7.27623707754043	-3.48747389993315 h
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-0.98915148021029	-1.80368373803005	8.02370552809893 c
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-1.04879062639276	3.72605615380338	-3.77237712224906 c
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-1.69542311881092	8.46915551196460	-5.90701936068680 c

-3.62521246249506 7.42725911478076 -4.44416169697200 c
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 \$end

F_{cis} @ RI-TPSS-D3(BJ)/def2-TZVP

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\$end

F_{trans} @ RI-TPSS-D3(BJ)/def2-TZVP

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 5.87424921428044 -1.74471774847141 6.07918825539394 c
 5.87746843237270 0.70601450314762 7.05345792796525 c
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BB_{cis} @ RI-TPSS-D3(BJ)/def2-TZVP

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BB_{trans} @ RI-TPSS-D3(BJ)/def2-TZVP

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\$end

CC_{trans} @ RI-TPSS-D3(BJ)/def2-TZVP

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CC_{transTS} @ RI-TPSS-D3(BJ)/def2-TZVP

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BB_{transTS} @ RI-TPSS-D3(BJ)/def2-TZVP

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Send

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\$coord

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BB_{cisTS} @ RI-TPSS-D3(BJ)/def2-TZVP

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CC_{cisTS} @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord
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B_{cis} @ RI-TPSS/def2-TZVP (no dispersion correction)

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-1.85566885006846   8.79088657923438  -6.14159659552674 c
-3.81200790018374   7.30752749096786  -5.22466069624508 c
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3.86509085406589   5.54012381792191  -3.51227415709275 c
4.75533827616742   3.17365313774121  -3.18643951000710 n
7.23146960707732   2.85965125500645  -2.75475881042798 c
8.96895082281041   4.82439882592078  -2.57991506755475 c
8.05117173433148   7.28347380410799  -2.80173514499017 c
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 -1.51358115612567 -5.76803774470552 -3.50775916525500 c
 -4.09466089098163 -5.32657811280488 -3.09628242188208 c
 -5.91441696665529 -6.73390870403448 -4.38073750906410 c
 -5.18534821806324 -8.56644244549443 -6.13081722445310 c
 -2.62339991999242 -8.97789923446234 -6.58788193804726 c
 -0.79745180979247 -7.59743417391974 -5.28014956985933 c
 -4.68104784092625 -3.86349316271566 -1.78119925457847 h
 -7.90726227334287 -6.39018474634963 -4.02209907442677 h
 -6.60481866133947 -9.64793082337442 -7.14660428690018 h
 -2.03371842377022 -10.37255726588462 -7.97513744519609 h
 1.18653627275458 -7.92531924069677 -5.67563693153647 h
 -2.45875978057384 -0.21778196505809 3.89279171699574 c
 -1.90839770010018 -1.35388973827466 6.21964505477003 c
 -3.76565696693078 -2.70786201336365 7.51312468783513 c
 -6.18983201539248 -2.93822823932727 6.50634514087886 c
 -6.74638231763799 -1.83235155831350 4.17691176142691 c
 -4.89152599317473 -0.49325770879712 2.87027597056481 c
 -0.02914063720322 -1.20109663865209 7.02396574927395 h
 -3.30576481991763 -3.58971198212999 9.30961615714871 h
 -7.63391566464742 -3.98645092191172 7.52302568518728 h
 -8.62474955063305 -2.00738652861607 3.36674522463461 h
 -5.33410398644672 0.35730107985572 1.05425706275342 h
 2.83143608126358 1.45565692244701 3.81876430699256 c
 3.13451340215651 2.39545894234845 6.28529671877694 c
 5.45222213068348 2.19184413283724 7.51773934985652 c
 7.51237919437216 1.08108233393165 6.29600310320419 c
 7.24129099538027 0.18278227428639 3.83506094617321 c
 4.91344140402386 0.37085967695457 2.60686472750619 c
 1.56308871669243 3.31601091246349 7.23183478793653 h
 5.65552855088881 2.92232351072744 9.42629119388676 h
 9.32461429676798 0.94311236851186 7.25224083722284 h
 8.84317751052094 -0.65359634461186 2.85901320254847 h
 4.70062202405273 -0.28618750629481 0.67436449464356 h
 -1.06412504082660 4.95781195869963 3.22696448714651 c
 -2.93730546391529 5.38213555484573 5.04883367741592 c
 -3.30798159382426 7.79801349190508 6.04496946499839 c
 -1.82621834377712 9.81422670967814 5.22706466173106 c
 0.02427436902032 9.41123301458172 3.38877356508478 c
 0.40488148903724 7.00433747789547 2.39763667790171 c
 -4.10400516207385 3.83174721741564 5.71048942305936 h
 -4.76894832392223 8.09410804973690 7.45721977943157 h
 -2.11682059260413 11.69256464044946 6.00455550290767 h
 1.17989807452551 10.97428854993463 2.72674105375335 h
 1.87019439288104 6.70783819277579 0.99539918271458 h

\$end

BB_{cis} @ RI-TPSS/def2-TZVP (no dispersion correction)

\$coord
 -0.46922713880075 -4.89719914203633 -4.09904952499592 c
 1.33764296689443 -6.63183066179716 -5.02145842692096 c
 3.16634601226644 -5.91515014434738 -6.81895593907253 c
 3.18377547292783 -3.40599802033179 -7.68067294876870 c
 1.42386458928953 -1.66841814206589 -6.80848078026962 c
 -0.37143184558593 -2.42120178417496 -5.04299269375821 c
 4.61833046506139 -2.86512280456250 -9.04390937638633 h
 1.43764052772940 0.26187310456882 -7.50735955282301 h
 -1.76217779071050 -1.07716320665100 -4.36387090586670 h
 5.14482390698418 -7.60430726812749 -7.90462107220859 c
 7.51918239320188 -6.68439617446675 -7.85845646794125 n
 9.35962723333675 -8.08277577306115 -8.89391690463901 c
 8.95070053991438 -10.41275128489492 -10.04917926724396 c
 6.48202079336681 -11.32867238029232 -10.15187274397019 c
 4.55301233136077 -9.91331962212125 -9.06398087894681 c
 11.25268139406673 -7.28168420669247 -8.79325772412566 h
 10.51685089409830 -11.46369030500273 -10.85873696871375 h

6.06232636762911 -13.11663235847944 -11.07064517350588 h
 2.61099349364877 -10.56523546816861 -9.12336415568928 h
 -2.52218550649093 -5.54941923070390 -2.27880149907481 c
 -2.87361041066965 -4.27717311846313 0.03908309700810 c
 -4.83699985537477 -5.08112486381125 1.62785265531427 c
 -6.47595178178004 -7.02755582169749 0.94184435827919 c
 -6.19295324050545 -8.20945624573972 -1.39610876122984 c
 -4.22642684399612 -7.47133253761016 -2.97461741645882 c
 -5.09892662076726 -4.17790912839244 3.45451814995577 h
 -7.97611735225426 -7.59876481436413 2.22510766418003 h
 -7.47752554324188 -9.70133171841256 -1.98012143569453 h
 -3.97824344559959 -8.39475415028555 -4.79315494136074 h
 -0.59817113666538 -1.39507212264991 1.38473496992946 pd
 1.51672831963406 -10.31124812536869 -3.41153250285283 i
 2.69447737199268 1.41921930276651 3.15610328372557 p
 -3.80419030512925 1.51113329810980 0.65893176512515 p
 2.46016581425234 -5.20582948643138 2.58810192114063 i
 3.90147359834159 0.24159890843949 6.20421124748975 c
 6.44520125633601 0.40568621321583 6.90812612927428 c
 7.22706924721115 -0.42900891821177 9.28490639113964 c
 5.47692290627440 -1.41236445530177 10.99234711181565 c
 2.93702727169052 -1.58748459722022 10.30246997215906 c
 2.16048180956715 -0.78655628429083 7.91753483003315 c
 7.83455046923406 1.14201687795324 5.59188033288193 h
 9.21372613816308 -0.31777427032135 9.79360320014434 h
 6.09179025630044 -2.06458406276205 12.83990972656520 h
 1.56570529970389 -2.38905232824526 11.60401611218835 h
 0.19895340940130 -1.00123037408318 7.35338469114284 h
 2.18090037001505 4.79951330699759 3.94515150136395 c
 1.72648704054817 5.58987930990247 6.43431694428899 c
 1.33865325861741 8.13837248359457 6.99072963844097 c
 1.39089861949448 9.94595192774293 5.07459604337981 c
 1.82629044606780 9.18273914659550 2.58792337353908 c
 2.21462930152669 6.63783678119329 2.03076292546092 c
 1.70966635287076 4.21717595560231 7.95751888260980 h
 1.00839151080198 8.70606401576246 8.93670240854210 h
 1.10600906663319 11.93180625050979 5.51374159156931 h
 1.88249044877641 10.56996322244500 1.07408155165079 h
 2.59770642482505 6.09101101541602 0.09298556320395 h
 5.46545866102668 1.65262109331533 1.05907259032370 c
 7.33910413406131 3.50345197058890 1.41717379637696 c
 9.43417748438612 3.61080209660565 -0.17593331302239 c
 9.68627482585826 1.88169655066566 -2.15442138915084 c
 7.83002144390571 0.05182496422173 -2.54083269363764 c
 5.73086553975418 -0.05865773680949 -0.94626842578007 c
 7.15215236212626 4.87689841096059 2.93057233358187 h
 10.86974412802291 5.04762020762916 0.13087299627838 h
 11.32365378889258 1.96700510663632 -3.39172008009259 h
 8.00538364500459 -1.30709588335420 -4.07032150554066 h
 4.30558401267854 -1.50537829737435 -1.23760310949666 h
 -3.26378597325691 3.82022140441471 -1.88394383257459 c
 -0.87436732450321 3.97640996082563 -3.01064338810904 c
 -0.42324482355029 5.67897392677799 -4.97469113925039 c
 -2.36228858052301 7.24050783173518 -5.83837633605424 c
 -4.76059794996420 7.08231617007413 -4.74626147116189 c
 -5.21544737837443 5.37604048426112 -2.79225105331893 c
 0.62087798172869 2.72483552854988 -2.36312149610321 h
 1.43963895213428 5.77096069797708 -5.83438897460447 h
 -2.01698678350264 8.55968607497538 -7.37378903557831 h
 -6.28544739044051 8.27564156449061 -5.43020972450727 h
 -7.09948970259204 5.22741941761949 -1.99074445171721 h
 -4.45086795299263 3.35535220039977 3.53440948425249 c
 -4.93509638195941 5.95603039876068 3.55345132558006 c
 -5.56157486427604 7.17607951860826 5.80663640174333 c
 -5.72321486239843 5.81679307795183 8.05868790346545 c
 -5.21898355916208 3.22736863315380 8.06243825730397 c
 -4.57065122546501 2.00992433979522 5.81858419777623 c
 -4.80932476347221 7.04105364301228 1.81783824887609 h
 -5.91728360602093 9.19835137469143 5.79631274950035 h
 -6.21939948687736 6.77278432952154 9.80693698759073 h

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-5.31895731498409  2.15608734415668  9.81148921877345 h
-4.16130423370147 -0.00457095439426  5.82186658887693 h
-6.99915693158489  0.38603260574732  -0.17514196610287 c
-9.06077248139771  0.57748302444790  1.47410234363637 c
-11.43945130302195 -0.31158675578671  0.75288087489041 c
-11.78855480340672 -1.39895796279863  -1.61906698263907 c
-9.74380269579448  -1.59615277528097  -3.27635118992300 c
-7.37134269054537  -0.71691727768000  -2.55999750486097 c
-8.82682539181004  1.42693600059824  3.32522742755685 h
-13.01776458339682 -0.14484644952707  2.05636125378614 h
-13.63865589404896 -2.09414826106384  -2.17599112631878 h
-9.98963751568542  -2.45391861948443  -5.12508297134996 h
-5.80073508335515  -0.90024469879003  -3.86582179029903 h
$end

```

3 @ RI-TPSS-D3(BJ)/def2-TZVP (UKS triplet configuration)

```

$coord
-0.49736404876538   1.30105873562000  1.74742388205849 pd
 0.74414389077187  -1.28539830069939  -1.69839441981040 p
 2.88967236079392   3.21237936898802  2.88078191312427 n
-1.72084838952370   3.24296240093659  4.68377399921981 c
-4.23172003391821   0.37808919768951  1.64760483253057 c
 4.01012390703300  -1.20943103426000  -2.84473029692501 c
 0.28863876009869  -4.67524733191276  -1.18547374077128 c
-1.05714022685059  -0.47962788589363  -4.54369239377897 c
 2.52943106903196   4.69506440463653  5.05729114358417 c
 5.17383564185890   3.20901409122961  1.78475234382373 c
 0.02433691224861   4.69698330444236  6.02815721084929 c
-4.27517392593558   3.05688648029371  5.36684545822038 c
-5.69540696945299   1.49153860720361  3.70779104241368 c
-5.56642473093267  -1.10024305449846  -0.07863105786848 c
 4.72703256158909   0.30626158565552  -4.89274887126965 c
 5.88084143146261  -2.51604960693448  -1.48926332006256 c
-1.13474097879032  -5.46369499551359  0.90307635338437 c
 1.35738668802440  -6.50071280964204  -2.78772045749074 c
-1.94793983527215   2.00960949844527  -4.71827157988193 c
-1.57204920377616  -2.18175464265405  -6.50292980447484 c
 4.59728150091456   6.06257542911894  6.06994369242729 c
 5.34835621622750   2.06657949115281  0.09599545272876 h
 7.24046573518453   4.54584513931602  2.69601459869350 c
-0.91178932910979   6.05106432689855  8.22573340672868 c
-5.18489369168287   4.42909115958633  7.57803046173100 c
-8.32727290835617   1.02428368866550  3.94154186743052 c
-4.60182294664075  -1.96616641253654  -1.66809101797698 h
-8.17106873256762  -1.53696584570693  0.17058048141141 c
 3.29819963242788   1.32723547033950  -5.95410329087390 h
 7.26659916527195   0.51027921075211  -5.57328845159762 c
 5.34831019631631  -3.68064153256556  0.11548920929049 h
 8.41193570687006  -2.31514448180463  -2.17921417061855 c
-1.91983070520163  -4.04852089595907  2.16506943964867 h
-1.52871898187335  -8.03092813237598  1.35209149420682 c
 2.53874189012806  -5.91456203138847  -4.36066490990701 h
 0.95859254980388  -9.06345541907404  -2.33609937870147 c
-1.60819145615383   3.30092026402765  -3.15447569766983 h
-3.29847183292111   2.79565925884155  -6.83884842024042 c
-0.93347348235315  -4.12625619671338  -6.37095977459972 h
-2.94486425061661  -1.39849320137257  -8.61048530711676 c
 4.30702933753061   7.17818485766909  7.76679300299255 h
 6.92901737378227   5.99498862702699  4.91495929419373 c
 9.03201805675875   4.44502608363476  1.70778252392775 h
 0.35439571750654   7.21880381254642  9.34410828832732 h
-3.46501716880293   5.87361527964371  8.92790946058762 c
-7.14963235251074   4.31731855580957  8.15400947405069 h
-9.37695675969519   1.86655482992348  5.49171880447157 h
-9.54433610866219  -0.47988916287702  2.18323392744451 c
-9.13640842974841  -2.71514185488604  -1.20869103191569 h
 7.79826861361504   1.69096858461270  -7.16641174263747 h

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 9.11326347163025      -0.79668079334256      -4.22128747187935      c
 9.83996659093209      -3.33616922111669      -1.11510122573411      h
-2.63496137769037      -8.61965642791996      2.97781047013489      h
-0.49412568789838      -9.83176287941369      -0.27059693144500      c
 1.79239998404848      -10.46164179760838      -3.58723040072979      h
-3.98295265060317      4.72735816911342      -6.95370109536083      h
-3.80029340013489      1.09139118855487      -8.78682793079374      c
-3.3515147655347      -2.73517240766613      -10.11498762226070      h
 8.50414968094308      7.05312407994631      5.69876839731341      h
-4.09942142759617      6.91109886157202      10.58341569350400      h
-11.55953547121537     -0.83999613634518      2.34564889047690      h
 11.08901418971982     -0.63520517507907      -4.75373113784975      h
-0.79664066577929     -11.83145851079271      0.08305457675319      h
-4.87244590593890     1.69425413466032      -10.43054813544116      h

```

\$end

[{C^N^C}PdPPh₃] @ RI-TPSS-D3(BJ)/def2-TZVP

\$coord

-0.46232514815002	1.10939070061242	1.73803708584297	pd
0.77915141621946	-1.02204979089798	-1.69961205193712	p
2.81117630539010	2.91653375912581	2.98395835677585	c
-1.89764321565281	3.12276382981925	4.65852554833384	n
-4.20647377928012	-0.15574414600726	1.64326979138268	c
4.07185585849528	-0.95158841725831	-2.75731858680328	c
0.19433016145800	-4.41352745287774	-1.31912479656093	c
-0.85284742613696	-0.05815066900409	-4.59752243551018	c
2.28999029949205	4.59670373678625	5.03576921449203	c
5.34825412176170	2.71713230399187	2.26513718265899	c
-0.33410129436411	4.71495027084796	5.91107364881340	c
-4.39430218088877	2.88803890409073	5.16890205636572	c
-5.68753351095045	1.03959692583223	3.55931124664454	c
-5.46381232212952	-1.94509246589868	0.14976196393124	c
4.97049413550260	1.20477204727376	-4.01281939733625	c
5.75719966771994	-2.90709009834214	-2.18256735355633	c
0.16611109210385	-5.35959732740521	1.15434048991834	c
-0.19788596942801	-6.06863099721734	-3.34570633369336	c
-2.98092864534971	1.50569197808767	-4.43134490833545	c
0.00875001536767	-0.81912647522642	-6.98961879429993	c
4.20564075585255	6.00982659310494	6.20120862239833	c
5.88487878506326	1.44182575672852	0.75468039602557	h
7.26459407602579	4.11454763862011	3.43444747069166	c
-1.33099879434455	6.21824146435989	7.84750962846103	c
-5.44543579181445	4.36321027409649	7.09745549728405	c
-8.25033417131645	0.45250285536547	3.90338929280627	c
-4.44873412818737	-2.92919143430041	-1.33993902566406	h
-8.01555027850226	-2.53597953116132	0.49110878316860	c
3.68263142836976	2.74671286855357	-4.43361830015855	h
7.50306374705653	1.38651411140580	-4.69818447260767	c
5.08353719929773	-4.57900203874509	-1.20274283379728	h
8.29835106297610	-2.71434280633121	-2.86121403141659	c
0.40476052551909	-4.04881310343936	2.71960396921619	h
-0.21602148932039	-7.92814296025841	1.59302498689879	c
-0.22286854177984	-5.35554158492450	-5.26831944980264	h
-0.60420758263314	-8.63332984647556	-2.90146248421932	c
-3.61840175864521	2.11791737182918	-2.57968350733487	h
-4.25565329575382	2.25516188354894	-6.61263881405108	c
1.71057914942425	-1.95485303383023	-7.15114572058652	h
-1.27281170860532	-0.07423935433697	-9.16487850474926	c
3.75863353443849	7.27993289183535	7.75425116893096	h
6.69828487561778	5.78213265195007	5.39620621019974	c
9.20969228264637	3.89498492326827	2.80534016005377	h
-0.12270143456014	7.51157567813382	8.87818148177997	h
-3.89192428416504	6.02480442653651	8.42244004718886	c
-7.43934950216735	4.21680787765829	7.54187613479967	h
-9.33672398102888	1.38075267749932	5.38064680532598	h
-9.42137016413393	-1.33400157819299	2.37132000894446	c
-8.90760729787796	-3.93991061703414	-0.71700925555861	h

8.17704378427343	3.06540458954570	-5.66819997457341	h
9.17558190810079	-0.57256708263787	-4.12091388875614	c
9.59017917403790	-4.24331890290884	-2.40503257369557	h
-0.23792085152208	-8.64161246032008	3.51757731292132	h
-0.60473023561096	-9.56821993505606	-0.43457333572293	c
-0.92825359991193	-9.90147661276896	-4.48326527197001	h
-5.90333588765210	3.46957462226958	-6.45789537710704	h
-3.41333270551107	1.45839673064749	-8.97910800666338	c
-0.59113430572734	-0.67598940783678	-11.00570672012779	h
8.18153012685051	6.87599907101943	6.30073106775105	h
-4.68744153836140	7.18414786665385	9.91890359467524	h
-11.40462286680632	-1.78872805087582	2.64397772822738	h
11.15402410368618	-0.42548038152394	-4.64822118881208	h
-0.92589962979157	-11.56726486930013	-0.09447104412751	h
-4.40510027468584	2.04605415129551	-10.67810851337341	h

\$end

[(C^N^C)PdPPh₃] @ RI-TPSS-D3(BJ)/def2-TZVP (UKS triplet configuration)

\$coord

-0.68252170022285	1.33214115093803	1.51483554333741	pd
0.64042459089765	-0.89435929551036	-1.92102210419996	p
2.60795473288169	2.09265357295767	3.55191393386571	c
-2.00047445181740	3.81312315976548	4.20897178515839	n
-4.32295675160029	-0.04400236713243	2.11977374408072	c
3.94429937792518	-0.44774652948899	-2.82473596809618	c
0.38820747018418	-4.30007253738137	-1.40851344426282	c
-1.03076666770830	-0.34075744003454	-4.89723833341868	c
2.31514856967941	4.27011896393162	5.11486621221057	c
5.02361452812291	1.09899103034436	3.16604072878221	c
-0.27082478532814	4.98690106286516	5.72130221018316	c
-4.49520049288218	3.67817794924956	4.85568758885547	c
-5.84776634109521	1.74671838233958	3.43987388174183	c
-5.47650349797738	-2.13524870331279	0.98909258305342	c
4.82498689843004	2.04082152989907	-3.07072964791940	c
5.61911494249794	-2.46084838024479	-3.19668399325807	c
0.85342763525956	-5.19856351257986	1.04201961419121	c
-0.24622943341039	-6.00826259045270	-3.32704494950916	c
-3.57224213678081	0.40486314972803	-4.81805599563150	c
0.16337683874388	-0.63542098037694	-7.24608298274587	c
4.47040963124791	5.49527411708045	6.06587547576699	c
5.28657673241173	-0.60066141409387	2.04712487891582	h
7.14133033458779	2.30711671916209	4.17120845734639	c
-1.10680242644484	6.48144448594433	7.72247138160382	c
-5.39530698880653	5.15201858419768	6.84549005644354	c
-8.49091416704799	1.48420646759664	3.41079076260410	c
-4.33870565597902	-3.56330930491051	0.04960422319787	h
-8.10059555927191	-2.39810039939238	1.02894312578957	c
3.54138182748411	3.60387277149352	-2.71247183665066	h
7.33205283885837	2.50442904306842	-3.71002527964187	c
4.95791085513069	-4.39198690925986	-2.98970902018121	h
8.14057938532593	-1.98833072614095	-3.81404270072820	c
1.26847787606250	-3.85156343554514	2.53805325815784	h
0.71847145830825	-7.77705072461427	1.55365144224391	c
-0.64104747186217	-5.31819323076896	-5.21887538257401	h
-0.39793303714608	-8.58743798832361	-2.80218674246408	c
-4.48592551228812	0.67796982220752	-3.00077064082121	h
-4.90714895793857	0.80508263147005	-7.05155330527051	c
2.14086100421716	-1.17846889955812	-7.32508399990380	h
-1.17481755647970	-0.21234927215233	-9.47631112761200	c
4.26120053608955	7.20687330791305	7.18518981295013	h
6.86469274415632	4.52343996242986	5.59540831978124	c
9.01134006661180	1.52187437920679	3.84156102576809	h
0.25024812043997	7.45445431573836	8.91245533442962	h
-3.69648468172023	6.62491707487205	8.23357004038439	c
-7.38126077788285	5.08891671804428	7.35184532678431	h
-9.66646222122573	2.89163249740640	4.33989521006422	h
-9.60827255194377	-0.56938046078739	2.21489330063066	c
-8.97413741024041	-4.03060756945844	0.13753527457385	h
7.99751177748257	4.43794553880325	-3.88776707630113	h

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 8.99852138873210      0.48900888211306      -4.07687769804694      c
 9.43172746651724     -3.56112030835161      -4.08787594400571      h
 1.07611126937254     -8.45897056661182       3.45651251956266      h
 0.09141145404997     -9.44740301024037      -0.36719709518889      c
 -0.90619884603018    -9.90260052693579      -4.29462498590487      h
 -6.87659073600072    1.37897908784392      -6.96729618955135      h
 -3.71247159126569    0.49990693110995      -9.38435086177710      c
 -0.23169028581104    -0.43584473746251      -11.28648382896432      h
 8.52073744989180     5.47158040917866      6.35253781170380      h
 -4.37078275229801    7.76604213404004      9.79967146380449      h
 -11.65148293241076   -0.76902427884665      2.22059885342315      h
 10.96294817347924   0.85266803487555      -4.54926159416331      h
 -0.03454916659117   -11.48339340087005      0.03785715103758      h
 -4.74999042957139   0.83349563302525      -11.12424960363566      h

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\$end

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