

## Experimental Section

### Trigonal bipyramidal Rhodium(I) Methyl and Phenyl Complexes: Precursors of Oxidative Methyl and Phenyl Radical Generation

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#### General Procedures

All manipulations of air or moisture sensitive compounds were performed on a standard vacuum line in flame-dried flasks under an atmosphere of argon. Solvents were distilled under argon from Na (toluene), Na/benzophenone (THF, diethyl ether), Na/benzophenone/tetraglyme (*n*-hexane), CaH<sub>2</sub> (CH<sub>2</sub>Cl<sub>2</sub>, chloroform, acetonitrile), P<sub>2</sub>O<sub>5</sub> (acetonitrile). Air sensitive compounds were stored and weighed in gloveboxes. Basic chemicals were ordered from commercial suppliers and used as received. [RhCl(trop<sub>3</sub>P)]<sup>1</sup> and FcOTf<sup>2</sup> were prepared according to literature methods. IR spectra were recorded on a Perkin-Elmer-Spectrum 2000 FT-IR-Raman spectrometer with the ATR technique. Mass spectra were recorded on a Finnigan MAT SSQ 7000 mass spectrometer using electron ionization and Bruker UltraFlex II – MALDI-TOF-MS. Melting points were determined with a Büchi melting point apparatus and are not corrected. Solution NMR spectra were recorded on Bruker Avance 400, 300, 250 and 200 spectrometers. Chemical shifts ( $\delta$ ) are measured and referenced according to IUPAC<sup>3</sup> are expressed in ppm. Electron paramagnetic resonance spectra were obtained with a Bruker EMX 080 equipped with a microwave-bridge ER 041 XG and the dielectric mixing resonator ER 4117 D-MVT. Data acquisition and analysis were carried out with ACQUISIT software (Bruker).

### Synthesis of methyl[tris(5*H*-dibenzo[*a,d*]cyclohepten-5-yl)phosphane]rhodium(I) (2)

Complex RhCl(trop<sub>3</sub>P)] Error! Reference source not found. (260 mg, 0.35 mmol, 1.0 equiv) was suspended in dry THF (25 ml) and cooled in an ice bath. A solution of MeLi in Et<sub>2</sub>O (1.6 M, 0.45 ml, 0.72 mmol, 2.0 equiv). was added dropwise until all the solids had dissolved The colour of the resulting solution changed from light yellow to a strong dark green. Conversion of the reaction was checked by <sup>31</sup>P NMR spectroscopy. Diethylether (1.5 ml, 1 % v/v water) was added carefully to the reaction mixture provoking an immediate colour change to light yellow. The resulting solution was concentrated to dryness and extracted twice with CH<sub>2</sub>Cl<sub>2</sub> (2 x 25 ml) to remove residual salts. The CH<sub>2</sub>Cl<sub>2</sub> solution was concentrated and the residue was extracted with hexane (3 x 50 ml). The combined extractions were concentrated to dryness and recrystallized from Et<sub>2</sub>O. The precipitated product was collected by filtration, washed with Et<sub>2</sub>O (2 x 3 mL), hexane (2 x 3 mL) and pentane (2 x 3 mL) and then dried in high vacuum. The obtained product was a microcrystalline light yellow powder. Yield: 95 mg (38 %).

M.p. 196 – 198 °C (decomposition).

IR (ATR):  $\tilde{\nu}$  = 3012(w,  $\nu_{CH}$ ), 2886(w,  $\nu_{CH}$ ), 2811(w,  $\nu_{CH}$ ), 1598(w), 1572(w), 1481(m), 1414(m), 1284(m), 1127(m), 1043(w), 936(w), 792(w), 732(s), 638(m) cm<sup>-1</sup>.

MS (EI): *m/z* 707 (M<sup>+</sup>–CH<sub>3</sub>), 382, 281, 207, 191 (C<sub>15</sub>H<sub>11</sub><sup>+</sup>, 100 %), 165.

HRMS (MALDI TOF, *m/z*) Calc for C<sub>46</sub>H<sub>36</sub>PRh 722.1610, found 722.1612

<sup>1</sup>H NMR (300 MHz, THF-d<sub>8</sub>, 25 °C):  $\delta$  = 6.82 ppm (dd, <sup>3</sup>*J*<sub>H-H</sub> = 7.3 Hz, <sup>4</sup>*J*<sub>H-H</sub> = 1.0 Hz, 6 H, CH<sub>aryl</sub>), 6.70 ppm (dd, <sup>3</sup>*J*<sub>H-H</sub> = 7.3 Hz, <sup>3</sup>*J*<sub>H-H</sub> = 7.3 Hz, 6 H, CH<sub>aryl</sub>), 6.60 ppm (dd, <sup>3</sup>*J*<sub>H-H</sub> = 7.3 Hz, 7.3 Hz, 6 H, CH<sub>aryl</sub>), 6.43 ppm (d, <sup>3</sup>*J*<sub>H-H</sub> = 7.3 Hz, 6 H, CH<sub>aryl</sub>), 5.06 ppm (dd, <sup>3</sup>*J*<sub>P-H</sub> = 3.2 Hz, <sup>2</sup>*J*<sub>Rh-H</sub> = 2.0 Hz, 6 H, CH<sub>olef</sub>), 4.15 ppm (d, <sup>2</sup>*J*<sub>PH</sub> = 12.6 Hz, 3 H, CH<sub>benz</sub>), –1.01 ppm (dd, <sup>3</sup>*J*<sub>PH</sub> = 5.6 Hz, <sup>2</sup>*J*<sub>RhH</sub> = 1.0 Hz, 3 H, CH<sub>3</sub>).

<sup>13</sup>C{<sup>1</sup>H} NMR (100.6 MHz, THF-d<sub>8</sub>, 25 °C):  $\delta$  = 137.5 ppm (d, *J*<sub>P-C</sub> = 3.1 Hz, 6 C, C<sub>aryl</sub>), 136.0 ppm (d, *J*<sub>P-C</sub> = 6.1 Hz, 6 C, C<sub>aryl</sub>), 130.8 ppm (s, 6 C, CH<sub>aryl</sub>), 128.0 ppm (d, *J*<sub>P-C</sub> = 5.9 Hz, 6 C, CH<sub>aryl</sub>), 126.9 ppm (s, 6 C, CH<sub>aryl</sub>), 125.8 (s, 6 C, CH<sub>aryl</sub>), 75.0 ppm (d, <sup>2</sup>*J*<sub>P-C</sub> = 6.9 Hz, 6 C, CH<sub>olef</sub>), 47.4 ppm (d, <sup>1</sup>*J*<sub>P-C</sub> = 11.3 Hz, 3 C, CH<sub>benz</sub>), 9.9 ppm (dd, <sup>2</sup>*J*<sub>P-C</sub> = 114 Hz, <sup>1</sup>*J*<sub>Rh-C</sub> = 20 Hz, 1 C, CH<sub>3</sub>).

<sup>31</sup>P{<sup>1</sup>H} NMR (121.5 MHz, THF-d<sub>8</sub>, 25 °C):  $\delta$  = 162.9 ppm (d, <sup>1</sup>*J*<sub>Rh-P</sub> = 106 Hz).

<sup>103</sup>Rh NMR (12.6 MHz, THF-d<sub>8</sub>, 25 °C):  $\delta$  = –859 ppm (d, <sup>1</sup>*J*<sub>Rh-P</sub> = 106 Hz).

EA: Calcd. for C<sub>46</sub>H<sub>36</sub>PRh: C: 76.45, H: 5.02, P: 4.29. Found: C: 76.23, H: 5.07, P: 4.33.

### Synthesis of phenyl[tris(5*H*-dibenzo[*a,d*]cyclohepten-5-yl)phosphane]rhodium(I) (**3**)

Complex [RhCl(trop<sub>3</sub>P)] **Error! Reference source not found.** (214 mg, 0.29 mmol, 1.0 equiv) was suspended in dry THF (15 ml) and a solution of PhLi in dibutylether (2.0 M, 0.29 ml, 0.58 mmol, 2.0 equiv) was added dropwise. Upon addition, the suspended starting material dissolved and the colour of the solution changed from light yellow to a strong dark green. Ethanol (50  $\mu$ L) was added to the dark green solution provoking an immediate colour change to orange. The solution was concentrated to dryness and the residue was extracted with dry toluene (2 x 15 ml). The toluene solution was concentrated to ca. 5 ml and cooled to -18 °C. After 16h, the precipitated product was collected by filtration and washed with diethyl ether (5 ml twice). After drying under high vacuum, complex **3** was isolated as yellow crystalline powder. Yield: 127 mg (56 %).

M.p.: 275 – 277 °C (decomposition).

IR (ATR):  $\tilde{\nu}$  = 3036(w,  $\nu_{\text{CH}}$ ), 2876(w,  $\nu_{\text{CH}}$ ), 1597(w), 1567(w), 1471(m), 1416(w), 1283(w), 1218(w), 1094(m), 1011(m), 790(m), 727(s), 704(s), 639(w)  $\text{cm}^{-1}$ .

<sup>1</sup>H NMR (300.1 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C):  $\delta$  = 8.14 (dd, <sup>3</sup>*J*<sub>HH</sub> = 7.8 Hz, <sup>4</sup>*J*<sub>P,H</sub> = 5.1 Hz, 2 H, H<sub>o</sub>-phenyl), 7.77 (ddd, <sup>3</sup>*J*<sub>HH</sub> = 7.8 Hz, 7.1 Hz, <sup>5</sup>*J*<sub>PH</sub> = 1.7 Hz, 2 H, H<sub>m</sub>-phenyl), 7.55 (t, <sup>3</sup>*J*<sub>HH</sub> = 7.1 Hz 1 H, H<sub>p</sub>-phenyl), 6.80 (ddd, <sup>3</sup>*J*<sub>HH</sub> = 7.4 Hz, <sup>3</sup>*J*<sub>HH</sub> = 7.4 Hz, <sup>4</sup>*J*<sub>HH</sub> = 1.0 Hz, 6 H, H<sub>aryl</sub>), 6.71 (dd, <sup>3</sup>*J*<sub>HH</sub> = 7.4 Hz, <sup>4</sup>*J*<sub>HH</sub> = 1.0 Hz, 6 H, H<sub>aryl</sub>), 6.60 (dd, <sup>3</sup>*J*<sub>HH</sub> = 7.4 Hz, 7.4 Hz, 6 H, H<sub>aryl</sub>), 6.40 (d, <sup>3</sup>*J*<sub>HH</sub> = 7.4 Hz, 6 H, H<sub>aryl</sub>), 5.85 (dd, <sup>3</sup>*J*<sub>PH</sub> = 2.9 Hz, <sup>2</sup>*J*<sub>RhH</sub> = 2.0 Hz, 6 H, H<sub>olef</sub>), 3.65 (d, <sup>2</sup>*J*<sub>PH</sub> = 12.6 Hz, 3 H, H<sub>benz</sub>) ppm.

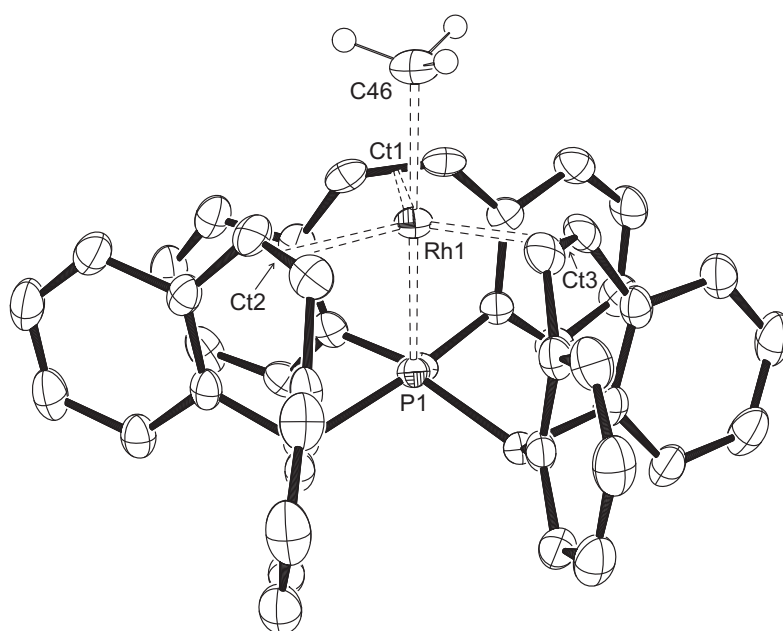
<sup>13</sup>C{<sup>1</sup>H} NMR (75.5 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 25 °C):  $\delta$  = 166.8 (dd, <sup>2</sup>*J*<sub>PC</sub> = 124.0 Hz, <sup>1</sup>*J*<sub>RhC</sub> = 26.5 Hz, 1 C, C<sub>ipso</sub>-phenyl), 136.5 (d, *J*<sub>PC</sub> = 2.9 Hz, 6 C, C<sub>aryl</sub>, quat), 134.7 (d, *J*<sub>PC</sub> = 6.3 Hz, 6 C, C<sub>aryl</sub>, quat), 134.0 (s, 2 C, C<sub>o/m</sub>-phenyl), 130.7 (d, *J*<sub>PC</sub> = 1.1 Hz, 6 C, C<sub>aryl</sub>), 127.5 (d, *J*<sub>PC</sub> = 6.0 Hz, 6 C, C<sub>aryl</sub>), 127.3 (d, *J*<sub>PC</sub> = 9.9 Hz, 2 C, C<sub>o/m</sub>-phenyl), 127.1 (s, 6 C, C<sub>aryl</sub>), 126.2 (s, 6 C, C<sub>aryl</sub>), 122.7 (s, 1 C, C<sub>p</sub>-phenyl), 75.8 (d, <sup>2</sup>*J*<sub>PC</sub> = 6.9 Hz, 6 C, C<sub>olef</sub>), 47.6 (d, <sup>1</sup>*J*<sub>PC</sub> = 13.6 Hz, 3 C, C<sub>benz</sub>) ppm.

<sup>31</sup>P{<sup>1</sup>H} NMR (121.5 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C):  $\delta$  = 162.3 (d, <sup>1</sup>*J*<sub>RhP</sub> = 102 Hz) ppm.

EA: Calcd. for C<sub>51</sub>H<sub>38</sub>PRh: C: 78.06, H: 4.88, P: 3.95. Found: C: 78.02, H: 5.01, P: 3.98.

### Crystallographic data of complexes **2** and **3**.

Data collection for the X-ray structure determinations were performed on a Bruker SMART 1K platform with graphite-monochromated Mo- $K_{\alpha}$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The reflex intensities were measured by CCD area detectors. The collected frames were processed with the proprietary software SAINT<sup>4</sup> and an absorption correction was applied (SADABS).<sup>5</sup> Solution and refinement of the structures was performed with SHELXS-97<sup>6</sup> and SHELXL-97<sup>7</sup> respectively. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in their idealized positions and allowed to ride on the respective carbon atoms. Associated crystallographic data and other experimental details of complexes **2** and **3** are summarized in Tables S1 and S2. Note that the data quality of the obtained structure **2** is limited ( $\sin(\theta_{\text{max}}/\lambda) > 0.6$ ) due to weakly diffracting crystals. The 'Squeeze' routine implemented in the OLEX 1.3. software package was used to treat further residual solvent peaks. However, the general connectivity of all atoms could be determined and hence the general structure of **2** is confirmed with certainty. CCDC 631208 contains the supplementary crystallographic data for **3**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

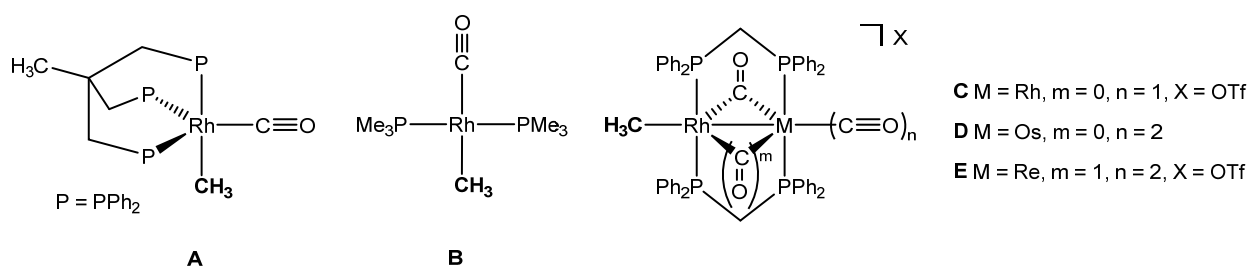


**Figure S1.** ORTEP plot of [Rh(Me)(trop<sub>3</sub>P)] **2** (thermal ellipsoids at 50 % probability, hydrogen atoms and solvent molecules omitted for clarity).

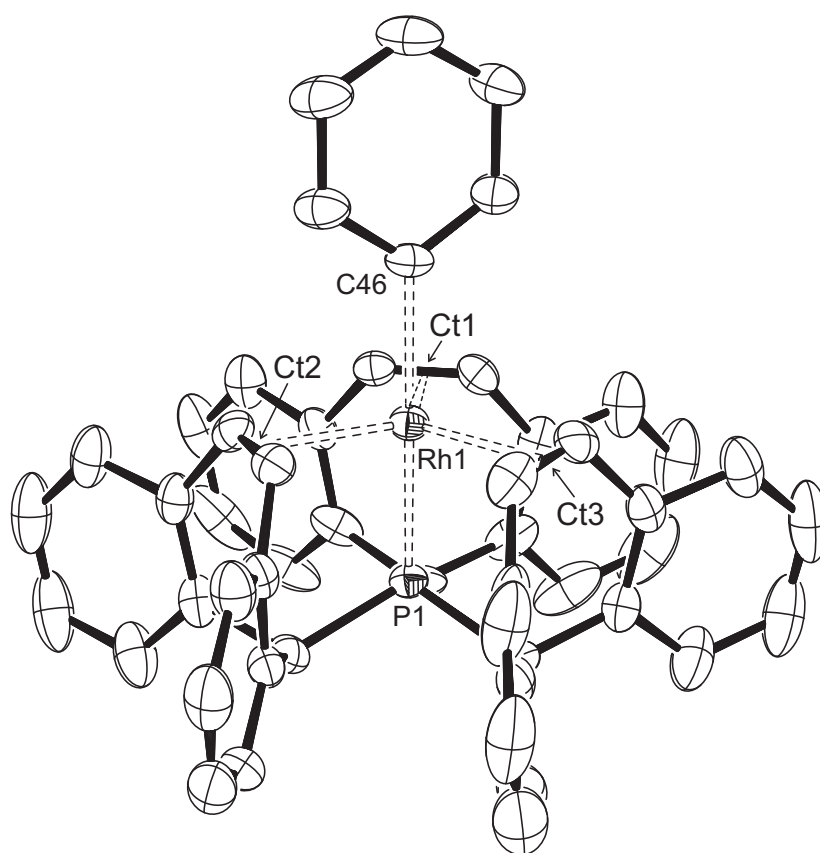
**Table S1.** Crystallographic data for [Rh(trop<sub>3</sub>P)(CH<sub>3</sub>)] × 0.5[C<sub>7</sub>H<sub>8</sub>] (**2**)

Empirical formula	C <sub>46</sub> H <sub>36</sub> PRh × 0.5[C <sub>7</sub> H <sub>8</sub> ]	
Temperature	200(0) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /n	
Unit cell dimensions	a = 11.3304(8) Å	α = 90°
	b = 18.7435(14) Å	β = 92.2700(10)°
	c = 16.9067(13) Å	γ = 90°
Volume	3587.7(5) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.443 gcm <sup>-3</sup>	
Absorption coefficient	0.558 mm <sup>-1</sup>	
F(000)	1608	
Crystal size	0.30 × 0.28 × 0.15 mm <sup>3</sup>	
Data collection	SMART APEX PLATFORM	
	with CCD area detector	
	Mo Kα, graphite monochromator	
Detector distance	50 mm	
Exposure time/frame	60 s	
Solution by	direct methods, SHELXTL 97	
Refinement method	full matrix least-squares on F <sup>2</sup>	
Theta range for data collection	2.10° to 23.25°	
Index range	-12 ≤ h ≤ 12, -20 ≤ k ≤ 20, -18 ≤ l ≤ 18	
Reflections collected	23901	
Independent reflections	5156 [R(int) = 0.0354]	
Absorption correction	Empirical (SADABS)	
Data / restraints / parameters	5156 / 0 / 474	
Goodness-of-fit on F <sup>2</sup>	1.016	
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0313, wR <sub>2</sub> = 0.0781	
R indices (all data)	R <sub>1</sub> = 0.0437, wR <sub>2</sub> = 0.0838	
Largest diff. peak and hole	0.530 and -0.476 eÅ <sup>-3</sup>	

Some related structures to complex **2** are displayed in Scheme S1.<sup>8-12</sup> The most similar structure is the triphos carbonyl complex **A**.<sup>8</sup> Other comparable structures do not have the same geometrical features, but consist of the more common square planar coordination sphere. In compound **B**,<sup>9</sup> the methyl group is located *trans* to a carbonyl and *cis* to two trimethylphosphane ligands. Other crystal structures that can be regarded as derived from square planar rhodium(I) species include the dimeric structures **C**,<sup>10</sup> **D**<sup>11</sup> and **E**,<sup>12</sup> where the second metal occupies the position *trans* to the methyl group and additional bridging carbonyl ligands interact with the rhodium center.



**Scheme S1.** Reported examples of methyl rhodium(I) complexes.



**Figure S2.** ORTEP plot of  $[\text{Rh}(\text{trop}_3\text{P})(\text{Ph})]$  **3** (thermal ellipsoids at 50 % probability, hydrogen atoms and solvent molecules omitted for clarity). Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ]: Rh1–P1: 2.2099(7); Rh1–C46: 2.149(3); P1–Rh1–P2: 178.37(8). Sum of bond angles of the three substituents at P1:  $318^\circ$ .



**Table S2.** Crystallographic data for [Rh(trop<sub>3</sub>P)(C<sub>6</sub>H<sub>5</sub>)] × 1.5 [C<sub>7</sub>H<sub>8</sub>] (**3**)

Empirical formula	C <sub>51</sub> H <sub>38</sub> PRh x 1.5[C <sub>7</sub> H <sub>8</sub> ]
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n
Unit cell dimensions	a = 12.5251(5) Å      α = 90° b = 18.7769(8) Å      β = 90.0430(10)° c = 18.8788(8) Å      γ = 90°
Volume	4440.0(3) Å <sup>3</sup>
Z	4
Density (calculated)	1.381 gcm <sup>-3</sup>
Absorption coefficient	0.463 mm <sup>-1</sup>
F(000)	1916
Crystal size	0.63 × 0.53 × 0.43 mm <sup>3</sup>
Data collection	SMART 1K PLATFORM with CCD area detector Mo Kα, graphite monochromator
Detector distance	50 mm
Exposure time/frame	15 s
Solution by	direct methods, SHELXTL 97
Refinement method	full matrix least-squares on F <sup>2</sup>
Theta range for data collection	1.95° to 28.32°
Index range	-15 ≤ h ≤ 16, -24 ≤ k ≤ 23, -25 ≤ l ≤ 24
Reflections collected	38905
Independent reflections	10456 [R(int) = 0.0208]
Absorption correction	Empirical (SADABS)
Data / restraints / parameters	10456 / 19 / 660
Goodness-of-fit on F <sup>2</sup>	1.053
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0350, wR <sub>2</sub> = 0.0864
R indices (all data)	R <sub>1</sub> = 0.0430, wR <sub>2</sub> = 0.0910
Largest diff. peak and hole	0.824 and -0.415 eÅ <sup>-3</sup>

## DFT Calculations

All calculations were carried out with the ORCA program package.<sup>13</sup> Unless stated otherwise, all calculations were carried out on isolated molecules. Density fitting techniques, also called resolution-of-identity approximation (RI),<sup>14</sup> were used for GGA and *meta*-GGA calculations and the RIJCOSX<sup>15</sup> approximation was used for hybrid-GGA and CASSCF calculations. Atom-pairwise dispersion corrections with the Becke-Johnson damping (D3BJ)<sup>16,17</sup> were used for all DFT calculations (D3(0) in case of M06). All geometries were obtained using the B97-3c method developed by the Grimme group.<sup>18</sup> Final energy calculations were performed using the M06<sup>19</sup> functional, the def2-TZVPP<sup>20</sup> basis set and the CPCM<sup>21</sup> model for THF.

Table S3: Calculated dissociation energies of complexes **2** and **3** or **2<sup>+</sup>** and **3<sup>+</sup>** into [Rh(P(trop)<sub>3</sub>)] or [Rh(P(trop)<sub>3</sub>)]<sup>+</sup>, respectively and methyl or phenyl radicals.

	<b>2</b>	<b>2<sup>+</sup></b>	<b>3</b>	<b>3<sup>+</sup></b>
$\Delta E$ [kcal·mol <sup>-1</sup> ]	60.6	13.8	70.3	23.5

## Cartesian coordinates of optimized species

### Methyl radical

C	5.71031301958893	3.25866265797977	15.46443986419341
H	6.72582193115919	3.39528555030522	15.79570171698112
H	5.20224876736606	4.05229231510776	14.94315185013092
H	5.20224628188581	2.32829947660724	15.65423656869453

### Phenyl radical

C	5.60863880050725	3.20892987927204	15.16706155667644
C	4.25890865290151	3.36712766711561	15.01180069320834
C	3.73686030614963	3.10379188074123	13.74283831669016
H	3.61429755607240	3.68047196692915	15.82309956923013
C	4.57803524456269	2.70274669484796	12.71321189957439
H	2.67386270654431	3.21448502704581	13.56837831088366
C	5.94227578199907	2.55856367946245	12.92904491320221

H	4.16651469768846	2.50071106681141	11.73338392482985
C	6.48320488644902	2.81723012975315	14.19102593694699
H	6.59310996375374	2.24545735493300	12.12217711769581
H	7.54486140337189	2.70863465308817	14.37269776106197

[Rh( $\eta^4$ -P(trop)<sub>3</sub>)]

P	6.33575142678996	15.62862603024745	11.76259663196886
C	7.00829511087029	17.37492315394128	11.76494082107933
H	6.66748173075639	17.89343329851059	10.86819569023535
C	6.45746479426550	18.08452071446429	12.97193520293159
C	6.67368652408632	17.57718250496687	14.26748309456934
C	7.48324407356970	16.39171703086377	14.56866054642265
C	8.70860269823598	16.10204780453299	13.94613891755526
C	9.27652646757304	16.88630554697822	12.85708638368774
C	8.51810556902515	17.46102664536833	11.81647989604519
C	5.74879306238150	19.26671517466886	12.79968053067015
H	5.59839754176670	19.64526918359810	11.79607985454275
C	5.22831842581482	19.95788985647323	13.88045850840169
H	4.67224641153216	20.87258683645272	13.72433191883267
C	5.41183610915244	19.45332995465207	15.15866303191785
H	4.99568349247353	19.96799645099924	16.01438312229919
C	6.11957625735236	18.28019211516594	15.34097697516507
H	6.25987913703509	17.89268542457756	16.34103730735025
C	10.65930944126643	17.09416272484414	12.85928456168253
H	11.24562026568970	16.64719797779318	13.65260527246049
C	11.28538925826149	17.86612831062908	11.89923705664284
H	12.35673358746206	18.01361730766497	11.93695569922570
C	10.53264014392172	18.43712821105197	10.88485813739381
H	11.00604784097831	19.03061605246091	10.11446646220023
C	9.16468795896878	18.22749721448327	10.85388822516351
H	8.57889033363589	18.66183520852700	10.05383815957192
C	6.72688034084308	14.81605179935048	10.12258935788057
H	6.14282395239550	15.29341000794022	9.33502424877853
C	8.18876507951791	15.02573778880724	9.83574966101780
C	9.17127007969231	14.58123826676006	10.74118949598119
C	8.88762679405528	13.83537510460052	11.97117957073098
C	7.93892743677167	12.80650100101416	12.06227346099954
C	7.04597973830923	12.41947958227936	10.97817434978368
C	6.44643246186887	13.32960175143696	10.08324478642815
C	8.56713527281610	15.64524230667882	8.65159404505314
H	7.79776260522187	15.97539596367425	7.96443692716387
C	9.90052312998178	15.85440803428361	8.34307267443270
H	10.17423833123684	16.34595015506762	7.41910997195433
C	10.87550786070904	15.44509880488144	9.23984238189367
H	11.92180046559787	15.61797717379204	9.02610386340175

C	10.50953937072553	14.82421814092318	10.41915446389300
H	11.27505505444869	14.50678730418940	11.11424898285524
C	6.78577700011584	11.05619171858242	10.80755092093870
H	7.23799398557758	10.35545141834610	11.49842368546096
C	5.99455362217447	10.58533146754902	9.77720881705407
H	5.82148470880821	9.52261584652337	9.66939915631225
C	5.41682310718819	11.48442552771394	8.89421372481337
H	4.78042191011843	11.13704241850944	8.09164352981946
C	5.64634549575380	12.83969084207221	9.05761833173201
H	5.18306253579954	13.54238935533723	8.37683621770292
C	4.48042900289471	15.67964931267741	12.00158596649831
H	4.04320603957895	16.37448331245760	11.28378582185221
C	3.93738163067247	14.30231399449985	11.73359436463553
C	4.39972082106349	13.19060185656053	12.46394265261087
C	5.36605017734878	13.26599947905875	13.56447895770406
C	5.35183133359504	14.26405246458330	14.55191064812152
C	4.44051280665652	15.40136772190443	14.55044814454319
C	4.04365171188252	16.09596634046989	13.38930137732445
C	2.95099805420841	14.13708857196112	10.76968249932338
H	2.60253680398372	15.00486358290455	10.22321705645742
C	2.41696703894659	12.89009194834062	10.49293377465497
H	1.65480249785319	12.78140421212594	9.73295796263485
C	2.88458642458679	11.78423617737730	11.18619820894616
H	2.49495678388131	10.79854164367788	10.96955865007367
C	3.86276979341701	11.93870581694831	12.15037981336550
H	4.22206706207506	11.07184219722132	12.68830179757969
C	3.91606827991244	15.81446412905754	15.77904553962771
H	4.22469763670387	15.28804284814347	16.67373064868323
C	3.00637300325172	16.85012075600998	15.87589092128166
H	2.61496926763621	17.13849822393415	16.84264322813100
C	2.61266997504956	17.52256087918032	14.72938068327498
H	1.91490852955747	18.34700387841730	14.78606231836037
C	3.13462633901004	17.14111957021789	13.50531813223259
H	2.83819417053483	17.67566029638111	12.61182486259021
Rh	7.24511859532028	14.50023907753552	13.37658952138141
H	7.39351467276216	16.06731720848186	15.59709697501373
H	9.74968120287160	13.73456202587200	12.61726009834924
H	9.44394200637250	15.59558701987583	14.55940281564883
H	5.68226099563464	13.96066366681754	15.53772757764793
H	8.16856779537357	12.00884984781032	12.75779385486846
H	5.72112154477126	12.29554942526634	13.88540049248421

[Rh( $\eta^4$ -P(trop)<sub>3</sub>)]<sup>+</sup>

P	6.36787959769677	15.58905965479193	11.81983058979983
C	7.03368020079745	17.33365695331804	11.80289278311002

H	6.65610190209574	17.77254479956328	10.87767836939905
C	6.46519559463420	18.07901047157700	12.97663368525472
C	6.67196344815420	17.59665658967896	14.27999608319205
C	7.48950459971428	16.42372728863033	14.58298093278576
C	8.69730947885901	16.11010523352243	13.93743567061027
C	9.29111667591069	16.89151886954465	12.86291591230477
C	8.53449090367977	17.45418804855870	11.82220524153291
C	5.75725436472130	19.25518679115296	12.77238201625424
H	5.61539842996310	19.62136717948728	11.76349322202718
C	5.23289678428219	19.96161564861183	13.84155462261149
H	4.68449182442370	20.87703709249559	13.66898665930792
C	5.40605917190399	19.47911242536701	15.13061571155761
H	4.98938556797426	20.01414067688546	15.97239099095405
C	6.10931994480514	18.30829435388661	15.34216904386875
H	6.24489622000194	17.94070526477345	16.35000773197032
C	10.67166028471474	17.10194790909024	12.87778830221710
H	11.25989268441677	16.66430172986111	13.67409083580149
C	11.28945256877024	17.88196533778556	11.91833925111248
H	12.35711220036471	18.04646744784804	11.96134192763334
C	10.53469844408079	18.44440695194589	10.89980213565640
H	11.00769920252873	19.04535123657015	10.13603847653076
C	9.16855645477157	18.22408807032250	10.85597127013828
H	8.58390792480202	18.65434050351084	10.05376594004048
C	6.74234133558810	14.78880083633910	10.17477955267283
H	6.11671585652362	15.31664723293824	9.45281477347264
C	8.18962169649255	15.01862436784594	9.84422427343275
C	9.18897399353332	14.57741146896821	10.72799217368303
C	8.90811120972607	13.82399281075466	11.94842989251631
C	7.93144018595813	12.81954259275633	12.05323340831862
C	7.04778608541971	12.40503347522664	10.97379572706971
C	6.44469309240367	13.31515377969902	10.09044619446113
C	8.53695800632068	15.64449999973125	8.65514534746205
H	7.75701210110229	15.96939063614878	7.97821963882845
C	9.86540369366375	15.85675791438059	8.32760671315815
H	10.12260841530786	16.34451515051001	7.39783662899532
C	10.85941803130160	15.45130940327482	9.20627958197706
H	11.89957803876119	15.62442563759348	8.96850502230485
C	10.52155421886355	14.82808677321625	10.39269676378315
H	11.30145190113867	14.51032565287821	11.07091713471179
C	6.80202104736295	11.04106756976426	10.80217177111495
H	7.25930498682267	10.33617692983008	11.48455645322291
C	6.01716624761076	10.57815911402587	9.76277773246852
H	5.85635025302631	9.51628958473927	9.63876445474482
C	5.43353413190328	11.48168358212668	8.88728812353820
H	4.80667843630287	11.13327413305348	8.07866888020393
C	5.64666976607843	12.83892417849740	9.05862282876493

H	5.18050999751368	13.54184748384349	8.38104260143364
C	4.51541286579118	15.65598944479444	12.04725988868978
H	4.16374081202482	16.37230643256622	11.30272238436626
C	3.94233849266841	14.30059833230522	11.74524081219521
C	4.38233423734302	13.17715814983544	12.46551995383102
C	5.33563920608065	13.25343534104939	13.57089141137934
C	5.34810607900224	14.27168008251220	14.53861494348827
C	4.43235886167302	15.40239836213811	14.56543745055601
C	4.04599777780679	16.09762319862206	13.40803667298459
C	2.96175839910038	14.16512397955265	10.77238365066895
H	2.62351062691594	15.04087094139629	10.23318653411579
C	2.41395918695164	12.92613302077884	10.48599385127644
H	1.64984007577381	12.83431402876003	9.72689704439420
C	2.86245540161420	11.80563859800995	11.16997656618454
H	2.45291372685113	10.83088640324437	10.94506924505644
C	3.83913409709632	11.93222699825842	12.13962518254120
H	4.18061701762129	11.05532118887167	12.67217607936782
C	3.90446942918377	15.80176316442823	15.79509939726628
H	4.20409558365190	15.27309386228468	16.69084353234777
C	2.98661462101332	16.83162896867458	15.88197595598778
H	2.57691085944490	17.11042083466547	16.84282056051494
C	2.60079768692311	17.50685470908811	14.73367038626329
H	1.89418956426182	18.32278388765238	14.78991302655129
C	3.13411093678212	17.13997428327188	13.50978079053104
H	2.84009656019915	17.67628156762499	12.61736106851791
Rh	7.25588348582474	14.48698572098422	13.38502851394250
H	7.39314813318643	16.07861467343877	15.60414317314256
H	9.76245224874421	13.72566886355491	12.60550438632431
H	9.41754742930650	15.55994920152930	14.53422740921622
H	5.72406126650855	13.98447196806886	15.51520615646762
H	8.13935219104217	12.03922563043603	12.77823050652397
H	5.70944593681902	12.28953132467909	13.89063038729472

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P	6.36065219312036	15.60040086177611	11.80538030355349
C	6.99974904210812	17.36021808987681	11.77245399144767
H	6.63651847019216	17.85537452665247	10.87171965684799
C	6.45644241302074	18.07850209009751	12.97733999922369
C	6.67994832059736	17.57686849037006	14.27397061576789
C	7.50043028166536	16.40248515696022	14.57803387122487
C	8.71100491576414	16.10345567579839	13.93128613191137
C	9.27019543771840	16.89103236951395	12.83881694219420
C	8.50623914417502	17.46432103467632	11.80459151668497
C	5.74729445955469	19.26016576096333	12.80365321406933
H	5.59301871415635	19.63564527989065	11.79950929703337

C	5.23082325729443	19.95423641470375	13.88420900136562
H	4.67508910566473	20.86902406714512	13.72752494847615
C	5.41821168398365	19.45333365096386	15.16374151347078
H	5.00459196106061	19.97061690262005	16.01904184544132
C	6.12695807053523	18.28146493386656	15.34760852965153
H	6.27201345092875	17.89704584863803	16.34819402809118
C	10.65141316502450	17.10729887537275	12.84045726987911
H	11.24238749948006	16.66033496564754	13.63000881303888
C	11.26889698610868	17.88654403398075	11.88056716016899
H	12.33914722874811	18.04190204241688	11.91565463728781
C	10.50965836583821	18.45363408118338	10.86868141879199
H	10.97781468790339	19.05060456120845	10.09780675173531
C	9.14272236242247	18.23598488684299	10.84001986300929
H	8.55146291317170	18.66755522797111	10.04257767836509
C	6.73231615893442	14.82534549043592	10.14185339666420
H	6.14369040597666	15.32727994769360	9.37367173587870
C	8.19385257359998	15.02646901486752	9.84756693728716
C	9.17710755681824	14.57377274733593	10.74837303695033
C	8.89595441617048	13.81838841760682	11.97113529999939
C	7.92286706068603	12.80966564735129	12.06245645418891
C	7.03289469630740	12.43077218809052	10.97115523488409
C	6.44026127853076	13.34478636147933	10.07923443592641
C	8.57122383171995	15.64585944651753	8.66299227592222
H	7.80146130663347	15.97983988068376	7.97812644277902
C	9.90436610574715	15.84997184187256	8.35135271407887
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C	10.88051994601945	15.43602183145520	9.24524037733543
H	11.92675299178344	15.60559961910667	9.02885042252731
C	10.51573230439265	14.81401791136230	10.42399305097662
H	11.28152158742032	14.49133741981351	11.11636589208989
C	6.77691184733160	11.06827014502651	10.79083181026786
H	7.22487645936090	10.36375051249035	11.48029504580691
C	5.99118677534793	10.60483537008164	9.75269876891766
H	5.81987023135387	9.54287860893463	9.63565515046992
C	5.41546994991852	11.51000472241219	8.87450629075281
H	4.78169068886118	11.16743681434315	8.06780594491361
C	5.64322362341268	12.86462854160499	9.04720829588129
H	5.18282203030555	13.57234240719341	8.36973517888715
C	4.50002939477825	15.67079884383392	12.00322518039076
H	4.08849517885854	16.36293039409629	11.26830903627172
C	3.94858111090704	14.29591243134335	11.74154150194169
C	4.40528619280180	13.18615903719901	12.47849571712675
C	5.35979348898039	13.26353649100183	13.58667271424301
C	5.35709308575445	14.28205511297110	14.55348902799485
C	4.44204715821500	15.41749461870443	14.54168954319301
C	4.04708289874350	16.10358473521821	13.37752771098219

C	2.96293563421747	14.12989951967849	10.77702310706586
H	2.61767109334688	14.99621414436095	10.22625705971939
C	2.42673922836882	12.88323361648684	10.50430956322107
H	1.66475870602199	12.77345148718495	9.74432582159695
C	2.89158410619494	11.77820866772526	11.20144599788129
H	2.49978401536845	10.79286687262439	10.98747523865554
C	3.86806260165093	11.93350393294731	12.16676241839533
H	4.22519198276401	11.06810880176631	12.70847012859971
C	3.90819621398628	15.82886259560679	15.76650149449418
H	4.21605475597792	15.30804918218496	16.66446562763609
C	2.99121541657024	16.85916913383461	15.85337629559167
H	2.58967695048692	17.14682262229917	16.81609012892944
C	2.60236963759227	17.52689879889709	14.70233254904455
H	1.90109267530201	18.34875026302853	14.75285455353142
C	3.13346321229180	17.14538664451708	13.48204121610058
H	2.84071602139367	17.67566673051567	12.58489414029656
Rh	7.28649945794946	14.45449210179413	13.43573393940554
C	8.18214020059723	13.34480272301166	15.01555996901519
H	7.60980751145718	12.44158580426852	15.24287234553639
H	8.24147981906173	13.93467666569139	15.93403595389896
H	9.19841994882478	13.03411374078534	14.75833557449265
H	7.42874175530726	16.08167230203202	15.60735751474056
H	9.75836533530232	13.69397468686209	12.61038668501154
H	9.45400003399289	15.60575263318161	14.53789928062327
H	5.67985017331545	13.98913813006166	15.54227771272456
H	8.15028707668764	12.00176676995377	12.74308386468486
H	5.70815153081255	12.29829664522698	13.92533454308727

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P	6.38917485977150	15.55661966303973	11.83833174178423
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C	6.46773412990138	18.04350842776475	12.99779288362572
C	6.63934222875371	17.54448849099862	14.30148115646471
C	7.45281120298416	16.37732088966865	14.63301590993209
C	8.69831950855133	16.10223517703952	14.03967042145563
C	9.28410088409754	16.80861869061497	12.92582173950932
C	8.54520891854318	17.39425966646873	11.87481556330354
C	5.77549558733306	19.22809928246832	12.79708155251065
H	5.65559033683956	19.60677077607703	11.79017195674398
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H	4.70352594716493	20.85391253311820	13.68957778210644
C	5.37805982794335	19.43377591553761	15.15132959894186
H	4.95147811354064	19.96444020809054	15.99071374163357
C	6.06381100683207	18.25289923630089	15.36128531773268



H	6.17683439916309	17.87187451588614	16.36671427426370
C	10.68010906100254	16.95843252723219	12.93112594042229
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C	11.32656648972630	17.71515349329270	11.97751297876877
H	12.39955041434731	17.83912464754666	12.01840828453528
C	10.58835985018961	18.31329507273707	10.96421055058854
H	11.08200481214926	18.90361093263453	10.20524012781384
C	9.21443233625834	18.14016707659225	10.91587320142111
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C	6.76521131745833	14.79119895839754	10.16101453825060
H	6.10819228001066	15.27457478402899	9.43807463338046
C	8.19021600120427	15.06535707599437	9.77196353172331
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C	9.10544716852403	13.80979809190874	11.76736720145117
C	8.17104007125628	12.82068941970939	11.95280226126071
C	7.16754894214329	12.41428231201939	10.98444711539101
C	6.51276200025921	13.30594102948247	10.11418700317575
C	8.45528077907920	15.73934983242012	8.58684031506733
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C	9.75505498157340	15.99823612502798	8.18502224797028
H	9.93976579251324	16.51747827165597	7.25490338333483
C	10.81389706250171	15.59741427280692	8.98693429592377
H	11.83237013043613	15.80317633291214	8.68905499486865
C	10.56504956975692	14.93641730695925	10.17340408712628
H	11.39182999138937	14.62172357037709	10.79504221808725
C	6.88685519615932	11.04673411965600	10.88633031299177
H	7.38098495572270	10.36236572107538	11.56381191140856
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H	5.85211109547681	9.49367287014444	9.84388260070106
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C	5.65236317257889	12.79685508263600	9.15002319986395
H	5.14886231513726	13.47991202546909	8.47939456495567
C	4.52286114437654	15.69030119504247	11.99469399454236
H	4.16820642672309	16.40528676958198	11.25277209127354
C	3.92940465408074	14.34308447436021	11.70658836374293
C	4.35678251702310	13.21803953068180	12.43992897492149
C	5.28660872634790	13.28495604637621	13.55250871692617
C	5.31332744712357	14.29629950744681	14.54762250359931
C	4.40462573018420	15.43581765055611	14.53050652489686
C	4.04447936481523	16.12763757483302	13.36014320835099
C	2.95002895787493	14.20097463053108	10.73553613227745
H	2.62238565351682	15.07187040263090	10.18262383772310
C	2.37952542892275	12.96484860371411	10.47465254770050
H	1.60710968890948	12.87442275416555	9.72368770114928
C	2.81480313108871	11.84519821590489	11.16995275385773

H	2.38737530652681	10.87450478416226	10.96187988586572
C	3.80408874614212	11.96984873017690	12.12490941212873
H	4.14177960418782	11.09610600883554	12.66472793179026
C	3.83737502802425	15.82934927615188	15.74559751802140
H	4.11646211683990	15.29889387801359	16.64679224891047
C	2.91292282176484	16.85445330873376	15.81243098880652
H	2.47517495811348	17.12810683903816	16.76226198216925
C	2.55872321251341	17.53038494091058	14.65509501073854
H	1.84620863182243	18.34249781714883	14.69153021171853
C	3.12649944402848	17.16607957229708	13.44498805477479
H	2.84981250673347	17.70020734875395	12.54563627926979
Rh	7.25201926804358	14.40346646484164	13.54526351442462
C	8.20884758662430	13.39896848297480	15.14295177856607
H	7.67242032609046	12.45452399070519	15.26793594439617
H	8.16360855383854	13.94667221502555	16.08322928150622
H	9.25112803172399	13.16986487591075	14.92138653275041
H	7.36284636075805	16.06966200324980	15.66464155743668
H	9.94715072824333	13.81345398112271	12.44686830663215
H	9.41507153174426	15.60171515964962	14.67379408031923
H	5.56874632580454	13.95754551104027	15.54235193912545
H	8.39824944700879	12.09139010572956	12.71997246834838
H	5.66391243330398	12.31657961961556	13.85782601098333

3

Rh	11.00499813282420	15.09287602310813	15.45156847270314
P	12.99471405491978	14.84935569684467	14.53463314398300
C	13.94134154713344	16.46405169214223	14.48658768961255
H	14.83846359220045	16.32310066934455	13.88333961562000
C	13.15374571173123	17.61735179981634	13.91721794901636
C	11.92018698284918	18.00848959627214	14.46833541727106
C	11.27339042755685	17.33357271778158	15.58443603295727
H	10.26967898940354	17.67389169735099	15.77878310139100
C	11.93983574881914	16.80637836243318	16.69615701163615
H	11.35836923647497	16.75567396659515	17.60552078368131
C	13.38201559227018	16.91655204448997	16.91181600640508
C	14.34682940473106	16.81457463807374	15.89161985158720
C	13.70585330274617	18.36817334250225	12.88673463452573
H	14.65250795981336	18.05929057380891	12.46235448786018
C	13.06734422926159	19.48920824331043	12.38453410807368
H	13.51563097771986	20.04841641695359	11.57456945005996
C	11.84480115121983	19.87338397044763	12.91454094196000
H	11.32970117084972	20.74316814336694	12.52879509646643
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H	10.32600037135247	19.42861868179154	14.35053193701688
C	13.82800809489022	17.21571658726150	18.20294135369561

H	13.10007208966722	17.27629680936575	19.00060092912731
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C	16.09973328059241	17.37820443536084	17.45635375180681
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H	16.41224039408053	16.98146428858419	15.37688097807923
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H	15.07030130171208	13.65244862221895	15.03135323547994
C	13.48801721133038	12.24844463043297	15.25328769605115
C	12.14632048135535	11.98666506465577	15.58658747875870
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C	14.15861738705493	13.87187291073120	16.93901472092383
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H	14.43194436935233	9.17676486346910	14.16397165561784
C	12.46258264844346	9.69379699631688	14.85131509061180
H	12.04988469831831	8.70844978230315	14.68166473004932
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H	10.62004531730767	10.48854941766703	15.57908264008053
C	13.16760708035919	14.09607738984062	19.12219830821709
H	12.28214229619454	14.16447481266014	19.74144325115876
C	14.41853857028232	14.13332920706440	19.70796885567620
H	14.51089520752911	14.23782826676923	20.78088627558705
C	15.55045083852659	14.04972129736346	18.91092450222732
H	16.53730222951974	14.09550771917840	19.35121098522474
C	15.41058059107640	13.92333321499762	17.53952287477609
H	16.29336609016810	13.87235471542771	16.91515596048724
C	12.86236161159367	14.22829793175250	12.77430299545444
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H	9.01007175569845	13.91574618306356	14.09610535793423
C	10.20951863416412	15.48556904831146	13.36245874610619
H	9.37449938779534	16.14411812705897	13.54020518551340
C	11.06670469623257	15.92697818998372	12.26139079328412
C	12.29785513125556	15.33344358724245	11.92681112476268
C	12.47768239732716	11.90551863319741	11.94262109001679
H	13.51182236906688	11.90826677285756	11.62259766613152
C	11.68676298124974	10.79925213804889	11.68284779013721

H	12.10395077599143	9.94713765874358	11.16351334791776
C	10.36721835760942	10.78862117016777	12.10872181978465
H	9.73724037595979	9.92969071538004	11.91870767339734
C	9.86180291151688	11.87962333421199	12.78999024852602
H	8.83232312184800	11.87482920730993	13.12497056202314
C	10.60589488737532	16.96965995814347	11.45160172877623
H	9.67168913390936	17.45060265648945	11.70846576357440
C	11.30238619306128	17.38426210024920	10.33247808430520
H	10.91502916076981	18.19353595272418	9.72816928162898
C	12.49883200857026	16.76913228134021	9.99453512849909
H	13.05309397354460	17.08755376895643	9.12182408701751
C	12.98848077373856	15.75327220601883	10.79736854939168
H	13.92961770441478	15.27735416361002	10.55058111310474
C	9.04807032554543	15.31380096108302	16.27255968809263
C	6.37550047139992	15.58052728013084	17.23912210500494
C	8.49094870921897	14.42737616349063	17.20250687605777
C	7.19111711465713	14.55068126688144	17.68107188974502
C	6.88441585988326	16.47283721680946	16.30891301488188
C	8.18700554712603	16.33356311205924	15.84323940528380
H	6.81688576368538	13.83378175021939	18.40288453269419
H	9.06267936839723	13.59080758789823	17.58499691889129
H	8.51939318289502	17.06022127656624	15.11164410961948
H	5.36263294902216	15.68184192226850	17.60747273735754
H	6.26731730511080	17.28396880248285	15.93985809628840

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Rh	10.88310296682599	15.21354354098930	15.47004349311792
P	12.92772493256245	14.83898168585841	14.58085960383196
C	13.91190857429240	16.43316619494654	14.48073155925665
H	14.78815617804052	16.25124424328800	13.85880927533806
C	13.14361437749508	17.60029804106615	13.90951447388253
C	11.92628328622632	18.02533554860488	14.46968117722943
C	11.27428612535328	17.35740377449608	15.58639700960313
H	10.31041430519350	17.77334765222069	15.83596366983760
C	11.97242196173343	16.80450740519328	16.68837978278794
H	11.39924514663944	16.71709125174250	17.60313061523912
C	13.40600685696776	16.90286552192791	16.90000592869865
C	14.35658433799833	16.79898769988395	15.86611603468693
C	13.71097509255152	18.34170846970546	12.88186734417580
H	14.64891081055698	18.01628785036869	12.45186372567509
C	13.09978502026935	19.48637290072206	12.39679812483100
H	13.56267233576819	20.04408036730787	11.59474564769553
C	11.89385873919079	19.90532793475842	12.93802656463288
H	11.40831551465964	20.79754795314944	12.56797561577739
C	11.31281796956172	19.17083676817231	13.95406123245262

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C	13.85748018577288	17.20989012059198	18.18978955420999
H	13.13892349404202	17.27007108221087	18.99547266876230
C	15.18994547204779	17.47356347017516	18.43752806508444
H	15.51030285302761	17.73006568361573	19.43746989625785
C	16.11366178233280	17.40272078327830	17.40371424575747
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C	15.69419196515808	17.05088348885430	16.13060264307548
H	16.41564463764735	16.97768168861272	15.32698588421106
C	14.02918968387022	13.60721777435277	15.48445892919661
H	15.02557262822758	13.73177998487822	15.05977678817260
C	13.56933071335726	12.20183341110712	15.22455490574400
C	12.26574724717609	11.79914851771928	15.56987079060482
C	11.32629112848833	12.63880114338257	16.29373753450995
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C	11.64132825460887	13.51948275160009	17.29143335446302
H	10.83419337065377	13.84094485129535	17.93528938069215
C	12.97320877397602	13.80382071722209	17.78736150827703
C	14.11816030922962	13.82614941674323	16.97153333856235
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H	15.44914191478502	11.59884699460260	14.40512377902811
C	14.05185812957615	9.97900618288679	14.41575506083590
H	14.74918719557489	9.27673320392984	13.98048408327191
C	12.75723830710195	9.58325775602620	14.72099278229459
H	12.43612656424382	8.57028509752534	14.52305624866867
C	11.87444564014198	10.48778440885340	15.27726055608963
H	10.86814886265296	10.17550158870662	15.52042440066776
C	13.12032353363246	14.00626604419813	19.16501274337645
H	12.23696560436805	14.00470899948902	19.79048672875005
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H	14.45992177997668	14.28751241887371	20.80660896279763
C	15.49693944797424	14.14190298213504	18.93146809402349
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C	15.36507607450889	13.98754977590904	17.56249634231822
H	16.24734574321834	14.00220408558338	16.93707904686320
C	12.79399609963948	14.20990359635267	12.82221630700471
H	13.79474814540304	13.94211450448600	12.48426282604098
C	11.90134976013109	13.00720329369769	12.68365205111600
C	10.56038078423123	13.02818349844606	13.12153426922484
C	9.90947380946712	14.18289061761581	13.69098343476990
H	8.91477733499877	13.98869452197543	14.06549374920393
C	10.17375844533933	15.53174961529643	13.37062007884183
H	9.33670293560314	16.19656942731784	13.51845287871303
C	11.05341503754457	15.95468201446626	12.28381958671612
C	12.26618404799566	15.32169332292709	11.96038021378565
C	12.38057952683295	11.87949096328718	12.03307227508324

H	13.40628969473879	11.86473773875718	11.69086536524891
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H	11.97392445638575	9.90952216003953	11.30655270025030
C	10.26422059288869	10.77134404062693	12.28051092582509
H	9.63193857302921	9.90831198427682	12.12597873882061
C	9.77435956956253	11.87962724411739	12.93737204469486
H	8.75056813303590	11.88983638300291	13.28784165737776
C	10.61760676452267	17.00437970981612	11.46911227235746
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C	11.32846597594577	17.38927205512310	10.34853804661393
H	10.96332913347612	18.19796857309663	9.73134401166516
C	12.50881389073369	16.73817875639747	10.02256663137964
H	13.07018078481024	17.03020294849025	9.14599610596771
C	12.97366451642516	15.71561353819695	10.83449506025202
H	13.90135485444244	15.21432078434893	10.58990445096313
C	8.95378792295723	15.44265217556728	16.16818430187364
C	6.33392263854288	15.72671529668268	17.20448829498526
C	8.38090160411590	14.47897925064765	17.01702432571106
C	7.10524376269360	14.62176921627568	17.54018833788652
C	6.85229165997950	16.67791388614837	16.33376276880536
C	8.12859092496559	16.52559074497914	15.81760678093213
H	6.70795413978949	13.86535094762244	18.20458316603792
H	8.92851805942275	13.58685689997157	17.28869396505567
H	8.48136182974690	17.28380404825040	15.13008280168835
H	5.33486571729611	15.83761004508309	17.60323503980810
H	6.25579306155824	17.53651159054977	16.05372877768617

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