

Supporting Information for

**Propene Oxidation Catalysis and Electronic Structure of
M₅₅ Particle (M= Pd or Rh): Differences and Similarities
between Pd₅₅ and Rh₅₅**

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Table of Contents

| | |
|---|-----------|
| Stability of icosahedral (I_h) and octahedral (O_h) Pd_{55} cluster..... | S4 |
| Table S1. The relative energies (in kcal/mol) of icosahedral (I_h) and octahedral (O_h) Pd_{55} cluster and Pd-O bond energies of $Pd_{55}(O)$ ($E_b(O)$, eV) and $Pd_{55}(O)_2$ ($E_b(2O)$, eV) with I_h and O_h structures..... | S4 |
| Spin multiplicity (S)..... | S4 |
| Table S2. Spin multiplicities of important species..... | S4 |
| d-band center..... | S5 |
| Table S3. The d-band center (ε_d , eV) of 4d orbital in $M_{55}(O^{fcc})_2$ and M_{55} , ($M = Pd, Rh$) in the level of PBE, PBE0 and HSE06..... | S5 |
| Table S4. The Fermi level (ε_F , eV), d-valance band top (ε_{VB} , eV), d-conduction band bottom (ε_{CB} , eV), and band gap (ΔE , eV) in $M_{55}(O^{fcc})_2$ and M_{55} , ($M = Pd, Rh$) in the level of PBE, PBE0 and HSE06..... | S6 |
| Table S5. The electron populations (in e) of H^1 and C atoms and allyl species..... | S6 |
| O_2 dissociative adsorption on the Pd_{55} cluster..... | S7 |
| Figure S1. Energy profile of O_2 dissociative adsorption on the Pd surface..... | S7 |
| Active species..... | S7 |
| Figure S2. The relative energies (in kcal/mol) of $Pd_{55}(O^{hcp})_1$ and other $Pd_{55}(O)_1$ species. The numbers below the structure represent the relative energy to $Pd_{55}(O^{hcp})_1$ | S7 |
| Figure S3. The relative energies (in kcal/mol) of 1_Pd_a and 1_Pd_b of $Pd_{55}(O)_2$ species. The numbers below the structure represent the relative energy to 1_Pd_a | S7 |
| Figure S4. The relative energy (ΔE relative to $Rh_{55}(O^{fcc})_1$, in kcal/mol) of $Rh_{55}(O)_1$ species..... | S8 |
| Stepwise C-H activation of CH_3 group on Pd_{55} cluster..... | S8 |
| Figure S5. Energy profile of stepwise C-H activation of CH_3 group on Pd_{55} cluster.. | S8 |
| One-step C-H activation of CH_3 group on Rh cluster..... | S9 |
| Figure S6. Energy profile of one-step C-H activation of CH_3 group on Rh_{55} particle .. | S9 |
| Partial Density of states (DOS) | S9 |

| | |
|--|------------|
| Figure S7. Partial density of states (PDOS) of 4d orbital in $M_{55}(O^{fcc})_2$ and M_{55} , ($M=Pd, Rh$) by PBE0 functional..... | S9 |
| Figure S8. Partial density of states (PDOS) of 4d orbital in $M_{55}(O^{fcc})_2$ and M_{55} , ($M=Pd, Rh$) by PBE functional..... | S10 |
| Allyl alkoxide formation on Pd_{55} and Rh_{55} cluster..... | S10 |
| Figure S9. Energy profile of allyl alkoxide formation on Pd_{55} cluster..... | S10 |
| Figure S10. Energy profile of allyl alkoxide formation on Rh_{55} cluster..... | S11 |
| Second C-H bond cleavage on Pd_{55} and Rh_{55} cluster..... | S11 |
| Figure S11. Energy profile of the second C-H activation via step-wise H-transfer and acrolein formation on Pd_{55} | S11 |
| Figure S12. Energy profile of the second C-H bond cleavage via oxidative addition to Rh_{55} cluster..... | S12 |
| Electron density difference of propene adsorption 2_Pd..... | S12 |
| Figure S13. The electron density difference of propene coordinated intermediate 2_Pd. Blue: electron increase, purplish red: electron decrease..... | S12 |
| Structure change of Pd_{55} cluster during the reaction via H-transfer mechanism..... | S13 |
| Table S7. The Pd-Pd distances and changes (in Å)..... | S13 |
| Election population change of key Pd centers during the reaction via H-transfer mechanism..... | S15 |
| Table S8. Atomic populations and their changes (in e)..... | S15 |
| Changes in Pd-Pd distance and Pd atomic population in the reaction via H-transfer mechanism..... | S16 |
| Changes in electron population of Pd centers during the reaction via H-transfer mechanism..... | S19 |
| Figure S14. Changes in electron population (in e)..... | S19 |
| Coordinate Cartesian..... | S20 |

Stability of icosahedral (I_h) and octahedral (O_h) Pd_{55} cluster.

Table S1. The relative energies (in kcal/mol) of icosahedral (I_h) and octahedral (O_h) Pd_{55} cluster and Pd-O bond energy BDE(Pd-O) (in eV) of $Pd_{55}(O)$ with I_h and O_h structures.

| | ΔE | BDE(Pd-O) |
|-------|------------|-----------|
| I_h | 0.00 | 6.63 |
| O_h | 8.53 | 6.35 |

The I_h structure is more stable than the O_h but the Pd-O bond energy is similar between the I_h and O_h structures. These computational results do not provide strong support to the use of icosahedral M_{55} as a model, because the lowest energy species is not always good catalyst. However, these results are not inconsistent with the use of icosahedral M_{55} . Also, we performed full geometry optimization of intermediate and transition state without any constraint.

Spin multiplicity (S)

Table S2. Spin multiplicities of important species.

(A) Spin multiplicities of important species in **Figure 1**.

| 1_Pda | 2_Pd | TS1_Pd _{C1} | 3_Pd _{C1} | TS1_Pd _{C2} |
|--------------------|---------------------|----------------------|---------------------|----------------------|
| 15et | 13et | 21et | 17et | 21et |
| <hr/> | | | | |
| 3_Pd _{C2} | TS2_Pd _C | 4_Pd _C | TS3_Pd _C | 5_Pd _C |
| 19et | 23et | 21et | 23et | 23et |

(B) Spin multiplicities of important species in **Figure 2**.

| 1_Rha | 2_Rh | TS1_Rh _{C1} | 3_Rh _{C1} | TS1_Rh _{C2} | 3_Rh _{C2} | 4_Rh _C | 5_Rh _C |
|-------|------|----------------------|--------------------|----------------------|--------------------|-------------------|-------------------|
| | | | | | | | |

| | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|
| 2et | 2et | 6et | 2et | 2et | 2et | 6et | 2et |
|-----|-----|-----|-----|-----|-----|-----|-----|

(C) Spin multiplicities of important species in **Figure 3**.

| TS1_Pd | 3_Pd | TS2_Pd _{OH} | 4_Pd _{OH} | TS3_Pd _{OH} |
|-----------------------|--------|----------------------|--------------------|----------------------|
| 13et | 19et | 15et | 13et | 23et |
| 4_Pd _{OH} _2 | TS4_Pd | 5_Pd | TS5_Pd | 6_Pd |
| 21et | 23et | 25et | 23et | 23et |

(D) Spin multiplicities of important species in **Figure 4**.

| TS1_Rh_S | 3_Rh_S | TS2_Rh_S | 3_Rh | TS3_Rh _{OH} |
|--------------------|-----------------------|----------|------|----------------------|
| 4et | 6et | 2et | 2et | 2et |
| 4_Rh _{OH} | 4_Rh _{OH} _2 | TS4_Rh | 5_Rh | 6_Rh |
| 2et | 6et | 4et | 2et | 4et |

d-Band center

Table S3. The d-band center (ε_d , eV) of 4d orbital in $M_{55}(O^{fcc})_2$ and M_{55} , ($M = Pd, Rh$) in the level of PBE, PBE0 and HSE06.

| ε_d | Pd ₅₅ | Rh ₅₅ | Pd ₅₅ (O ^{fcc}) ₂ | Rh ₅₅ (O ^{fcc}) ₂ |
|-----------------|------------------|------------------|---|---|
| PBE | -1.97 | -2.48 | -2.04 | -2.57 |
| PBE0 | -2.50 | -3.10 | -2.56 | -3.20 |
| HSE06 | -2.37 | -3.02 | -2.69 | -3.05 |

We firstly tried to discuss the results using d-band center, because it has been used as one important property in discussing the catalytic activity. The d-band centers of Pd₅₅, Pd₅₅(O^{fcc})₂, Rh₅₅ and Rh₅₅(O^{fcc})₂ are calculated using PBE, PBE0, and HSE06 functionals. As listed in Table S3 in the Supporting Information, the d-band centers of Pd₅₅ and Pd₅₅(O^{fcc})₂ are at higher energy than those of Rh₅₅ and Rh₅₅(O^{fcc})₂, respectively. As discussed in the main text, propene adsorption occurs mainly through back-donation

from metal surface to propene and the binding energy of propene is larger in $\text{Rh}_{55}(\text{O})_2$ than in $\text{Pd}_{55}(\text{O})_2$. These results suggest that the high energy d orbital leads to the formation of strong propene adsorption. However, the d-band center of $\text{Rh}_{55}(\text{O})_2$ is at lower energy than that of $\text{Pd}_{55}(\text{O})_2$ (Table S3), which is not consistent with the larger binding energy of propene with $\text{Rh}_{55}(\text{O})_2$ than with $\text{Pd}_{55}(\text{O})_2$.

We expected that not all the d-orbitals but some of d-orbitals plays important roles for interaction of propene with metal particle. It has been discussed for long time that frontier orbitals such as the highest energy occupied orbital (HOMO) and the lowest energy unoccupied orbital (LUMO) play important roles in the intermolecular interaction and chemical reaction. The HOMO corresponds to the valence band-top. Actually, the d-valence band-top is calculated at higher energy in Rh_{55} and $\text{Rh}_{55}(\text{O}^{\text{fcc}})_2$ than that in Pd_{55} and $\text{Pd}_{55}(\text{O}^{\text{fcc}})_2$, respectively (Table S4). We wish to propose that the d-valence band-top, as well as the d-band center, is useful for discussion of the interaction and reaction of substrate with metal particle.

Table S4. The Fermi level (ε_F , eV), d-valance band top (ε_{VB} , eV), d-conduction band bottom (ε_{CB} , eV), and band gap (ΔE , eV) in $\text{M}_{55}(\text{O}^{\text{fcc}})_2$ and M_{55} , (M= Pd, Rh) in the level of PBE, PBE0 and HSE06.

| Pd ₅₅ | | | Rh ₅₅ | | | Pd ₅₅ (O ^{fcc}) ₂ | | | Pd ₅₅ (O ^{fcc}) ₂ | | | |
|---------------------------|-------|-------|------------------|-------|-------|---|-------|-------|---|-------|-------|-------|
| PBE | PBE0 | HSE06 | PBE | PBE0 | HSE06 | PBE | PBE0 | HSE06 | PBE | PBE0 | HSE06 | |
| ε_F | -3.99 | -4.22 | -3.93 | -3.81 | -4.04 | -3.78 | -4.05 | -4.34 | -4.03 | -3.89 | -4.01 | -3.82 |
| ε_{VB} | -3.99 | -4.28 | -3.99 | -3.82 | -4.08 | -3.80 | -4.14 | -4.41 | -4.12 | -4.08 | -4.14 | -3.90 |
| ε_{CB} | -3.97 | -3.50 | -3.78 | -3.79 | -3.22 | -3.54 | -3.97 | -3.62 | -3.74 | -3.83 | -3.31 | -3.54 |
| ΔE | 0.02 | 0.78 | 0.21 | 0.03 | 0.86 | 0.26 | 0.17 | 0.79 | 0.38 | 0.25 | 0.83 | 0.36 |

Table S5. The electron populations (in e) of H¹ and C atoms and allyl species.

| Species | C ¹ | C ² | C ³ | H ¹ | C ₃ H ₅ |
|-----------------|----------------|----------------|----------------|----------------|-------------------------------|
| 2_Pd | 4.113 | 4.110 | 4.141 | 0.901 | 17.000 |
| TS1_Pd | 4.539 | 4.171 | 4.467 | 0.654 | 17.113 |
| 3_Pd | 4.154 | 4.110 | 4.111 | 0.372 | 16.956 |
| 2_Rh | 4.133 | 4.105 | 4.290 | 0.921 | 17.100 |
| TS1_Rh_S | 4.250 | 4.116 | 4.258 | 0.993 | 16.999 |

| | | | | | |
|---------------|-------|-------|-------|-------|--------|
| 3_Rh_S | 4.101 | 4.188 | 4.216 | 1.126 | 17.050 |
|---------------|-------|-------|-------|-------|--------|

O₂ dissociative adsorption on the Pd₅₅ cluster.

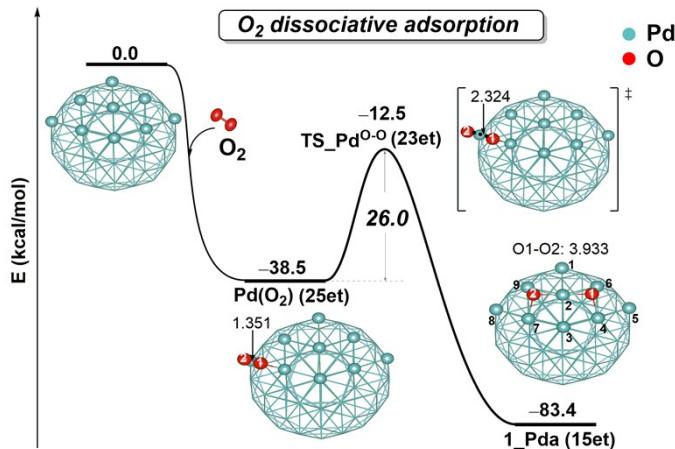


Figure S1. Energy profile of O₂ dissociative adsorption on the Pd surface.

Active species

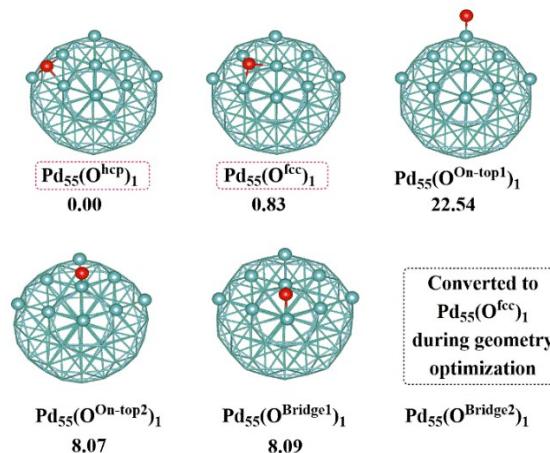


Figure S2. The relative energies (in kcal/mol) of Pd₅₅(O^{hcp})₁ and other Pd₅₅(O)₁ species. The numbers below the structure represent the relative energy to Pd₅₅(O^{hcp})₁.

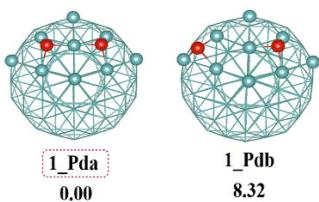


Figure S3. The relative energies (in kcal/mol) of **1_Pd_a** and **1_Pd_b** of $\text{Pd}_{55}(\text{O})_2$ species. The numbers below the structure represent the relative energy to **1_Pd_a**.

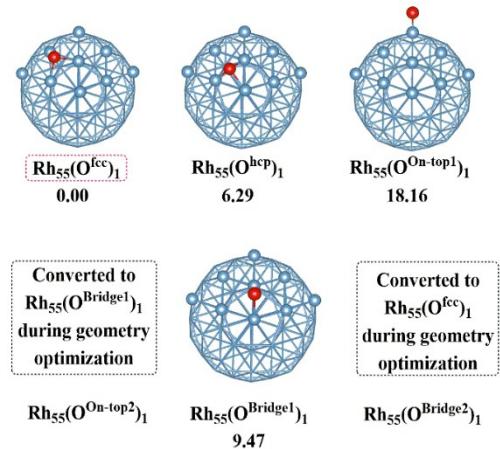


Figure S4. The relative energy (ΔE relative to $\text{Rh}_{55}(\text{O}^{\text{fcc}})_1$, in kcal/mol) of $\text{Rh}_{55}(\text{O})_1$ species.

Stepwise C-H activation of CH_3 group on Pd_{55} cluster

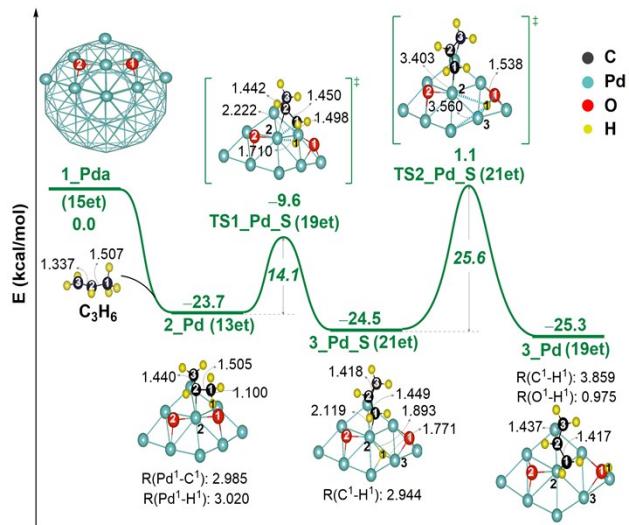


Figure S5. Energy profile of stepwise C-H activation of CH_3 group on Pd_{55} cluster.

One-step C-H activation of CH₃ group on Rh cluster

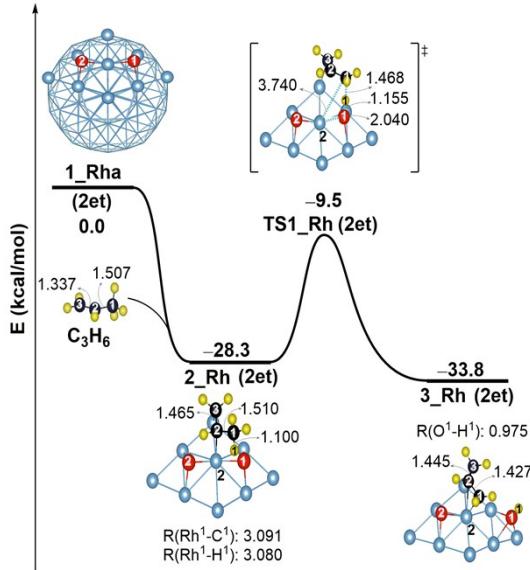


Figure S6. Energy profile of one-step C-H activation of CH₃ group on Rh₅₅ cluster.

Partial Density of states (DOS)

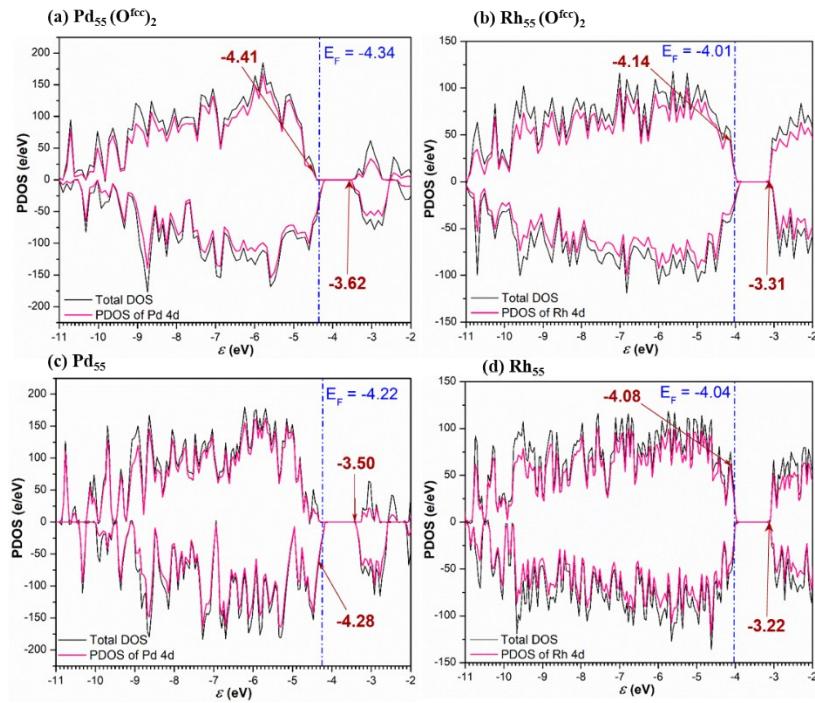


Figure S7. PBE0-calculated Partial density of states (PDOS) of 4d orbital in M₅₅(O^{fcc})₂ and M₅₅, (M = Pd, Rh).

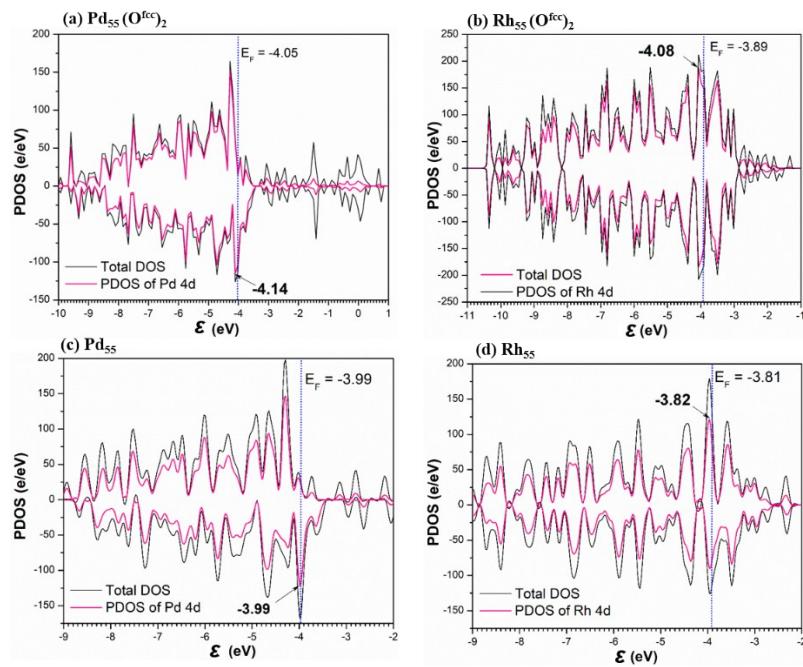


Figure S8. PBE-calculated Partial density of states (PDOS) of 4d orbital in $\text{M}_{55}(\text{O}^{\text{fcc}})_2$ and M_{55} , (M= Pd, Rh).

Allyl alkoxide formation on Pd_{55} and Rh_{55} cluster

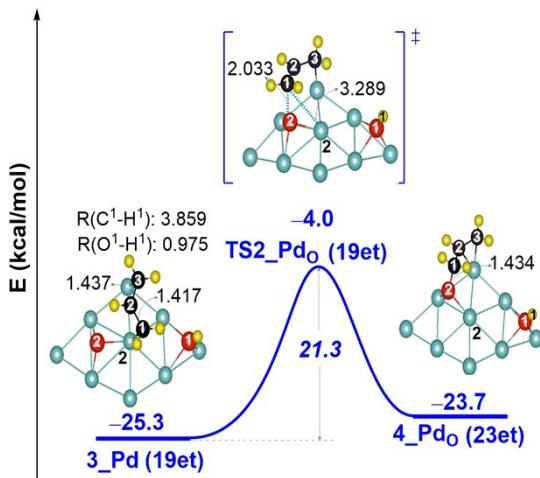


Figure S9. Energy profile of allyl alkoxide formation on Pd_{55} cluster.

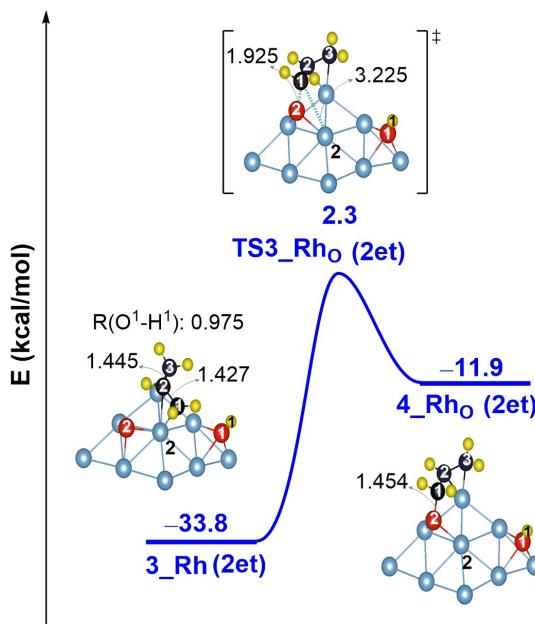


Figure S10. Energy profile of allyl alkoxide formation on Rh_{55} cluster.

Second C-H bond cleavage on Pd_{55} and Rh_{55} cluster

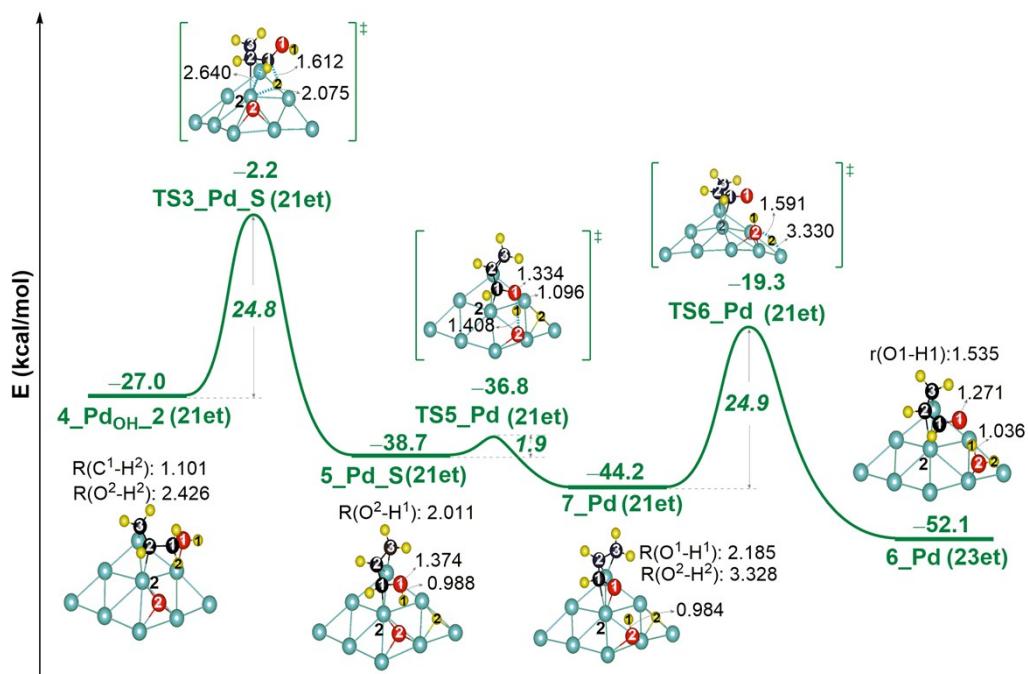


Figure S11. Energy profile of the second C-H activation via step-wise H-transfer and acrolein formation on Pd_{55} .

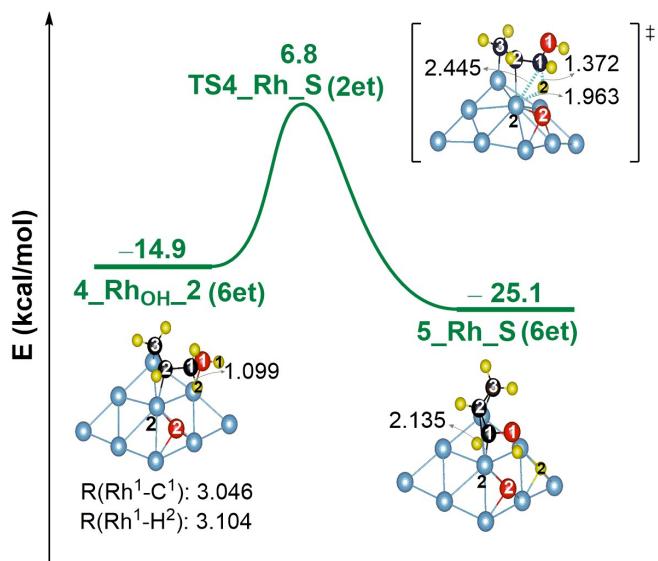


Figure S12. Energy profile of the second C-H bond cleavage via oxidative addition to Rh₅₅ cluster.

Electron density difference of propene adsorption 2_Pd

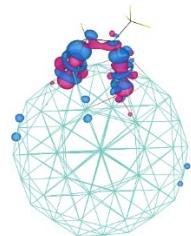


Figure S13. The difference $\Delta\rho$ in electron density by propene adsorption to Pd₅₅(O)₂.
2_Pd, where $\Delta\rho = \rho(2\text{-Pd}) - \{\rho(1\text{-Pd}) + \rho(\text{C}_3\text{H}_6)\}$. Blue represents increase in electron density and purplish red represents decrease in electron density.

Figure 13 clearly shows that charge transfer (CT) occurs mainly from the surface Pd¹ and Pd² atoms to propene π^* orbital, while the other Pd atoms do not participate very much in the CT. The moderate decrease in density in propene π orbital indicates that CT also occurs from propene to the Pd surface, but its decrease is much less than the density increase in the π^* orbital. These features are consistent with the results of the Bader charge (Table S6) showing that the back-donation to propene from Pd particle is stronger than the donation to Pd particle from propene.

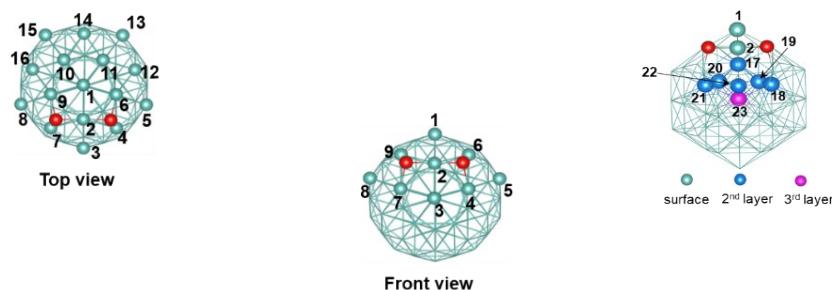
Bader charge

Table S6. The C atomic population (in e) in **C₃H₆**, **2_Pd** and **2_Rh**.

| Species | C ¹ | C ² | C ³ |
|-----------------------------------|----------------|----------------|----------------|
| C₃H₆ | 4.135 | 4.178 | 4.068 |
| 2_Pd | 4.113 | 4.110 | 4.141 |
| 2_Rh | 4.133 | 4.105 | 4.290 |

Structure change of Pd₅₅ cluster during the reaction via H-transfer mechanism.

Table S7. The Pd-Pd distances and changes (in Å).^a



| 1_Pda | 2_Pd | TS1_Pd | 3_Pd | TS2_Pd _{OH} | 4_Pd _{OH} |
|-------|------|--------|------|----------------------|--------------------|
| | | | | | |

| | | Pd¹-C² | | Pd¹-C² | |
|--|--|--|--|--|--|
| | | Pd¹-C³ | Pd¹-C² | Pd¹-C³ | Pd¹-C² |
| Pd¹-Pd² | Pd⁸-Pd¹ | 2.721 (-0.103) | 2.774(-0.048) | 2.781 (-0.043) | 2.801(-0.023) |
| Pd¹-Pd⁶ | Pd⁷-Pd¹ | 2.772 (-0.024) | 2.727(-0.069) | 2.737 (-0.059) | 2.852(0.056) |
| Pd¹-Pd⁹ | Pd⁶-O¹ | 2.791 (-0.005) | 2.863(0.067) | 2.818 (-0.022) | 2.772 (-0.024) |
| Pd¹-Pd¹⁰ | Pd²-O² | 2.759 | 2.828(-0.069) | 2.851(0.092) | 2.755(-0.060) |
| Pd¹-Pd¹¹ | Pd⁷-O² | 2.761 | 2.844(-0.053) | 2.792 (0.031) | 2.768(-0.077) |
| Pd²-Pd³ | Pd⁷-O² | 2.816 | 2.791(-0.025) | 2.796 (-0.02) | 2.802(-0.014) |
| Pd⁴-Pd⁵ | Pd²-O² | 2.770 | 2.808(-0.128) | 2.793 (-0.023) | 3.012(0.242) |
| Pd⁴-Pd⁶ | | 2.976 | 2.848(-0.128) | 3.058(0.080) | 2.878(-0.098) |
| Pd⁵-Pd⁶ | | 2.771 | 2.750 (-0.021) | 2.711(-0.060) | 2.986 (0.215) |
| Pd⁸-Pd⁹ | | 2.770 | 2.754 (-0.016) | 2.797 (0.027) | 2.770 (0.000) |
| Pd¹⁰-Pd¹⁵ | | 2.764 | 2.772 (0.008) | 2.786 (0.022) | 2.772 (0.008) |
| Pd¹¹-Pd¹³ | | 2.762 | 2.771 (0.009) | 2.764 (0.020) | 2.777 (0.015) |
| | | | | | 2.768 (0.006) |
| | | | | | 2.785 (0.023) |
| Pd¹-Pd¹⁷ | | 2.622 | 2.669 (0.047) | 2.599 (-0.023) | 2.656 (0.034) |
| Pd²-Pd¹⁷ | | 2.919 | 2.844 (-0.075) | 2.916 (-0.003) | 2.839 (-0.080) |
| Pd¹⁷-Pd¹⁸ | | 2.735 | 2.775 (0.040) | 2.748 (0.013) | 2.783 (0.048) |
| Pd¹⁸-Pd²³ | | 2.575 | 2.591 (0.016) | 2.579 (0.004) | 2.599 (0.024) |
| Pd¹⁷-Pd²³ | | 2.597 | 2.599 (0.002) | 2.660 (0.063) | 2.619 (0.022) |
| | | | | | 2.595 (-0.002) |
| | | | | | 2.614 (0.017) |
| TS3_Pd | | 4_Pd_{OH}_2 | TS4_Pd | 5_Pd | TS5_Pd |
| | | | | | 6_Pd |
| | | | | | |
| | | | Pd¹-C³ | Pd¹-C³ | Pd¹-C³ |
| | | Pd¹-C² | Pd²-C¹ | Pd¹-C² | Pd¹-C³ |
| | | Pd¹-C³ | Pd²-C² | Pd²-C² | Pd¹-C² |
| | Pd⁶-O¹H¹ | Pd⁶-O¹H¹ | Pd⁶-O¹H¹ | Pd²-C² | Pd¹-C² |
| | Pd²-O² | Pd²-O² | Pd²-O²H² | Pd⁶-O¹H¹ | Pd²-C² |
| | Pd³-O² | Pd³-O² | Pd³-O²H² | Pd³-O²H² | Pd²-C² |
| | | Pd⁴-O² | Pd⁴-O²H² | Pd⁴-O²H² | Pd⁴-O²(H)₂ |
| Pd¹-Pd² | | 2.713(-0.111) | 2.678 (-0.146) | 2.693 (-0.131) | 2.712(-0.112) |
| Pd¹-Pd⁶ | | 2.877(0.081) | 2.938 (0.142) | 2.839 (0.043) | 2.761(-0.035) |
| Pd¹-Pd⁹ | | 2.740(-0.056) | 2.694(-0.102) | 2.809 (0.013) | 2.838(0.042) |
| Pd¹-Pd¹⁰ | | 2.733(-0.026) | 2.709 (-0.05) | 2.763(0.004) | 2.837(0.078) |
| Pd¹-Pd¹¹ | | 2.785(0.024) | 2.795(0.034) | 2.773(0.012) | 2.812(0.051) |
| Pd²-Pd³ | | 2.942(0.126) | 2.951(0.135) | 2.917 (0.101) | 2.785(-0.031) |
| Pd⁴-Pd⁵ | | 2.785(0.015) | 2.775(0.005) | 2.693(-0.077) | 2.726(-0.044) |
| Pd⁴-Pd⁶ | | 2.868(-0.108) | 2.932(-0.044) | 2.842(-0.134) | 2.854(-0.122) |
| Pd⁵-Pd⁶ | | 2.743(-0.028) | 2.765(-0.006) | 2.819 (0.048) | 2.794 (0.023) |
| Pd⁸-Pd⁹ | | 2.766(-0.004) | 2.739(-0.031) | 2.749(-0.021) | 2.746(-0.024) |
| | | | | | 2.754(-0.016) |
| | | | | | 2.776 (0.006) |

| | | | | | | |
|--|---------------|---------------|---------------|---------------|---------------|---------------|
| Pd¹⁰-Pd¹⁵ | 2.773(0.009) | 2.768(0.004) | 2.780(0.016) | 2.790(0.026) | 2.788(0.024) | 2.784(0.020) |
| Pd¹¹-Pd¹³ | 2.777(0.015) | 2.788(0.026) | 2.773(0.011) | 2.786(0.024) | 2.779(0.017) | 2.798(0.036) |
| Pd¹-Pd¹⁷ | 2.633(0.011) | 2.645(0.023) | 2.656(0.034) | 2.666 (0.044) | 2.665(0.043) | 2.669(0.047) |
| Pd²-Pd¹⁷ | 2.851(-0.068) | 2.827(-0.092) | 2.764(-0.155) | 2.773(-0.146) | 2.779(-0.140) | 2.800(-0.119) |
| Pd¹⁷-Pd¹⁸ | 2.688(-0.047) | 2.698(-0.037) | 2.760(0.025) | 2.754(0.019) | 2.765(0.030) | 2.760(0.025) |
| Pd¹⁸-Pd²³ | 2.610(0.035) | 2.609(0.034) | 2.604(0.029) | 2.613(0.038) | 2.612(0.037) | 2.604(0.029) |
| Pd¹⁷-Pd²³ | 2.611(0.014) | 2.606(0.009) | 2.612(0.015) | 2.614(0.017) | 2.609(0.012) | 2.598(0.001) |

^a In parenthesis is difference of Pd-Pd distance relative to that in **1_Pda**.

Election population change of key Pd centers during the reaction via H-transfer mechanism.

Table S8. Pd atomic populations and their changes (in e^-).^a

| | 1_Pda | 2_Pd | TS1_Pd | 3_Pd | TS2_Pd_{OH} | 4_Pd_{OH} |
|-------------------------------------|--------------|-------------------------------------|-------------------------------------|--|--|--|
| | | Pd¹-C² | Pd¹-C² | Pd¹-C² | | |
| Pd²-O¹ | | Pd¹-C³ | Pd¹-C³ | Pd¹-C³ | Pd¹-C² | Pd¹-C² |
| Pd⁴-O¹ | | Pd²-C¹ | Pd²-O¹ | Pd²-C¹ | Pd¹-C³ | Pd¹-C³ |
| Pd⁶-O¹ | | Pd²-O¹ | Pd⁴-O¹ | Pd⁴-O¹H¹ | Pd⁶-O¹H¹ | Pd⁶-O¹H¹ |
| Pd²-O² | | Pd⁴-O¹ | Pd⁶-O¹ | Pd⁵-O¹H¹ | Pd²-O² | Pd²-O² |
| Pd⁷-O² | | Pd⁶-O¹ | Pd²-O² | Pd⁶-O¹H¹ | Pd⁷-O² | Pd⁷-O² |
| Pd⁹-O² | | Pd²-O² | Pd⁷-O² | Pd²-O² | Pd⁹-O² | Pd⁹-O² |
| | | Pd⁹-O² | Pd⁹-O² | Pd⁹-O² | | |
| Pd¹ | 10.059 | 9.959 (-0.100) | 9.931(-0.128) | 9.963(-0.095) | 9.922(-0.137) | 9.951(-0.108) |
| Pd² | 9.499 | 9.454 (-0.046) | 9.637(0.138) | 9.686(0.187) | 9.762(0.263) | 9.705(0.206) |
| Pd³ | 10.056 | 10.069 (0.013) | 10.007(-0.049) | 10.054(-0.001) | 10.056(0.000) | 10.078(0.022) |
| Pd⁴ | 9.748 | 9.756 (0.007) | 9.863(0.115) | 9.864(0.116) | 10.024(0.277) | 10.042(0.294) |
| Pd⁵ | 10.055 | 10.045(-0.010) | 10.008(-0.047) | 9.870(-0.185) | 10.051(-0.004) | 10.105(0.050) |
| Pd⁶ | 9.752 | 9.762(0.011) | 9.834(0.083) | 9.849(0.098) | 9.792(0.040) | 9.903(0.152) |
| Pd⁷ | 9.755 | 9.751(-0.005) | 9.817(0.061) | 9.741(-0.015) | 9.751(-0.005) | 9.749(-0.006) |
| Pd⁸ | 10.040 | 10.048(0.008) | 9.997(-0.043) | 10.048(0.008) | 10.056(0.016) | 10.048(0.008) |
| Pd⁹ | 9.749 | 9.769(0.020) | 9.825(0.076) | 9.762(0.013) | 9.759(0.010) | 9.761(0.012) |
| Pd¹⁰ | 10.023 | 10.043(0.020) | 10.024(0.002) | 10.053(0.030) | 10.026(0.004) | 10.045(0.022) |
| Pd¹¹ | 10.016 | 10.047(0.031) | 10.024(0.008) | 10.025(0.009) | 10.009(-0.007) | 10.025(0.009) |
| Pd¹² | 10.015 | 10.021(0.006) | 10.023(0.008) | 10.010(-0.005) | 9.997(-0.018) | 10.006(-0.009) |
| Pd¹³ | 10.064 | 10.069(0.004) | 10.011(-0.053) | 10.069(0.005) | 10.065(0.001) | 10.069(0.004) |
| Pd¹⁴ | 10.012 | 10.011(-0.001) | 10.021(0.009) | 10.009(-0.003) | 10.009(-0.003) | 10.014(0.002) |
| Pd¹⁵ | 10.068 | 10.067(0.001) | 10.014(-0.054) | 10.065(-0.004) | 10.076(0.008) | 10.072(0.004) |
| Pd¹⁶ | 10.021 | 10.023(0.002) | 10.025(0.003) | 10.026(0.004) | 10.023(0.002) | 10.022(0.001) |
| Pd¹⁷ | 9.947 | 9.963 (0.016) | 9.982 (0.035) | 9.978(0.031) | 9.982(0.035) | 9.963(0.016) |

| Pd¹⁸ | 9.937 | 9.934 (-0.003) | 9.963(0.026) | 9.930(-0.007) | 9.950(0.013) | 9.925(-0.012) |
|------------------------|--|--|---|---|---|---|
| Pd²³ | 10.027 | 10.023(-0.004) | 9.985(-0.042) | 10.024(-0.003) | 10.027(0.000) | 10.021(-0.006) |
| TS3_Pd | 4_Pd_{OH}_2 | TS4_Pd | 5_Pd | TS5_Pd | 6_Pd | |
| | | | Pd¹-C³ | Pd¹-C³ | Pd¹-C³ | |
| | Pd¹-C² | Pd¹-C³ | Pd²-C¹ | Pd¹-C² | Pd¹-C³ | Pd¹-C³ |
| | Pd¹-C³ | Pd²-C² | Pd²-C² | Pd¹-C² | Pd¹-C² | Pd¹-C³ |
| | Pd⁶-O¹H¹ | Pd⁶-O¹H¹ | Pd⁶-O¹H¹ | Pd⁶-O¹H¹ | Pd²-C² | Pd¹-C² |
| | Pd²-O² | Pd²-O² | Pd²-O² H² | Pd³-O² H² | Pd³-O² H² | Pd²-C² |
| | Pd³-O² | Pd⁴-O² | Pd³-O² H² | Pd⁴-O² H² | Pd⁴-O² H² | Pd⁴-O² (H)₂ |
| | | | Pd⁴-O² H² | | | |
| Pd¹ | 9.978(-0.081) | 9.975(-0.083) | 9.975(-0.083) | 9.969(-0.090) | 9.962(-0.097) | 9.9590(-0.010) |
| Pd² | 9.679(0.180) | 9.724(0.225) | 9.873(0.374) | 9.887(0.387) | 9.887(0.388) | 9.899(0.400) |
| Pd³ | 9.754(-0.301) | 9.802(-0.253) | 9.814(-0.242) | 9.904(-0.152) | 9.937(-0.119) | 10.055(-0.001) |
| Pd⁴ | 9.975(0.227) | 9.781(0.033) | 9.785(0.036) | 9.838(0.090) | 9.856(0.107) | 10.055(0.307) |
| Pd⁵ | 10.092(0.037) | 10.092(0.037) | 10.071(0.016) | 10.062(0.008) | 10.066(0.011) | 10.079(0.023) |
| Pd⁶ | 9.879(0.129) | 9.886(0.135) | 9.965(0.213) | 9.838(0.090) | 9.989(0.237) | 9.982(0.231) |
| Pd⁷ | 9.994(0.239) | 10.028(0.273) | 10.028(0.272) | 10.038(0.283) | 10.026(0.270) | 10.017(0.262) |
| Pd⁸ | 10.070(0.030) | 10.073(0.033) | 10.073(0.034) | 10.072(0.032) | 10.072(0.032) | 10.076(0.036) |
| Pd⁹ | 10.008(0.259) | 10.020(0.271) | 10.020(0.271) | 10.012(0.263) | 10.013(0.264) | 10.012(0.263) |
| Pd¹⁰ | 10.029(0.006) | 10.028(0.006) | 10.027(0.005) | 10.030(0.007) | 10.028(0.005) | 10.026(0.003) |
| Pd¹¹ | 10.026(0.001) | 10.027(0.011) | 10.026(0.001) | 10.032(0.016) | 10.028(0.012) | 10.029(0.013) |
| Pd¹² | 10.006(-0.009) | 10.009(-0.006) | 10.001(-0.014) | 10.000(-0.015) | 9.995(-0.020) | 9.999(-0.016) |
| Pd¹³ | 10.065(0.001) | 10.070(0.006) | 10.070(0.006) | 10.070(0.007) | 10.075(0.010) | 10.077(0.012) |
| Pd¹⁴ | 10.011(-0.001) | 10.010(-0.002) | 10.001(-0.011) | 10.010(-0.002) | 10.006(-0.006) | 10.004(-0.008) |
| Pd¹⁵ | 10.070(0.001) | 10.069(0.001) | 10.073(0.004) | 10.065(-0.003) | 10.065(-0.003) | 10.071(0.002) |
| Pd¹⁶ | 10.006(-0.016) | 10.007(-0.015) | 10.006(-0.016) | 10.011(-0.010) | 10.016(-0.005) | 10.010(-0.011) |
| Pd¹⁷ | 9.956(0.009) | 9.951(0.004) | 9.954(0.007) | 9.963(0.016) | 9.953(0.006) | 9.949(0.002) |
| Pd¹⁸ | 9.930(-0.007) | 9.943(0.006) | 9.940(0.003) | 9.944(0.007) | 9.935(-0.002) | 9.938(0.001) |
| Pd²³ | 10.025(-0.002) | 10.029(0.002) | 10.029(0.002) | 10.032(0.005) | 10.029(0.002) | 10.035(0.008) |

^a In parenthesis is difference of Pd atomic population relative to that in **1_Pda**.

Changes in Pd-Pd distance and Pd atomic population in the reaction via H-transfer mechanism

We explored here how much Pd-Pd distance and Pd atomic population change in the H-transfer mechanism, as shown in Tables S7 and S8 and Figure S14. In the discussion below, we will describe “the Pd-Pd distance substantially changes” when its change is more than 0.1 Å, “considerably changes” when its change is less than 0.1 Å but larger than 0.02 Å, and “somewhat changes” when its change is less than 0.02 Å but more than 0.01 Å. We will describe “the Pd atomic population substantially changes” when its change is larger than 0.1 e, “considerably changes” when its change

is less than 0.1 e but larger than 0.02 e , and “somewhat changes” when its change is less than 0.02 e but larger than 0.01 e .

In the first step, propene is adsorbed at Pd¹ (**1_Pda** → **2_Pd**). We found that Pd¹-Pd², Pd⁴-Pd⁵, and Pd⁴-Pd⁶ distances substantially change (by more than 0.1 Å), Pd¹-Pd¹⁰ and Pd¹-Pd¹¹ distances considerably change (by more than 0.05 Å), and Pd¹-Pd⁶ distance somewhat changes. Other Pd-Pd distances on the surface change little or moderately. The Pd¹-Pd¹⁷, Pd²-Pd¹⁷ and Pd¹⁷-Pd¹⁸ distances somewhat change, while the Pd¹⁷-Pd²³ distance changes little. Because Pd¹⁷ belonging to the Pd₁₃ core is just below Pd¹ and Pd²³ is at the center of Pd₅₅, Pd atoms in the second layer are not influenced very much by propene adsorption except for the Pd¹⁷ atom and the Pd²³ atom at the center of Pd₅₅ is influenced little by propene adsorption. Consistent with these changes in Pd-Pd distance, Pd¹ atomic population decreases substantially, Pd², Pd⁹, Pd¹⁰, and Pd¹¹ atomic populations considerably change, and the Pd³ and Pd⁶ atomic populations somewhat change. However, other Pd atomic populations change little; see Table S8 and Figure S14. It is likely that the Pd atomic population is less sensitive to the reaction than the Pd-Pd distance.

In the first C-H activation process (**2_Pd** → **3_Pd**), the O atom interacting with the Pd⁴, Pd⁵, and Pd⁶ in **2_Pd** reacts with the H¹ atom to afford an OH¹ group on the Pd⁶ in **3_Pd**. The Pd⁴-Pd⁵ and Pd⁵-Pd⁶ distances substantially changes (by about 0.1 Å and 0.23 Å, respectively), and the Pd¹-Pd², Pd¹-Pd⁶, Pd¹-Pd¹⁰, Pd¹-Pd¹¹, and Pd⁴-Pd⁶ distances considerably change, and the Pd¹-Pd⁹ and Pd²-Pd³ distances somewhat change. But, other Pd-Pd distances change moderately or little. In the inside core, the Pd¹-Pd¹⁷ and Pd¹⁷-Pd²³ distances somewhat change, where Pd¹⁷ could be considerably influenced by the reaction because it exists below Pd⁵. The Pd¹⁷-Pd²³ distance considerably increases at **TS1_Pd** but then decreases. These results indicate the geometry changes occur around the Pd¹, Pd⁵ and Pd⁶ but other moiety does not change very much; remember that the Pd¹ bonding nature significantly change in this step because the C-C double bond of propene interacts with Pd¹ in **2_Pd** but it is converted to π-allyl interacting mainly with Pd¹ in **3_Pd**. The Pd², Pd⁴, and Pd⁵ atomic populations substantially change, the Pd⁶ and Pd¹¹ atomic populations considerably change, and Pd³, Pd⁷, and Pd¹⁰ atomic populations somewhat change. Other Pd atomic populations change moderately or little; see Table S4 and Figure S8. These results show again that the Pd atomic populations change in limited area on which the propene is converted to π-allyl.

The next is the allyl-alcohol formation process (**3_Pd** → **4_PdOH**). In this process, the OH group on the Pd⁶ reacts with the C¹ atom of the π-allyl group which is bound on the Pd¹ atom. The Pd¹-Pd¹⁰ and Pd⁵-Pd⁶ distances substantially change, the Pd¹-Pd², Pd¹-Pd⁹, Pd¹-Pd¹⁰, Pd²-Pd³, Pd⁴-Pd⁶, and Pd⁸-Pd⁹ distances considerably change, and the Pd¹⁰-Pd¹⁵ distances somewhat changes; see Table S3. In the core part, the Pd¹-Pd¹⁷ and Pd²-Pd¹⁷ distances considerably change and the Pd¹⁸-Pd²³ distance somewhat changes. The Pd¹⁷-Pd²³ distance changes little in this step. These results indicate that the geometry changes occur around the Pd atoms bound with the π-allyl and OH groups. The Pd⁴ and Pd⁵ atomic populations substantially change, the Pd², Pd³, and Pd⁶ atomic

populations considerably change, and the Pd¹ atomic population somewhat changes. In the Pd₁₃ core, the Pd¹⁷ atomic population somewhat changes but other Pd atomic populations change little. Again, these Pd-Pd distance and Pd atomic population change around the Pd atoms which directly participate in the reaction.

After the O² atom migration on the surface, the second C-H² activation of the CH₂OH group of allyl alcohol occurs to afford OH-substituted π-allyl group (**4_Pd_{OH}_2** → **5_Pd**). In this step, the H² moves to the O² atom bound with the Pd², Pd³, and Pd⁴ atoms on the surface and the Pd¹ interacts with the C¹-C² double bond in **4_Pd_{OH}_2** but the Pd¹ and Pd² interact with π-allyl in **5_Pd**. The Pd¹-Pd⁶ and Pd²-Pd³ distances substantially change, the Pd¹-Pd², Pd¹-Pd⁹, Pd¹-Pd¹⁰, Pd¹-Pd¹¹, Pd⁴-Pd⁵, Pd⁴-Pd⁶, Pd¹⁰-Pd¹⁵ distances considerably change, and the Pd¹-Pd¹¹ and Pd⁵-Pd⁶ distances somewhat change. Other Pd-Pd distances on the surface moderately change or little. In the Pd₁₃ core, the Pd¹-Pd¹⁷, Pd²-Pd¹⁷, and Pd¹⁷-Pd¹⁸ distances somewhat change. The Pd² and Pd³ atomic populations substantially change and the Pd⁴, Pd⁵, and Pd⁶ atomic populations considerably change, while other Pd atomic populations change moderately or little; Table S4 and Figure S8. The Pd-Pd distance and the Pd atomic population change in the limited area close to the reaction site.

The last step is H transfer from the OH group of the OH-substituted π-allyl to the O²H group on the Pd⁴, Pd⁵ and Pd⁶ atoms (**5_Pd** → **6_Pd**) to afford H₂O on the Pd⁴, Pd⁵ and Pd⁶ atoms, in which the Pd¹ interacts with the terminal C of OH-substituted π-allyl in **5_Pd** but interacts with the C-C double bond of acrolein in **6_Pd**. The geometry changes occur much less than in other elementary steps; the Pd¹-Pd⁹ and Pd⁴-Pd⁵ distances considerably change and the Pd²-Pd³, Pd⁴-Pd⁶, and Pd¹¹-Pd¹³ distances somewhat change. In the Pd₁₃ core part, Pd²-Pd¹⁷ distance considerably changes and the Pd¹⁷-Pd²³ distance somewhat changes. Other Pd-Pd distances change little or moderately. On the other hand, the Pd atomic populations change more than expected by the geometry changes. For instance, the Pd³, Pd⁴, and Pd⁶ atomic populations substantially change, the Pd⁷ atomic population considerably changes, and Pd², Pd⁵, and Pd¹⁷ atomic populations somewhat change. These results are reasonable because the OH group on the Pd⁴ is converted to H₂O in this step and the OH and H₂O are bound with Pd⁴, Pd⁵, and Pd⁶ atoms; in other words, the H₂O formation from H and OH induces significantly large changes in electron distribution.

During whole reaction, the Pd², Pd³, Pd⁴, Pd⁶, and Pd⁹ atomic populations significantly change, while other Pd atomic populations change moderately or little, as shown in Figure S8.

On the basis of the above results, it should be concluded that the geometry and electron distribution change around the Pd atoms on which the chemical reaction occurs. The influence to other part and inside is moderate except for several limited cases.

**Changes in electron population of Pd centers during the reaction via
H-transfer mechanism**

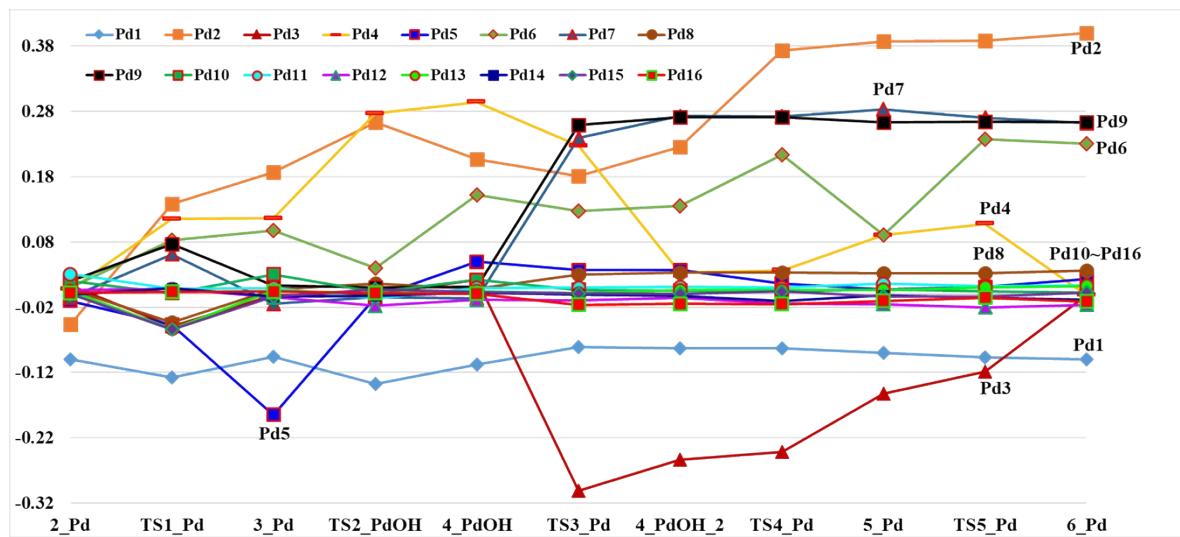


Figure S14. Changes in Pd atomic population (in e) relative to **1_Pd**.

Coordinate Cartesian

Pd₅₅ (Ih)

| | | | |
|----|-------------|-------------|-------------|
| Pd | 10.23417500 | 11.76377500 | 16.35482500 |
| Pd | 12.50000000 | 12.50000000 | 17.76052500 |
| Pd | 12.50000000 | 10.11762500 | 16.35492500 |
| Pd | 11.09960000 | 14.42742500 | 16.35487500 |
| Pd | 8.02537500 | 11.04615000 | 14.85230000 |
| Pd | 14.76582500 | 11.76377500 | 16.35482500 |
| Pd | 13.90040000 | 14.42742500 | 16.35487500 |
| Pd | 10.23422500 | 9.38140000 | 14.88237500 |
| Pd | 8.83397500 | 13.69117500 | 14.88235000 |
| Pd | 12.50000000 | 7.79502500 | 14.85260000 |
| Pd | 9.73440000 | 16.30642500 | 14.85250000 |
| Pd | 12.50000000 | 12.50000000 | 15.10350000 |
| Pd | 14.76577500 | 9.38140000 | 14.88237500 |
| Pd | 12.50000000 | 16.35482500 | 14.88235000 |
| Pd | 10.28547500 | 11.78042500 | 13.66437500 |
| Pd | 16.97462500 | 11.04615000 | 14.85230000 |
| Pd | 16.16602500 | 13.69117500 | 14.88235000 |
| Pd | 15.26560000 | 16.30642500 | 14.85250000 |
| Pd | 12.50000000 | 10.17132500 | 13.66422500 |
| Pd | 11.13125000 | 14.38390000 | 13.66425000 |
| Pd | 8.83392500 | 9.83637500 | 12.50000000 |
| Pd | 7.96855000 | 12.50000000 | 12.50000000 |
| Pd | 14.71452500 | 11.78042500 | 13.66437500 |
| Pd | 11.09957500 | 8.19005000 | 12.50000000 |

| | | | |
|----|-------------|-------------|-------------|
| Pd | 13.86875000 | 14.38390000 | 13.66425000 |
| Pd | 8.83392500 | 15.16362500 | 12.50000000 |
| Pd | 13.90042500 | 8.19005000 | 12.50000000 |
| Pd | 12.50000000 | 12.50000000 | 12.50000000 |
| Pd | 11.09957500 | 16.80995000 | 12.50000000 |
| Pd | 16.16607500 | 9.83637500 | 12.50000000 |
| Pd | 11.13125000 | 10.61607500 | 11.33575000 |
| Pd | 13.90042500 | 16.80995000 | 12.50000000 |
| Pd | 10.28547500 | 13.21957500 | 11.33562500 |
| Pd | 17.03145000 | 12.50000000 | 12.50000000 |
| Pd | 16.16607500 | 15.16362500 | 12.50000000 |
| Pd | 13.86875000 | 10.61607500 | 11.33575000 |
| Pd | 12.50000000 | 14.82867500 | 11.33577500 |
| Pd | 9.73440000 | 8.69357500 | 10.14752500 |
| Pd | 8.83397500 | 11.30882500 | 10.11765000 |
| Pd | 8.02537500 | 13.95385000 | 10.14770000 |
| Pd | 14.71452500 | 13.21957500 | 11.33562500 |
| Pd | 12.50000000 | 8.64517500 | 10.11765000 |
| Pd | 10.23422500 | 15.61860000 | 10.11762500 |
| Pd | 12.50000000 | 12.50000000 | 9.89650000 |
| Pd | 15.26560000 | 8.69357500 | 10.14752500 |
| Pd | 12.50000000 | 17.20497500 | 10.14742500 |
| Pd | 16.16602500 | 11.30882500 | 10.11765000 |
| Pd | 16.97462500 | 13.95385000 | 10.14770000 |
| Pd | 10.23417500 | 13.23622500 | 8.64517500 |
| Pd | 14.76577500 | 15.61860000 | 10.11762500 |
| Pd | 11.09960000 | 10.57257500 | 8.64510000 |

| | | | |
|----|-------------|-------------|------------|
| Pd | 13.90040000 | 10.57257500 | 8.64510000 |
| Pd | 12.50000000 | 14.88237500 | 8.64505000 |
| Pd | 12.50000000 | 12.50000000 | 7.23947500 |
| Pd | 14.76585000 | 13.23622500 | 8.64517500 |

Pd₅₅(Oh)

| | | | |
|----|-------------|-------------|-------------|
| Pd | 12.50000000 | 8.72505000 | 8.72505000 |
| Pd | 10.61357500 | 10.61357500 | 8.63702500 |
| Pd | 12.50000000 | 12.50000000 | 8.55227500 |
| Pd | 14.38642500 | 10.61357500 | 8.63702500 |
| Pd | 16.27495000 | 12.50000000 | 8.72505000 |
| Pd | 14.38642500 | 14.38642500 | 8.63702500 |
| Pd | 12.50000000 | 16.27495000 | 8.72505000 |
| Pd | 10.61357500 | 14.38642500 | 8.63702500 |
| Pd | 10.61357500 | 8.63702500 | 10.61357500 |
| Pd | 14.38642500 | 8.63702500 | 10.61357500 |
| Pd | 16.36297500 | 10.61357500 | 10.61357500 |
| Pd | 12.50000000 | 10.60507500 | 10.60507500 |
| Pd | 8.63702500 | 10.61357500 | 10.61357500 |
| Pd | 14.39492500 | 12.50000000 | 10.60507500 |
| Pd | 8.72505000 | 12.50000000 | 8.72505000 |
| Pd | 16.36297500 | 14.38642500 | 10.61357500 |
| Pd | 12.50000000 | 14.39492500 | 10.60507500 |
| Pd | 14.38642500 | 16.36297500 | 10.61357500 |
| Pd | 10.61357500 | 16.36297500 | 10.61357500 |
| Pd | 8.63702500 | 14.38642500 | 10.61357500 |
| Pd | 10.60507500 | 12.50000000 | 10.60507500 |

| | | | |
|----|-------------|-------------|-------------|
| Pd | 8.72505000 | 16.27495000 | 12.50000000 |
| Pd | 10.60507500 | 14.39492500 | 12.50000000 |
| Pd | 8.55227500 | 12.50000000 | 12.50000000 |
| Pd | 10.60507500 | 10.60507500 | 12.50000000 |
| Pd | 8.72505000 | 8.72505000 | 12.50000000 |
| Pd | 12.50000000 | 8.55227500 | 12.50000000 |
| Pd | 16.27495000 | 8.72505000 | 12.50000000 |
| Pd | 14.39492500 | 10.60507500 | 12.50000000 |
| Pd | 16.44772500 | 12.50000000 | 12.50000000 |
| Pd | 12.50000000 | 12.50000000 | 12.50000000 |
| Pd | 14.39492500 | 14.39492500 | 12.50000000 |
| Pd | 16.27495000 | 16.27495000 | 12.50000000 |
| Pd | 12.50000000 | 16.44772500 | 12.50000000 |
| Pd | 10.61357500 | 16.36297500 | 14.38642500 |
| Pd | 14.38642500 | 16.36297500 | 14.38642500 |
| Pd | 8.63702500 | 14.38642500 | 14.38642500 |
| Pd | 12.50000000 | 14.39492500 | 14.39492500 |
| Pd | 16.36297500 | 14.38642500 | 14.38642500 |
| Pd | 10.60507500 | 12.50000000 | 14.39492500 |
| Pd | 14.39492500 | 12.50000000 | 14.39492500 |
| Pd | 8.63702500 | 10.61357500 | 14.38642500 |
| Pd | 12.50000000 | 10.60507500 | 14.39492500 |
| Pd | 16.36297500 | 10.61357500 | 14.38642500 |
| Pd | 10.61357500 | 8.63702500 | 14.38642500 |
| Pd | 14.38642500 | 8.63702500 | 14.38642500 |
| Pd | 12.50000000 | 8.72505000 | 16.27495000 |
| Pd | 14.38642500 | 10.61357500 | 16.36297500 |

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|----|-------------|-------------|-------------|
| Pd | 10.61357500 | 10.61357500 | 16.36297500 |
| Pd | 16.27495000 | 12.50000000 | 16.27495000 |
| Pd | 12.50000000 | 12.50000000 | 16.44772500 |
| Pd | 8.72505000 | 12.50000000 | 16.27495000 |
| Pd | 14.38642500 | 14.38642500 | 16.36297500 |
| Pd | 10.61357500 | 14.38642500 | 16.36297500 |
| Pd | 12.50000000 | 16.27495000 | 16.27495000 |

1_Pd_a

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.80732500 | 11.25940000 | 16.74027500 |
| Pd | 12.95042500 | 13.62665000 | 17.60292500 |
| Pd | 14.55715000 | 11.70600000 | 16.43260000 |
| Pd | 10.41070000 | 13.62932500 | 16.43357500 |
| Pd | 10.66887500 | 8.89730000 | 15.84575000 |
| Pd | 15.00355000 | 14.36895000 | 15.87140000 |
| Pd | 12.38737500 | 15.86837500 | 15.99412500 |
| Pd | 13.40410000 | 9.24035000 | 15.58745000 |
| Pd | 9.33307500 | 11.27777500 | 15.50772500 |
| Pd | 16.08730000 | 9.77902500 | 15.19047500 |
| Pd | 8.04727500 | 13.66725000 | 14.98487500 |
| Pd | 12.70632500 | 13.12780000 | 15.03980000 |
| Pd | 16.50690000 | 12.43572500 | 14.60567500 |
| Pd | 9.81962500 | 15.71400000 | 14.40042500 |
| Pd | 11.60367500 | 10.70172500 | 14.12555000 |
| Pd | 16.82462500 | 15.08837500 | 13.91192500 |
| Pd | 14.41685000 | 16.45757500 | 13.83422500 |
| Pd | 11.84175000 | 17.54485000 | 13.78795000 |

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|----|-------------|-------------|-------------|
| Pd | 14.22567500 | 11.13545000 | 13.85840000 |
| Pd | 10.29857500 | 13.08380000 | 13.74302500 |
| Pd | 11.92762500 | 8.12965000 | 13.51662500 |
| Pd | 9.40815000 | 9.32482500 | 13.44410000 |
| Pd | 14.63977500 | 13.78547500 | 13.21520000 |
| Pd | 14.62552500 | 8.58245000 | 13.18025000 |
| Pd | 12.18267500 | 15.01382500 | 13.23300000 |
| Pd | 8.07967500 | 11.74557500 | 13.03212500 |
| Pd | 16.54750000 | 10.48505000 | 12.56940000 |
| Pd | 12.49662500 | 12.53597500 | 12.51947500 |
| Pd | 8.41642500 | 14.47460000 | 12.38040000 |
| Pd | 16.93627500 | 13.19470000 | 11.93297500 |
| Pd | 12.80855000 | 10.04337500 | 11.77072500 |
| Pd | 10.33810000 | 16.40712500 | 11.77417500 |
| Pd | 10.36062500 | 11.25127500 | 11.75025000 |
| Pd | 15.61720000 | 15.64617500 | 11.49415000 |
| Pd | 13.09707500 | 16.84475000 | 11.43105000 |
| Pd | 14.70010000 | 11.92487500 | 11.26902500 |
| Pd | 10.75035000 | 13.88067500 | 11.15522500 |
| Pd | 13.15240000 | 7.44552500 | 11.13605000 |
| Pd | 10.67167500 | 8.60730000 | 11.08605000 |
| Pd | 8.18620000 | 9.86210000 | 11.03370000 |
| Pd | 13.39032500 | 14.29190000 | 10.83667500 |
| Pd | 15.06505000 | 9.30987500 | 10.53570000 |
| Pd | 8.51122500 | 12.49347500 | 10.34530000 |
| Pd | 12.29747500 | 11.95315000 | 9.97360000 |
| Pd | 16.95470000 | 11.26970000 | 9.97312500 |

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|----|-------------|-------------|-------------|
| Pd | 8.90477500 | 15.16475000 | 9.76315000 |
| Pd | 15.65917500 | 13.64507500 | 9.47305000 |
| Pd | 14.33067500 | 16.04727500 | 9.09115000 |
| Pd | 10.12862500 | 10.52657500 | 9.17402500 |
| Pd | 11.59850000 | 15.64217500 | 9.30825000 |
| Pd | 12.61387500 | 9.30620000 | 9.21007500 |
| Pd | 14.51690000 | 11.24675000 | 8.64617500 |
| Pd | 10.47392500 | 13.22767500 | 8.52517500 |
| Pd | 12.07482500 | 11.28580000 | 7.38547500 |
| Pd | 13.20622500 | 13.67790000 | 8.17710000 |
| O | 10.45742500 | 15.62072500 | 16.28997500 |
| O | 14.31255000 | 16.24020000 | 15.81690000 |

2_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.63895000 | 11.36767500 | 17.08685000 |
| Pd | 12.86910000 | 13.84400000 | 17.47015000 |
| Pd | 14.59845000 | 11.92190000 | 16.46337500 |
| Pd | 10.40757500 | 14.05097500 | 16.21432500 |
| Pd | 10.56885000 | 9.16977500 | 15.89215000 |
| Pd | 14.89175000 | 14.53550000 | 15.68497500 |
| Pd | 12.41167500 | 15.79835000 | 15.54455000 |
| Pd | 13.33622500 | 9.35302500 | 15.57612500 |
| Pd | 9.14910000 | 11.48115000 | 15.32295000 |
| Pd | 16.01260000 | 9.89542500 | 15.22127500 |
| Pd | 8.05957500 | 13.94115000 | 14.75440000 |
| Pd | 12.65282500 | 13.12455000 | 14.98150000 |
| Pd | 16.49055000 | 12.53915000 | 14.57955000 |

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|----|-------------|-------------|-------------|
| Pd | 9.97135000 | 15.85405000 | 14.19595000 |
| Pd | 11.55717500 | 10.87895000 | 14.14425000 |
| Pd | 16.84322500 | 15.17030000 | 13.82917500 |
| Pd | 14.47002500 | 16.54932500 | 13.67017500 |
| Pd | 11.95695000 | 17.65432500 | 13.54632500 |
| Pd | 14.25080000 | 11.24337500 | 13.81257500 |
| Pd | 10.30750000 | 13.24920000 | 13.57785000 |
| Pd | 11.83282500 | 8.24940000 | 13.53577500 |
| Pd | 9.33197500 | 9.51672500 | 13.38777500 |
| Pd | 14.64102500 | 13.88755000 | 13.13882500 |
| Pd | 14.57227500 | 8.61182500 | 13.23610000 |
| Pd | 12.27762500 | 15.08950000 | 13.00775000 |
| Pd | 8.05085000 | 11.92687500 | 12.85195000 |
| Pd | 16.55517500 | 10.50875000 | 12.61290000 |
| Pd | 12.52467500 | 12.58070000 | 12.42945000 |
| Pd | 8.47717500 | 14.61445000 | 12.14130000 |
| Pd | 16.96320000 | 13.20687500 | 11.87037500 |
| Pd | 12.78492500 | 10.05740000 | 11.81635000 |
| Pd | 10.48632500 | 16.49640000 | 11.49422500 |
| Pd | 10.39660000 | 11.27052500 | 11.67682500 |
| Pd | 15.68230000 | 15.60977500 | 11.35112500 |
| Pd | 13.21660000 | 16.86197500 | 11.20820000 |
| Pd | 14.73657500 | 11.89297500 | 11.25652500 |
| Pd | 10.78587500 | 13.89932500 | 11.02402500 |
| Pd | 13.10637500 | 7.48705000 | 11.19350000 |
| Pd | 10.60812500 | 8.64740000 | 11.01252500 |
| Pd | 8.19422500 | 9.98532500 | 10.90490000 |

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|----|-------------|-------------|-------------|
| Pd | 13.46755000 | 14.23755000 | 10.65777500 |
| Pd | 15.05217500 | 9.32650000 | 10.53355000 |
| Pd | 8.59727500 | 12.60752500 | 10.15730000 |
| Pd | 12.35790000 | 11.94950000 | 9.89760000 |
| Pd | 16.98280000 | 11.20427500 | 9.99395000 |
| Pd | 9.03067500 | 15.24537500 | 9.53275000 |
| Pd | 15.74675000 | 13.60980000 | 9.39045000 |
| Pd | 14.44720000 | 15.96110000 | 8.88762500 |
| Pd | 10.16560000 | 10.59717500 | 9.07715000 |
| Pd | 11.74660000 | 15.64367500 | 9.15547500 |
| Pd | 12.61410000 | 9.34710000 | 9.21855000 |
| Pd | 14.57170000 | 11.24755000 | 8.59467500 |
| Pd | 10.60912500 | 13.26195000 | 8.36745000 |
| Pd | 12.16727500 | 11.28200000 | 7.29010000 |
| Pd | 13.32370000 | 13.64642500 | 7.99050000 |
| O | 9.85537500 | 12.31505000 | 17.00620000 |
| O | 13.45255000 | 10.48972500 | 17.23225000 |
| C | 10.06287500 | 10.88437500 | 19.57482500 |
| C | 10.95067500 | 10.03922500 | 18.70110000 |
| C | 10.39295000 | 8.93582500 | 17.96210000 |
| H | 10.53915000 | 11.83225000 | 19.86032500 |
| H | 9.85272500 | 10.32712500 | 20.50667500 |
| H | 9.10657500 | 11.11090000 | 19.08550000 |
| H | 11.96915000 | 9.88035000 | 19.07717500 |
| H | 9.30090000 | 8.81240000 | 18.02780000 |
| H | 10.97155000 | 7.99822500 | 17.97695000 |

TS1_Pd_{C1}

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|----|-------------|-------------|-------------|
| Pd | 11.25967500 | 11.43880000 | 17.00665000 |
| Pd | 12.69535000 | 13.94977500 | 17.43540000 |
| Pd | 14.32532500 | 11.81747500 | 16.54467500 |
| Pd | 10.24680000 | 14.14990000 | 16.12142500 |
| Pd | 10.06212500 | 9.13270000 | 15.61210000 |
| Pd | 14.78357500 | 14.43320000 | 15.73977500 |
| Pd | 12.36972500 | 15.83545000 | 15.52882500 |
| Pd | 12.88207500 | 9.19087500 | 15.55632500 |
| Pd | 8.85907500 | 11.61232500 | 15.16272500 |
| Pd | 15.61652500 | 9.66945000 | 15.34232500 |
| Pd | 7.96005000 | 14.16657500 | 14.55477500 |
| Pd | 12.50665000 | 13.10695000 | 14.99832500 |
| Pd | 16.30367500 | 12.28722500 | 14.73145000 |
| Pd | 9.99375000 | 15.97655000 | 14.07630000 |
| Pd | 11.29247500 | 10.90230000 | 14.17655000 |
| Pd | 16.84175000 | 14.88022500 | 13.99275000 |
| Pd | 14.54340000 | 16.39505000 | 13.73907500 |
| Pd | 12.09432500 | 17.65477500 | 13.50880000 |
| Pd | 13.97912500 | 11.10240000 | 13.92755000 |
| Pd | 10.21342500 | 13.33362500 | 13.50535000 |
| Pd | 11.40525000 | 8.25350000 | 13.40770000 |
| Pd | 9.00380000 | 9.66895000 | 13.18747500 |
| Pd | 14.59897500 | 13.70222500 | 13.20077500 |
| Pd | 14.21337500 | 8.46925000 | 13.27820000 |
| Pd | 12.31075000 | 15.05287500 | 13.01185000 |

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|----|-------------|-------------|-------------|
| Pd | 7.91770000 | 12.17712500 | 12.63572500 |
| Pd | 16.32160000 | 10.26575000 | 12.78057500 |
| Pd | 12.41210000 | 12.52035000 | 12.45957500 |
| Pd | 8.53522500 | 14.83117500 | 11.97455000 |
| Pd | 16.94100000 | 12.93242500 | 12.05050000 |
| Pd | 12.54847500 | 10.01262500 | 11.82340000 |
| Pd | 10.67990000 | 16.58267500 | 11.41245000 |
| Pd | 10.27010000 | 11.34702500 | 11.59522500 |
| Pd | 15.80967500 | 15.41155000 | 11.49027500 |
| Pd | 13.43265000 | 16.78832500 | 11.24882500 |
| Pd | 14.64202500 | 11.70280000 | 11.37175000 |
| Pd | 10.82262500 | 13.95395000 | 10.96772500 |
| Pd | 12.75765000 | 7.45582500 | 11.17065000 |
| Pd | 10.35207500 | 8.74285000 | 10.82007500 |
| Pd | 8.03855000 | 10.23297500 | 10.69117500 |
| Pd | 13.54065000 | 14.15167500 | 10.73365000 |
| Pd | 14.85942500 | 9.16142500 | 10.61530000 |
| Pd | 8.61727500 | 12.82942500 | 9.97965000 |
| Pd | 12.35765000 | 11.94450000 | 9.89650000 |
| Pd | 16.91230000 | 10.92620000 | 10.18682500 |
| Pd | 9.23597500 | 15.43050000 | 9.39872500 |
| Pd | 15.82470000 | 13.40900000 | 9.56787500 |
| Pd | 14.72752500 | 15.84095000 | 8.98597500 |
| Pd | 10.13245000 | 10.76122500 | 8.95282500 |
| Pd | 11.99895000 | 15.66247500 | 9.15942500 |
| Pd | 12.49492500 | 9.36022500 | 9.17957500 |
| Pd | 14.58757500 | 11.12000000 | 8.67807500 |

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|----|-------------|-------------|-------------|
| Pd | 10.74865000 | 13.38100000 | 8.29235000 |
| Pd | 12.26067500 | 11.33680000 | 7.26522500 |
| Pd | 13.50690000 | 13.60705000 | 8.05180000 |
| O | 9.54510000 | 12.42387500 | 16.86177500 |
| O | 13.00192500 | 10.38360000 | 17.23670000 |
| C | 9.78067500 | 10.06327500 | 19.23710000 |
| C | 11.07160000 | 10.83530000 | 19.10620000 |
| C | 12.32990000 | 10.18815000 | 19.09120000 |
| H | 8.93282500 | 10.62107500 | 18.81705000 |
| H | 9.55882500 | 9.88090000 | 20.30397500 |
| H | 9.83997500 | 9.08652500 | 18.73427500 |
| H | 11.06042500 | 11.84635000 | 19.53552500 |
| H | 12.37595000 | 9.09762500 | 19.06660000 |
| H | 13.21135000 | 10.69907500 | 19.47915000 |

3_PdC1

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.44460000 | 11.56957500 | 16.83702500 |
| Pd | 12.57682500 | 14.06675000 | 17.42542500 |
| Pd | 14.21660000 | 12.00417500 | 16.57390000 |
| Pd | 10.18120000 | 14.20885000 | 16.08767500 |
| Pd | 10.21325000 | 9.24985000 | 15.75495000 |
| Pd | 14.70012500 | 14.61487500 | 15.75635000 |
| Pd | 12.25147500 | 15.94210000 | 15.46285000 |
| Pd | 13.03492500 | 9.55967500 | 15.81675000 |
| Pd | 8.91035000 | 11.66170000 | 15.25232500 |
| Pd | 15.72597500 | 9.90912500 | 15.48115000 |
| Pd | 7.91435000 | 14.13237500 | 14.52062500 |

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|----|-------------|-------------|-------------|
| Pd | 12.46955000 | 13.27420000 | 14.93945000 |
| Pd | 16.33415000 | 12.50000000 | 14.74990000 |
| Pd | 9.89710000 | 15.95682500 | 13.98225000 |
| Pd | 11.31612500 | 10.96235000 | 14.09685000 |
| Pd | 16.76790000 | 15.10100000 | 13.97522500 |
| Pd | 14.41762500 | 16.51617500 | 13.68297500 |
| Pd | 11.95482500 | 17.70945000 | 13.36977500 |
| Pd | 14.00040000 | 11.20630000 | 14.02807500 |
| Pd | 10.20252500 | 13.35627500 | 13.44540000 |
| Pd | 11.60125000 | 8.33647500 | 13.59310000 |
| Pd | 9.07925000 | 9.65390000 | 13.37875000 |
| Pd | 14.59145000 | 13.80435000 | 13.26385000 |
| Pd | 14.41997500 | 8.57642500 | 13.44617500 |
| Pd | 12.25872500 | 15.13615000 | 12.89435000 |
| Pd | 7.93155000 | 12.06742500 | 12.71877500 |
| Pd | 16.41060000 | 10.44610000 | 12.88297500 |
| Pd | 12.46227500 | 12.58802500 | 12.43767500 |
| Pd | 8.49202500 | 14.69035000 | 11.89732500 |
| Pd | 16.97692500 | 13.11560000 | 12.06390000 |
| Pd | 12.76097500 | 10.06290000 | 11.92097500 |
| Pd | 10.51885000 | 16.56305000 | 11.30282500 |
| Pd | 10.33485000 | 11.34105000 | 11.58537500 |
| Pd | 15.73395000 | 15.51725000 | 11.44280000 |
| Pd | 13.29107500 | 16.82897500 | 11.13205000 |
| Pd | 14.74552500 | 11.84510000 | 11.42625000 |
| Pd | 10.89305000 | 13.94977500 | 10.87570000 |
| Pd | 12.99400000 | 7.47942500 | 11.36995000 |

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|----|-------------|-------------|-------------|
| Pd | 10.53817500 | 8.71202500 | 11.07970000 |
| Pd | 8.13917500 | 10.08027500 | 10.83735000 |
| Pd | 13.59395000 | 14.15817500 | 10.69247500 |
| Pd | 15.01415000 | 9.21307500 | 10.75967500 |
| Pd | 8.62365000 | 12.66662500 | 10.01472500 |
| Pd | 12.42897500 | 11.86657500 | 9.93250000 |
| Pd | 16.98475000 | 11.06422500 | 10.25480000 |
| Pd | 9.19625000 | 15.26382500 | 9.28977500 |
| Pd | 15.87660000 | 13.48020000 | 9.51040000 |
| Pd | 14.65042500 | 15.85415000 | 8.91992500 |
| Pd | 10.18905000 | 10.59140000 | 9.04465000 |
| Pd | 11.90722500 | 15.59405000 | 9.05855000 |
| Pd | 12.61200000 | 9.25877500 | 9.31910000 |
| Pd | 14.66702500 | 11.10212500 | 8.74857500 |
| Pd | 10.73867500 | 13.19400000 | 8.28770000 |
| Pd | 12.32575000 | 11.13950000 | 7.34485000 |
| Pd | 13.48255000 | 13.52332500 | 8.05500000 |
| O | 9.58005000 | 12.50917500 | 16.92610000 |
| O | 11.72222500 | 8.54372500 | 17.06977500 |
| C | 10.07642500 | 10.81670000 | 19.34070000 |
| C | 11.37110000 | 10.51412500 | 18.62655000 |
| C | 11.64095000 | 9.01420000 | 18.42200000 |
| H | 9.91247500 | 11.89435000 | 19.47187500 |
| H | 10.09100000 | 10.35002500 | 20.34567500 |
| H | 9.21092500 | 10.40340000 | 18.80002500 |
| H | 12.23565000 | 11.01242500 | 19.09747500 |
| H | 10.83465000 | 8.43045000 | 18.90722500 |

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|---|-------------|------------|-------------|
| H | 12.59387500 | 8.74182500 | 18.91220000 |
|---|-------------|------------|-------------|

TS1_Pd_{C2}

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.98412500 | 11.22817500 | 17.10152500 |
| Pd | 13.14347500 | 13.72432500 | 17.51145000 |
| Pd | 14.87285000 | 11.84367500 | 16.40710000 |
| Pd | 10.58327500 | 13.85852500 | 16.41060000 |
| Pd | 10.63882500 | 9.10675000 | 15.99542500 |
| Pd | 15.04260000 | 14.46817500 | 15.65547500 |
| Pd | 12.50770000 | 15.67335000 | 15.63635000 |
| Pd | 13.54342500 | 9.28485000 | 15.56390000 |
| Pd | 9.25492500 | 11.37650000 | 15.38425000 |
| Pd | 16.24252500 | 9.85285000 | 15.07362500 |
| Pd | 8.16060000 | 13.79667500 | 14.96515000 |
| Pd | 12.82370000 | 13.06632500 | 15.00967500 |
| Pd | 16.66666667 | 12.51265000 | 14.49567500 |
| Pd | 10.03725000 | 15.74937500 | 14.39067500 |
| Pd | 11.68372500 | 10.79320000 | 14.25225000 |
| Pd | 16.91722500 | 15.14395000 | 13.73455000 |
| Pd | 14.50932500 | 16.47680000 | 13.75492500 |
| Pd | 11.99527500 | 17.57380000 | 13.65742500 |
| Pd | 14.39952500 | 11.20142500 | 13.77137500 |
| Pd | 10.40992500 | 13.19717500 | 13.75165000 |
| Pd | 11.94200000 | 8.15845000 | 13.65490000 |
| Pd | 9.43545000 | 9.36980000 | 13.47592500 |
| Pd | 14.72557500 | 13.82020000 | 13.05777500 |
| Pd | 14.69992500 | 8.55925000 | 13.20090000 |

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|----|-------------|-------------|-------------|
| Pd | 12.34960000 | 15.02970000 | 13.05870000 |
| Pd | 8.08060000 | 11.84045000 | 13.02090000 |
| Pd | 16.66666667 | 10.50477500 | 12.50292500 |
| Pd | 12.56157500 | 12.50000000 | 12.49582500 |
| Pd | 8.48947500 | 14.54870000 | 12.36402500 |
| Pd | 17.00430000 | 13.20587500 | 11.78612500 |
| Pd | 12.79595000 | 9.97800000 | 11.89700000 |
| Pd | 10.44220000 | 16.46337500 | 11.69460000 |
| Pd | 10.38972500 | 11.21915000 | 11.85607500 |
| Pd | 15.66700000 | 15.63192500 | 11.36085000 |
| Pd | 13.17997500 | 16.85040000 | 11.30835000 |
| Pd | 14.69037500 | 11.79237500 | 11.17045000 |
| Pd | 10.75200000 | 13.84000000 | 11.17250000 |
| Pd | 13.14252500 | 7.45527500 | 11.22737500 |
| Pd | 10.63722500 | 8.61545000 | 11.07940000 |
| Pd | 8.21195000 | 9.92690000 | 11.05467500 |
| Pd | 13.42182500 | 14.17195000 | 10.68685000 |
| Pd | 15.08272500 | 9.27772500 | 10.48182500 |
| Pd | 8.55972500 | 12.57872500 | 10.32970000 |
| Pd | 12.23642500 | 11.87445000 | 9.97635000 |
| Pd | 16.94987500 | 11.20502500 | 9.89820000 |
| Pd | 8.96597500 | 15.23567500 | 9.75160000 |
| Pd | 15.69877500 | 13.64010000 | 9.40710000 |
| Pd | 14.33180000 | 15.99275000 | 8.96262500 |
| Pd | 10.09185000 | 10.56497500 | 9.17030000 |
| Pd | 11.64562500 | 15.64835000 | 9.31545000 |
| Pd | 12.60592500 | 9.33375000 | 9.25302500 |

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|----|-------------|-------------|-------------|
| Pd | 14.52235000 | 11.25665000 | 8.57615000 |
| Pd | 10.50632500 | 13.26442500 | 8.50072500 |
| Pd | 12.04927500 | 11.29140000 | 7.37135000 |
| Pd | 13.22610000 | 13.66425000 | 8.07972500 |
| O | 10.11117500 | 11.97362500 | 17.16672500 |
| O | 13.75707500 | 10.40612500 | 17.20825000 |
| C | 7.92010000 | 11.29460000 | 18.48655000 |
| C | 9.24495000 | 10.61665000 | 18.36027500 |
| C | 9.37500000 | 9.34702500 | 17.71025000 |
| H | 8.03457500 | 12.36735000 | 18.69167500 |
| H | 7.36412500 | 10.84575000 | 19.32900000 |
| H | 7.31487500 | 11.16625000 | 17.57572500 |
| H | 9.96492500 | 10.83747500 | 19.15472500 |
| H | 8.43730000 | 8.93255000 | 17.31302500 |
| H | 10.01335000 | 8.62062500 | 18.24272500 |

3_Pd_{C2}

| | | | |
|----|-------------|-------------|-------------|
| Pd | 12.76282500 | 14.04535000 | 17.52860000 |
| Pd | 12.57652500 | 16.10865000 | 15.70795000 |
| Pd | 10.33927500 | 13.72332500 | 16.27507500 |
| Pd | 11.83322500 | 11.47877500 | 16.87125000 |
| Pd | 14.53865000 | 12.04457500 | 16.57202500 |
| Pd | 15.02755000 | 14.58292500 | 15.74772500 |
| Pd | 12.71262500 | 13.32237500 | 14.99060000 |
| Pd | 11.95402500 | 17.60502500 | 13.37517500 |
| Pd | 9.80402500 | 15.83957500 | 14.01867500 |
| Pd | 8.08505000 | 13.76625000 | 14.80205000 |

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|----|-------------|-------------|-------------|
| Pd | 9.32190000 | 11.40637500 | 15.49252500 |
| Pd | 10.68445000 | 9.09742500 | 16.07445000 |
| Pd | 13.40557500 | 9.44365000 | 15.83017500 |
| Pd | 16.08880000 | 9.97800000 | 15.47682500 |
| Pd | 16.56665000 | 12.56222500 | 14.66770000 |
| Pd | 16.89247500 | 15.12660000 | 13.72900000 |
| Pd | 14.53562500 | 16.54412500 | 13.41900000 |
| Pd | 13.18747500 | 16.67012500 | 11.05370000 |
| Pd | 10.43707500 | 16.21742500 | 11.39240000 |
| Pd | 8.45067500 | 14.37292500 | 12.09880000 |
| Pd | 8.11587500 | 11.73747500 | 12.97840000 |
| Pd | 9.45557500 | 9.32570000 | 13.61525000 |
| Pd | 11.97037500 | 8.17537500 | 13.83077500 |
| Pd | 14.70422500 | 8.59532500 | 13.53060000 |
| Pd | 16.62042500 | 10.44537500 | 12.80302500 |
| Pd | 17.05370000 | 13.11050000 | 11.93895000 |
| Pd | 15.73692500 | 15.47572500 | 11.23177500 |
| Pd | 12.24225000 | 15.03570000 | 13.02127500 |
| Pd | 14.69660000 | 13.83197500 | 13.12892500 |
| Pd | 14.28785000 | 11.27257500 | 14.04777500 |
| Pd | 12.57302500 | 12.50000000 | 12.52427500 |
| Pd | 10.34067500 | 13.21585000 | 13.61502500 |
| Pd | 11.64180000 | 10.85950000 | 14.31615000 |
| Pd | 12.92800000 | 9.93787500 | 12.08197500 |
| Pd | 10.85787500 | 13.65332500 | 10.95775000 |
| Pd | 10.44525000 | 11.10550000 | 11.91370000 |
| Pd | 8.28620000 | 9.69712500 | 11.17000000 |

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|----|-------------|-------------|-------------|
| Pd | 8.61317500 | 12.25955000 | 10.27325000 |
| Pd | 9.04142500 | 14.81705000 | 9.43395000 |
| Pd | 10.78335000 | 8.47140000 | 11.33920000 |
| Pd | 13.26172500 | 7.30502500 | 11.55727500 |
| Pd | 15.16577500 | 9.13842500 | 10.83265000 |
| Pd | 12.74552500 | 9.00252500 | 9.47647500 |
| Pd | 10.24295000 | 10.24142500 | 9.29670000 |
| Pd | 12.22780000 | 10.81732500 | 7.51230000 |
| Pd | 10.61132500 | 12.84895000 | 8.40530000 |
| Pd | 11.70075000 | 15.34847500 | 9.02040000 |
| Pd | 13.33325000 | 13.28360000 | 8.12030000 |
| Pd | 12.39757500 | 11.59952500 | 10.07532500 |
| Pd | 14.65060000 | 10.92890000 | 8.80755000 |
| Pd | 17.06467500 | 11.04707500 | 10.16290000 |
| Pd | 14.81445000 | 11.78015000 | 11.40780000 |
| Pd | 15.80070000 | 13.36142500 | 9.41935000 |
| Pd | 13.47510000 | 14.05830000 | 10.66635000 |
| Pd | 14.43325000 | 15.68840000 | 8.81587500 |
| O | 10.60067500 | 15.83947500 | 16.28680000 |
| O | 14.46377500 | 16.48137500 | 15.40047500 |
| C | 9.11872500 | 16.11327500 | 18.18737500 |
| C | 10.55192500 | 16.23997500 | 17.69710000 |
| C | 11.54785000 | 15.39385000 | 18.50692500 |
| H | 8.43810000 | 16.70382500 | 17.55782500 |
| H | 9.03520000 | 16.46432500 | 19.22697500 |
| H | 8.80155000 | 15.05620000 | 18.15060000 |
| H | 10.85882500 | 17.30227500 | 17.71432500 |

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|---|-------------|-------------|-------------|
| H | 11.03600000 | 14.72537500 | 19.22050000 |
| H | 12.30642500 | 16.00857500 | 19.02032500 |

TS2_PdC

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|----|-------------|-------------|-------------|
| Pd | 12.88240000 | 13.76447500 | 17.44377500 |
| Pd | 12.50502500 | 16.08505000 | 15.34757500 |
| Pd | 10.27762500 | 13.78272500 | 16.20395000 |
| Pd | 11.77105000 | 11.42900000 | 16.81562500 |
| Pd | 14.52210000 | 11.88010000 | 16.46415000 |
| Pd | 14.94052500 | 14.61987500 | 15.66795000 |
| Pd | 12.62840000 | 13.20262500 | 14.91372500 |
| Pd | 11.77065000 | 17.54180000 | 13.24435000 |
| Pd | 9.74767500 | 15.72680000 | 13.96950000 |
| Pd | 7.98430000 | 13.68127500 | 14.68802500 |
| Pd | 9.34932500 | 11.39770000 | 15.43105000 |
| Pd | 10.69872500 | 9.03007500 | 15.95687500 |
| Pd | 13.41345000 | 9.45077500 | 15.73900000 |
| Pd | 16.10582500 | 9.95922500 | 15.34065000 |
| Pd | 16.51642500 | 12.58835000 | 14.61020000 |
| Pd | 16.78360000 | 15.18380000 | 13.69175000 |
| Pd | 14.33255000 | 16.45962500 | 13.47542500 |
| Pd | 13.07627500 | 16.68687500 | 10.99130000 |
| Pd | 10.33050000 | 16.21412500 | 11.32365000 |
| Pd | 8.42405000 | 14.27755000 | 12.03477500 |
| Pd | 8.07722500 | 11.64507500 | 12.91552500 |
| Pd | 9.42262500 | 9.26190000 | 13.54730000 |
| Pd | 11.97025000 | 8.09970000 | 13.75480000 |

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|----|-------------|-------------|-------------|
| Pd | 14.71717500 | 8.57310000 | 13.43680000 |
| Pd | 16.62770000 | 10.45185000 | 12.70635000 |
| Pd | 16.98760000 | 13.11620000 | 11.89942500 |
| Pd | 15.68910000 | 15.47557500 | 11.18625000 |
| Pd | 12.09520000 | 14.95717500 | 12.90777500 |
| Pd | 14.59507500 | 13.85475000 | 13.13022500 |
| Pd | 14.31860000 | 11.28027500 | 13.90855000 |
| Pd | 12.53120000 | 12.44227500 | 12.42717500 |
| Pd | 10.28695000 | 13.11692500 | 13.54127500 |
| Pd | 11.63840000 | 10.72880000 | 14.17032500 |
| Pd | 12.95930000 | 9.91052500 | 11.95542500 |
| Pd | 10.81247500 | 13.57707500 | 10.84322500 |
| Pd | 10.42597500 | 11.05217500 | 11.79467500 |
| Pd | 8.27147500 | 9.63265000 | 11.09650000 |
| Pd | 8.55867500 | 12.21210000 | 10.19907500 |
| Pd | 8.98800000 | 14.80710000 | 9.37500000 |
| Pd | 10.77645000 | 8.44510000 | 11.27062500 |
| Pd | 13.28550000 | 7.29785000 | 11.47697500 |
| Pd | 15.18365000 | 9.13812500 | 10.73055000 |
| Pd | 12.73497500 | 9.00320000 | 9.39750000 |
| Pd | 10.22892500 | 10.23325000 | 9.22222500 |
| Pd | 12.23070000 | 10.82595000 | 7.41172500 |
| Pd | 10.54530000 | 12.83047500 | 8.30835000 |
| Pd | 11.64745000 | 15.31712500 | 9.00247500 |
| Pd | 13.29042500 | 13.28532500 | 8.06575000 |
| Pd | 12.42987500 | 11.62227500 | 9.95342500 |
| Pd | 14.65822500 | 10.91280000 | 8.66680000 |

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|----|-------------|-------------|-------------|
| Pd | 17.02885000 | 11.07115000 | 10.05595000 |
| Pd | 14.79660000 | 11.81795000 | 11.28720000 |
| Pd | 15.75825000 | 13.37732500 | 9.34112500 |
| Pd | 13.47255000 | 14.10432500 | 10.67522500 |
| Pd | 14.38557500 | 15.71412500 | 8.78992500 |
| O | 10.77685000 | 15.87740000 | 16.52897500 |
| O | 13.53347500 | 15.67852500 | 17.07260000 |
| C | 9.79015000 | 16.28222500 | 18.69472500 |
| C | 11.05830000 | 16.38147500 | 17.85032500 |
| C | 12.20765000 | 15.63310000 | 18.47917500 |
| H | 8.98095000 | 16.84507500 | 18.20932500 |
| H | 9.95015000 | 16.69180000 | 19.70297500 |
| H | 9.47997500 | 15.22855000 | 18.78412500 |
| H | 11.34415000 | 17.44215000 | 17.73010000 |
| H | 11.86390000 | 14.69085000 | 18.99210000 |
| H | 12.89270000 | 16.19740000 | 19.11462500 |

4_PdC

| | | | |
|----|-------------|-------------|-------------|
| Pd | 13.29267500 | 13.71942500 | 17.43960000 |
| Pd | 12.92542500 | 15.78772500 | 15.56157500 |
| Pd | 10.68067500 | 13.52422500 | 16.49855000 |
| Pd | 12.16037500 | 11.26755000 | 16.86537500 |
| Pd | 14.85035000 | 11.71477500 | 16.36880000 |
| Pd | 15.27985000 | 14.35745000 | 15.51667500 |
| Pd | 12.91855000 | 13.06355000 | 14.95965000 |
| Pd | 12.06435000 | 17.45442500 | 13.53997500 |
| Pd | 9.95955000 | 15.79625000 | 14.26412500 |

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|----|-------------|-------------|-------------|
| Pd | 8.34370000 | 13.70060000 | 15.11500000 |
| Pd | 9.59187500 | 11.24335000 | 15.61755000 |
| Pd | 10.98977500 | 8.89650000 | 16.03055000 |
| Pd | 13.67522500 | 9.27502500 | 15.62822500 |
| Pd | 16.30952500 | 9.75477500 | 15.07635000 |
| Pd | 16.76025000 | 12.37090000 | 14.31190000 |
| Pd | 17.04600000 | 14.99662500 | 13.47905000 |
| Pd | 14.65257500 | 16.35065000 | 13.52035000 |
| Pd | 13.18722500 | 16.68060000 | 11.16917500 |
| Pd | 10.46590000 | 16.24225000 | 11.64775000 |
| Pd | 8.53655000 | 14.37355000 | 12.41247500 |
| Pd | 8.21602500 | 11.71315000 | 13.23732500 |
| Pd | 9.51332500 | 9.23540000 | 13.69610000 |
| Pd | 12.03280000 | 8.05697500 | 13.67825000 |
| Pd | 14.76427500 | 8.47160000 | 13.19180000 |
| Pd | 16.67232500 | 10.34350000 | 12.37950000 |
| Pd | 17.05140000 | 13.01475000 | 11.60990000 |
| Pd | 15.74780000 | 15.43860000 | 11.09240000 |
| Pd | 12.31530000 | 14.91647500 | 13.13387500 |
| Pd | 14.77467500 | 13.75787500 | 12.99732500 |
| Pd | 14.47225000 | 11.15670000 | 13.80652500 |
| Pd | 12.61555000 | 12.40612500 | 12.48062500 |
| Pd | 10.48335000 | 13.10082500 | 13.78110000 |
| Pd | 11.81957500 | 10.66570000 | 14.24685000 |
| Pd | 12.95580000 | 9.89042500 | 11.89317500 |
| Pd | 10.79347500 | 13.61150000 | 11.08947500 |
| Pd | 10.46005000 | 11.03302500 | 11.97032500 |

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|----|-------------|-------------|-------------|
| Pd | 8.22277500 | 9.74205000 | 11.33292500 |
| Pd | 8.50900000 | 12.34247500 | 10.51310000 |
| Pd | 8.94452500 | 14.95017500 | 9.74855000 |
| Pd | 10.67360000 | 8.47750000 | 11.27927500 |
| Pd | 13.17640000 | 7.29747500 | 11.28640000 |
| Pd | 15.06395000 | 9.11610000 | 10.46707500 |
| Pd | 12.52510000 | 9.08372500 | 9.31652500 |
| Pd | 10.04525000 | 10.37662500 | 9.34875000 |
| Pd | 11.91830000 | 10.97720000 | 7.43602500 |
| Pd | 10.37887500 | 12.99920000 | 8.51470000 |
| Pd | 11.58147500 | 15.43320000 | 9.20917500 |
| Pd | 13.08570000 | 13.40040000 | 8.08290000 |
| Pd | 12.30357500 | 11.68277500 | 9.99642500 |
| Pd | 14.42290000 | 10.98852500 | 8.52732500 |
| Pd | 16.89842500 | 11.03405000 | 9.71965000 |
| Pd | 14.77245000 | 11.76382500 | 11.16222500 |
| Pd | 15.61607500 | 13.40462500 | 9.21302500 |
| Pd | 13.42047500 | 14.10937500 | 10.69482500 |
| Pd | 14.27185000 | 15.79715000 | 8.83325000 |
| O | 10.81145000 | 15.65847500 | 16.27085000 |
| O | 13.08995000 | 15.78445000 | 17.75295000 |
| C | 9.36562500 | 16.51072500 | 18.03147500 |
| C | 10.74787500 | 16.54287500 | 17.40752500 |
| C | 11.85930000 | 16.12765000 | 18.39140000 |
| H | 8.61170000 | 16.84410000 | 17.30417500 |
| H | 9.31327500 | 17.16585000 | 18.91442500 |
| H | 9.11950000 | 15.48217500 | 18.34142500 |

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|---|-------------|-------------|-------------|
| H | 10.98002500 | 17.55350000 | 17.02397500 |
| H | 11.49595000 | 15.27687500 | 19.00045000 |
| H | 12.05797500 | 16.97282500 | 19.07820000 |

TS3_Pd_C

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|----|-------------|-------------|-------------|
| Pd | 13.10195000 | 14.11862500 | 17.22532500 |
| Pd | 12.45042500 | 16.15080000 | 15.15060000 |
| Pd | 10.35232500 | 14.09115000 | 16.08352500 |
| Pd | 11.89305000 | 11.72520000 | 16.76982500 |
| Pd | 14.66082500 | 12.14277500 | 16.33370000 |
| Pd | 15.02465000 | 14.77107500 | 15.35977500 |
| Pd | 12.70172500 | 13.42842500 | 14.80345000 |
| Pd | 11.83802500 | 17.66302500 | 12.95897500 |
| Pd | 9.85892500 | 15.87042500 | 13.86135000 |
| Pd | 8.01000000 | 13.93427500 | 14.67522500 |
| Pd | 9.36075000 | 11.65737500 | 15.51345000 |
| Pd | 10.73982500 | 9.32675000 | 16.10712500 |
| Pd | 13.46252500 | 9.65602500 | 15.72667500 |
| Pd | 16.15077500 | 10.11910000 | 15.22387500 |
| Pd | 16.57695000 | 12.68552500 | 14.31150000 |
| Pd | 16.81595000 | 15.26325000 | 13.34407500 |
| Pd | 14.34145000 | 16.52387500 | 13.25110000 |
| Pd | 13.04410000 | 16.70745000 | 10.73155000 |
| Pd | 10.28707500 | 16.29567500 | 11.16020000 |
| Pd | 8.38275000 | 14.40000000 | 12.01585000 |
| Pd | 8.05042500 | 11.79142500 | 13.02925000 |

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|----|-------------|-------------|-------------|
| Pd | 9.42025000 | 9.44590000 | 13.70770000 |
| Pd | 11.94362500 | 8.26582500 | 13.87340000 |
| Pd | 14.69407500 | 8.68492500 | 13.39042500 |
| Pd | 16.59090000 | 10.53000000 | 12.54865000 |
| Pd | 16.91062500 | 13.15777500 | 11.57220000 |
| Pd | 15.59327500 | 15.51085000 | 10.89240000 |
| Pd | 12.15282500 | 15.06285000 | 12.67035000 |
| Pd | 14.62415000 | 13.87125000 | 12.90000000 |
| Pd | 14.24907500 | 11.35670000 | 13.86837500 |
| Pd | 12.49040000 | 12.52195000 | 12.34900000 |
| Pd | 10.28012500 | 13.28657500 | 13.47670000 |
| Pd | 11.55637500 | 10.99462500 | 14.22880000 |
| Pd | 12.79522500 | 9.95180000 | 12.03442500 |
| Pd | 10.75247500 | 13.65055000 | 10.77742500 |
| Pd | 10.34765000 | 11.16200000 | 11.78935000 |
| Pd | 8.16852500 | 9.71172500 | 11.29247500 |
| Pd | 8.43250000 | 12.25230000 | 10.27357500 |
| Pd | 8.86290000 | 14.81542500 | 9.33082500 |
| Pd | 10.63762500 | 8.47420000 | 11.40222500 |
| Pd | 13.14120000 | 7.34900000 | 11.57145000 |
| Pd | 15.03325000 | 9.13687500 | 10.65712500 |
| Pd | 12.54620000 | 8.97977500 | 9.44595000 |
| Pd | 10.03422500 | 10.19270000 | 9.30457500 |
| Pd | 11.99127500 | 10.71507500 | 7.41797500 |
| Pd | 10.36247500 | 12.76187500 | 8.31922500 |
| Pd | 11.51860000 | 15.27937500 | 8.85317500 |
| Pd | 13.07995000 | 13.19435000 | 7.90137500 |

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|----|-------------|-------------|-------------|
| Pd | 12.31277500 | 11.59490000 | 9.91445000 |
| Pd | 14.47137500 | 10.86027500 | 8.55770000 |
| Pd | 16.88700000 | 11.00090000 | 9.86465000 |
| Pd | 14.69492500 | 11.72600000 | 11.19490000 |
| Pd | 15.58967500 | 13.32512500 | 9.11425000 |
| Pd | 13.43972500 | 14.05047500 | 10.47005000 |
| Pd | 14.23332500 | 15.64340000 | 8.51407500 |
| O | 11.16380000 | 15.99140000 | 16.88507500 |
| O | 12.95635000 | 15.19740000 | 18.95460000 |
| C | 9.39872500 | 16.69482500 | 18.36835000 |
| C | 10.82250000 | 16.70062500 | 17.91435000 |
| C | 11.82630000 | 15.53165000 | 19.45330000 |
| H | 8.80477500 | 17.34447500 | 17.69982500 |
| H | 9.29495000 | 17.07875000 | 19.39350000 |
| H | 8.97687500 | 15.67990000 | 18.30155000 |
| H | 11.43907500 | 17.59115000 | 18.11787500 |
| H | 10.98295000 | 14.81862500 | 19.44490000 |
| H | 11.82407500 | 16.31810000 | 20.22840000 |

5_Pd_C

| | | | |
|----|-------------|-------------|-------------|
| Pd | 13.07147500 | 13.91032500 | 17.40802500 |
| Pd | 12.36995000 | 15.86937500 | 15.59725000 |
| Pd | 10.52897500 | 13.72600000 | 16.36647500 |
| Pd | 12.01095000 | 11.38447500 | 16.81807500 |
| Pd | 14.70392500 | 11.93445000 | 16.34515000 |
| Pd | 14.98222500 | 14.64592500 | 15.53800000 |
| Pd | 12.74432500 | 13.26350000 | 14.94970000 |

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|----|-------------|-------------|-------------|
| Pd | 11.83812500 | 17.57277500 | 13.40922500 |
| Pd | 9.89607500 | 15.76120000 | 14.49042500 |
| Pd | 8.08532500 | 13.67137500 | 15.10037500 |
| Pd | 9.42745000 | 11.31397500 | 15.65440000 |
| Pd | 10.86717500 | 8.99247500 | 16.04637500 |
| Pd | 13.56732500 | 9.40650000 | 15.62500000 |
| Pd | 16.21110000 | 9.97907500 | 15.10797500 |
| Pd | 16.57755000 | 12.59402500 | 14.34337500 |
| Pd | 16.79350000 | 15.20242500 | 13.51732500 |
| Pd | 14.31970000 | 16.43987500 | 13.53862500 |
| Pd | 12.92920000 | 16.81015000 | 11.10017500 |
| Pd | 10.19217500 | 16.33835000 | 11.64955000 |
| Pd | 8.37020000 | 14.41965000 | 12.47947500 |
| Pd | 8.05917500 | 11.69027500 | 13.26190000 |
| Pd | 9.46765000 | 9.31050000 | 13.69805000 |
| Pd | 11.98877500 | 8.13297500 | 13.71742500 |
| Pd | 14.70927500 | 8.63597500 | 13.19285000 |
| Pd | 16.56982500 | 10.55130000 | 12.43237500 |
| Pd | 16.84647500 | 13.24345000 | 11.60030000 |
| Pd | 15.48187500 | 15.62500000 | 11.12600000 |
| Pd | 12.12377500 | 15.01367500 | 12.93862500 |
| Pd | 14.61805000 | 13.79357500 | 13.02097500 |
| Pd | 14.25350000 | 11.23055000 | 13.85547500 |
| Pd | 12.45650000 | 12.48925000 | 12.46285000 |
| Pd | 10.28775000 | 13.14887500 | 13.73165000 |
| Pd | 11.60547500 | 10.81765000 | 14.26095000 |
| Pd | 12.73727500 | 9.95552500 | 11.94305000 |

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|----|-------------|-------------|-------------|
| Pd | 10.65777500 | 13.71615000 | 11.04137500 |
| Pd | 10.29810000 | 11.17225000 | 11.86695000 |
| Pd | 8.10655000 | 9.75115000 | 11.34122500 |
| Pd | 8.31945000 | 12.36037500 | 10.54470000 |
| Pd | 8.70760000 | 14.97742500 | 9.79427500 |
| Pd | 10.58280000 | 8.49875000 | 11.30485000 |
| Pd | 13.10097500 | 7.38832500 | 11.33282500 |
| Pd | 14.98230000 | 9.23757500 | 10.48867500 |
| Pd | 12.44607500 | 9.16200000 | 9.33725000 |
| Pd | 9.90652500 | 10.36455000 | 9.35190000 |
| Pd | 11.79695000 | 11.04745000 | 7.45762500 |
| Pd | 10.17595000 | 13.01475000 | 8.53952500 |
| Pd | 11.34785000 | 15.47935000 | 9.22400000 |
| Pd | 12.89155000 | 13.50007500 | 8.04280000 |
| Pd | 12.20215000 | 11.76362500 | 9.96642500 |
| Pd | 14.31792500 | 11.10147500 | 8.52525000 |
| Pd | 16.78132500 | 11.19452500 | 9.76880000 |
| Pd | 14.62030000 | 11.76817500 | 11.19320000 |
| Pd | 15.44050000 | 13.54790000 | 9.20520000 |
| Pd | 13.34215000 | 14.14480000 | 10.66035000 |
| Pd | 14.04967500 | 15.87615000 | 8.79752500 |
| O | 11.09257500 | 17.10730000 | 16.67945000 |
| O | 13.03175000 | 14.86012500 | 19.24645000 |
| C | 8.70855000 | 16.84435000 | 16.99417500 |
| C | 9.90010000 | 17.14390000 | 16.11710000 |
| C | 12.46640000 | 15.93775000 | 19.49520000 |
| H | 7.78290000 | 16.77015000 | 16.40540000 |

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|---|-------------|-------------|-------------|
| H | 8.58215000 | 17.66587500 | 17.72392500 |
| H | 8.86197500 | 15.90787500 | 17.55232500 |
| H | 9.75072500 | 17.95777500 | 15.36082500 |
| H | 11.88480000 | 16.48440000 | 18.72725000 |
| H | 12.55727500 | 16.34782500 | 20.51912500 |

TS1_Pd

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|----|-------------|-------------|-------------|
| Pd | 12.18055000 | 11.54962500 | 17.18257500 |
| Pd | 13.32327500 | 14.08825000 | 17.43680000 |
| Pd | 15.01585000 | 12.15507500 | 16.39262500 |
| Pd | 10.71805000 | 14.19802500 | 16.40542500 |
| Pd | 10.83230000 | 9.34470000 | 16.16892500 |
| Pd | 15.18655000 | 14.71662500 | 15.51435000 |
| Pd | 12.65467500 | 15.90490000 | 15.45772500 |
| Pd | 13.65290000 | 9.48747500 | 15.70175000 |
| Pd | 9.40165000 | 11.57917500 | 15.54047500 |
| Pd | 16.32470000 | 10.07362500 | 15.11772500 |
| Pd | 8.29552500 | 14.00132500 | 15.03040000 |
| Pd | 12.90120000 | 13.27750000 | 14.99350000 |
| Pd | 16.74062500 | 12.69130000 | 14.34712500 |
| Pd | 10.15485000 | 15.90812500 | 14.29792500 |
| Pd | 11.77187500 | 10.95437500 | 14.35727500 |
| Pd | 16.99607500 | 15.29790000 | 13.53155000 |
| Pd | 14.56505000 | 16.63560000 | 13.50075000 |
| Pd | 12.04640000 | 17.72500000 | 13.46085000 |
| Pd | 14.42792500 | 11.33782500 | 13.83587500 |
| Pd | 10.50102500 | 13.31990000 | 13.77252500 |

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|----|-------------|-------------|-------------|
| Pd | 12.05227500 | 8.31337500 | 13.80787500 |
| Pd | 9.53420000 | 9.53035000 | 13.70297500 |
| Pd | 14.76285000 | 13.94737500 | 13.02575000 |
| Pd | 14.77392500 | 8.70367500 | 13.29075000 |
| Pd | 12.38952500 | 15.14255000 | 12.91960000 |
| Pd | 8.18125000 | 11.95587500 | 13.18280000 |
| Pd | 16.68680000 | 10.61720000 | 12.47615000 |
| Pd | 12.62062500 | 12.59940000 | 12.49100000 |
| Pd | 8.58497500 | 14.60822500 | 12.37107500 |
| Pd | 17.03195000 | 13.29637500 | 11.62775000 |
| Pd | 12.85540000 | 10.06550000 | 11.97992500 |
| Pd | 10.49365000 | 16.48902500 | 11.56627500 |
| Pd | 10.45662500 | 11.28247500 | 11.93827500 |
| Pd | 15.64587500 | 15.64560000 | 11.14647500 |
| Pd | 13.20412500 | 16.90085000 | 11.07760000 |
| Pd | 14.77447500 | 11.90825000 | 11.21245000 |
| Pd | 10.78815000 | 13.82967500 | 11.10712500 |
| Pd | 13.18457500 | 7.50660000 | 11.39365000 |
| Pd | 10.67830000 | 8.64615000 | 11.27077500 |
| Pd | 8.25195000 | 9.96055000 | 11.29242500 |
| Pd | 13.42710000 | 14.21230000 | 10.59927500 |
| Pd | 15.07595000 | 9.34692500 | 10.55490000 |
| Pd | 8.54790000 | 12.56970000 | 10.44417500 |
| Pd | 12.33145000 | 11.85232500 | 10.00335000 |
| Pd | 16.95517500 | 11.22552500 | 9.82437500 |
| Pd | 8.94437500 | 15.17335000 | 9.69937500 |
| Pd | 15.65482500 | 13.60632500 | 9.24402500 |

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|----|-------------|-------------|-------------|
| Pd | 14.31152500 | 15.93060000 | 8.73462500 |
| Pd | 10.09832500 | 10.56207500 | 9.33755000 |
| Pd | 11.63280000 | 15.61570000 | 9.19305000 |
| Pd | 12.57597500 | 9.29625000 | 9.36435000 |
| Pd | 14.47745000 | 11.20187500 | 8.57892500 |
| Pd | 10.46720000 | 13.20047500 | 8.51827500 |
| Pd | 11.99122500 | 11.18970000 | 7.42650000 |
| Pd | 13.15292500 | 13.58792500 | 8.00837500 |
| O | 10.28065000 | 12.29892500 | 17.28987500 |
| O | 13.94872500 | 10.71590000 | 17.25670000 |
| C | 9.26370000 | 10.55967500 | 18.93140000 |
| C | 10.00555000 | 9.40217500 | 18.58517500 |
| C | 9.64290000 | 8.40915000 | 17.63547500 |
| H | 9.48597500 | 11.01107500 | 19.90412500 |
| H | 8.20952500 | 10.59115000 | 18.63167500 |
| H | 9.77235000 | 11.60487500 | 18.13000000 |
| H | 10.95115000 | 9.24665000 | 19.11832500 |
| H | 8.60980000 | 8.39097500 | 17.27035000 |
| H | 10.12225000 | 7.42697500 | 17.71802500 |

3_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.67352500 | 11.23267500 | 16.88415000 |
| Pd | 12.94955000 | 13.64377500 | 17.54022500 |
| Pd | 14.67115000 | 11.77922500 | 16.50250000 |
| Pd | 10.45027500 | 13.77395000 | 16.35765000 |
| Pd | 10.61475000 | 8.91995000 | 15.75882500 |
| Pd | 14.87975000 | 14.43925000 | 15.81687500 |

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|----|-------------|-------------|-------------|
| Pd | 12.34382500 | 15.63537500 | 15.72870000 |
| Pd | 13.40740000 | 9.25585000 | 15.52805000 |
| Pd | 9.31490000 | 11.30480000 | 15.38655000 |
| Pd | 16.09812500 | 9.82527500 | 15.18655000 |
| Pd | 8.00037500 | 13.87022500 | 14.61412500 |
| Pd | 12.66147500 | 12.97395000 | 15.03932500 |
| Pd | 16.55400000 | 12.47737500 | 14.64400000 |
| Pd | 9.91360000 | 15.76597500 | 14.27440000 |
| Pd | 11.59077500 | 10.74327500 | 14.09027500 |
| Pd | 16.82805000 | 15.12975000 | 14.00922500 |
| Pd | 14.43385000 | 16.47257500 | 13.85715000 |
| Pd | 11.92615000 | 17.54655000 | 13.75260000 |
| Pd | 14.31107500 | 11.18450000 | 13.78847500 |
| Pd | 10.31067500 | 13.17792500 | 13.61510000 |
| Pd | 11.90850000 | 8.15232500 | 13.45367500 |
| Pd | 9.38250000 | 9.40962500 | 13.32960000 |
| Pd | 14.67357500 | 13.81362500 | 13.27242500 |
| Pd | 14.64615000 | 8.58217500 | 13.18360000 |
| Pd | 12.28325000 | 15.01870000 | 13.20462500 |
| Pd | 8.06820000 | 11.83197500 | 12.79887500 |
| Pd | 16.60697500 | 10.54577500 | 12.59917500 |
| Pd | 12.55742500 | 12.55227500 | 12.46660000 |
| Pd | 8.44877500 | 14.55740000 | 12.15227500 |
| Pd | 17.01620000 | 13.23742500 | 11.96365000 |
| Pd | 12.86877500 | 10.06340000 | 11.73120000 |
| Pd | 10.47927500 | 16.47910000 | 11.64570000 |
| Pd | 10.43487500 | 11.26652500 | 11.69022500 |

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|----|-------------|-------------|-------------|
| Pd | 15.73785000 | 15.64425000 | 11.52255000 |
| Pd | 13.20650000 | 16.91192500 | 11.39080000 |
| Pd | 14.76112500 | 11.96592500 | 11.22102500 |
| Pd | 10.85470000 | 13.95120000 | 11.08745000 |
| Pd | 13.21770000 | 7.51735000 | 11.09195000 |
| Pd | 10.71362500 | 8.66152500 | 10.94432500 |
| Pd | 8.31032500 | 9.95002500 | 10.82157500 |
| Pd | 13.51557500 | 14.35085000 | 10.84620000 |
| Pd | 15.18330000 | 9.36492500 | 10.51417500 |
| Pd | 8.68807500 | 12.59775000 | 10.17002500 |
| Pd | 12.36510000 | 12.04132500 | 9.91685000 |
| Pd | 17.04965000 | 11.32480000 | 9.99430000 |
| Pd | 9.12127500 | 15.27305000 | 9.59072500 |
| Pd | 15.83632500 | 13.71245000 | 9.48717500 |
| Pd | 14.50690000 | 16.07985000 | 9.11240000 |
| Pd | 10.26185000 | 10.62777500 | 9.02457500 |
| Pd | 11.79495000 | 15.71212500 | 9.25297500 |
| Pd | 12.75905000 | 9.40920000 | 9.17737500 |
| Pd | 14.69055000 | 11.32140000 | 8.61012500 |
| Pd | 10.66157500 | 13.34040000 | 8.36780000 |
| Pd | 12.26727500 | 11.39175000 | 7.31772500 |
| Pd | 13.42075000 | 13.72985000 | 8.14940000 |
| O | 8.37735000 | 12.99165000 | 16.50662500 |
| O | 13.55657500 | 10.30880000 | 17.21110000 |
| C | 10.68582500 | 10.91987500 | 18.75447500 |
| C | 10.83722500 | 9.56695000 | 18.36307500 |
| C | 9.85572500 | 8.76287500 | 17.68925000 |

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|---|-------------|-------------|-------------|
| H | 11.35010000 | 11.32237500 | 19.52240000 |
| H | 9.70452500 | 11.39697500 | 18.67595000 |
| H | 7.77705000 | 12.97832500 | 17.27437500 |
| H | 11.76477500 | 9.07020000 | 18.66412500 |
| H | 8.82550000 | 9.14042500 | 17.66687500 |
| H | 9.94130000 | 7.67612500 | 17.82787500 |

TS2_PdOH

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|----|-------------|-------------|-------------|
| Pd | 11.85412500 | 12.07295000 | 16.96960000 |
| Pd | 13.23080000 | 14.45530000 | 17.35712500 |
| Pd | 14.78815000 | 12.31282500 | 16.52580000 |
| Pd | 10.74990000 | 14.53535000 | 16.19847500 |
| Pd | 10.68685000 | 9.63540000 | 16.23505000 |
| Pd | 15.21357500 | 14.86327500 | 15.50552500 |
| Pd | 12.77695000 | 16.21077500 | 15.30742500 |
| Pd | 13.43677500 | 9.77387500 | 15.91070000 |
| Pd | 9.39370000 | 12.12125000 | 15.70157500 |
| Pd | 16.12265000 | 10.16762500 | 15.40832500 |
| Pd | 8.32897500 | 14.52062500 | 14.81982500 |
| Pd | 12.94102500 | 13.52665000 | 14.91090000 |
| Pd | 16.64087500 | 12.69907500 | 14.51372500 |
| Pd | 10.27015000 | 16.27760000 | 13.98017500 |
| Pd | 11.65307500 | 11.19340000 | 14.35265000 |
| Pd | 17.10935000 | 15.22867500 | 13.54397500 |
| Pd | 14.76485000 | 16.66666667 | 13.34767500 |
| Pd | 12.32000000 | 17.91337500 | 13.16997500 |
| Pd | 14.35230000 | 11.44107500 | 13.90157500 |

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|----|-------------|-------------|-------------|
| Pd | 10.46985000 | 13.52600000 | 13.74210000 |
| Pd | 11.84165000 | 8.53965000 | 14.01320000 |
| Pd | 9.36692500 | 9.92250000 | 13.80562500 |
| Pd | 14.81927500 | 14.00160000 | 12.98160000 |
| Pd | 14.56730000 | 8.76620000 | 13.61585000 |
| Pd | 12.44470000 | 15.28705000 | 12.87185000 |
| Pd | 8.11537500 | 12.37075000 | 13.07060000 |
| Pd | 16.54137500 | 10.54602500 | 12.71537500 |
| Pd | 12.61555000 | 12.73677500 | 12.47510000 |
| Pd | 8.70405000 | 14.94000000 | 12.13272500 |
| Pd | 17.10352500 | 13.10125000 | 11.76055000 |
| Pd | 12.81217500 | 10.18207500 | 12.04442500 |
| Pd | 10.73417500 | 16.70150000 | 11.25087500 |
| Pd | 10.41000000 | 11.52082500 | 11.92612500 |
| Pd | 15.89085000 | 15.50175000 | 11.07037500 |
| Pd | 13.48152500 | 16.87022500 | 10.88512500 |
| Pd | 14.75457500 | 11.93655000 | 11.21672500 |
| Pd | 10.89987500 | 14.06310000 | 11.03830000 |
| Pd | 12.98002500 | 7.56990000 | 11.70507500 |
| Pd | 10.53422500 | 8.84357500 | 11.51007500 |
| Pd | 8.17700000 | 10.24602500 | 11.32782500 |
| Pd | 13.53980000 | 14.24870000 | 10.55057500 |
| Pd | 15.00277500 | 9.22865000 | 10.83295000 |
| Pd | 8.63625000 | 12.76527500 | 10.34915000 |
| Pd | 12.28525000 | 11.93437500 | 10.01792500 |
| Pd | 16.94637500 | 10.98565000 | 10.01085000 |
| Pd | 9.19995000 | 15.31462500 | 9.44087500 |

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|----|-------------|-------------|-------------|
| Pd | 15.83422500 | 13.38092500 | 9.28097500 |
| Pd | 14.59892500 | 15.76082500 | 8.61742500 |
| Pd | 10.08342500 | 10.57862500 | 9.38042500 |
| Pd | 11.89210000 | 15.58270000 | 8.95005000 |
| Pd | 12.52632500 | 9.25490000 | 9.57587500 |
| Pd | 14.51040000 | 10.97742500 | 8.73332500 |
| Pd | 10.60640000 | 13.18187500 | 8.41032500 |
| Pd | 12.04087500 | 11.04965000 | 7.50240000 |
| Pd | 13.37167500 | 13.39370000 | 7.98920000 |
| O | 8.25337500 | 11.58230000 | 17.25755000 |
| O | 13.52147500 | 11.06905000 | 17.43935000 |
| C | 8.49722500 | 9.59410000 | 18.31522500 |
| C | 9.73360000 | 8.95372500 | 18.23575000 |
| C | 10.04487500 | 7.95567500 | 17.25712500 |
| H | 8.24262500 | 10.19202500 | 19.18857500 |
| H | 7.67247500 | 9.28727500 | 17.67325000 |
| H | 8.54575000 | 12.16532500 | 17.98795000 |
| H | 10.48397500 | 9.18435000 | 18.99802500 |
| H | 9.22655000 | 7.51282500 | 16.67757500 |
| H | 10.89415000 | 7.28992500 | 17.43725000 |

4_PdOH

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.50250000 | 11.36452500 | 16.78425000 |
| Pd | 12.79555000 | 13.70605000 | 17.49575000 |
| Pd | 14.50605000 | 11.76185000 | 16.52185000 |
| Pd | 10.39652500 | 13.92575000 | 16.15790000 |
| Pd | 10.52802500 | 9.09180000 | 15.72795000 |

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|----|-------------|-------------|-------------|
| Pd | 14.87690000 | 14.39382500 | 15.81460000 |
| Pd | 12.43472500 | 15.70952500 | 15.60510000 |
| Pd | 13.26435000 | 9.26752500 | 15.55205000 |
| Pd | 9.17942500 | 11.56670000 | 15.28347500 |
| Pd | 15.94585000 | 9.77042500 | 15.26320000 |
| Pd | 8.06942500 | 13.98655000 | 14.64112500 |
| Pd | 12.65440000 | 13.06465000 | 14.96545000 |
| Pd | 16.45870000 | 12.40560000 | 14.69040000 |
| Pd | 10.00780000 | 15.86055000 | 14.13352500 |
| Pd | 11.53595000 | 10.82097500 | 14.00610000 |
| Pd | 16.86912500 | 15.05192500 | 14.04142500 |
| Pd | 14.50450000 | 16.44987500 | 13.83497500 |
| Pd | 12.03772500 | 17.62817500 | 13.62647500 |
| Pd | 14.23542500 | 11.17770000 | 13.81172500 |
| Pd | 10.31935000 | 13.19007500 | 13.55920000 |
| Pd | 11.81070000 | 8.19080000 | 13.44035000 |
| Pd | 9.34665000 | 9.56070000 | 13.21157500 |
| Pd | 14.68372500 | 13.81990000 | 13.21852500 |
| Pd | 14.54970000 | 8.56410000 | 13.22110000 |
| Pd | 12.30380000 | 15.06297500 | 13.07007500 |
| Pd | 8.06197500 | 12.00725000 | 12.67570000 |
| Pd | 16.55987500 | 10.45210000 | 12.68165000 |
| Pd | 12.56345000 | 12.58300000 | 12.40187500 |
| Pd | 8.56795000 | 14.68855000 | 12.04387500 |
| Pd | 17.05160000 | 13.14175000 | 12.02727500 |
| Pd | 12.81272500 | 10.06875000 | 11.74905000 |
| Pd | 10.61300000 | 16.57880000 | 11.49867500 |

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|----|-------------|-------------|-------------|
| Pd | 10.43165000 | 11.36565000 | 11.53930000 |
| Pd | 15.79870000 | 15.56890000 | 11.52772500 |
| Pd | 13.36260000 | 16.89410000 | 11.31740000 |
| Pd | 14.78902500 | 11.91967500 | 11.27037500 |
| Pd | 10.87992500 | 13.99390000 | 11.01072500 |
| Pd | 13.11927500 | 7.52322500 | 11.11102500 |
| Pd | 10.63805000 | 8.73300000 | 10.88515000 |
| Pd | 8.25557500 | 10.10020000 | 10.70712500 |
| Pd | 13.54910000 | 14.31730000 | 10.72977500 |
| Pd | 15.12440000 | 9.35262500 | 10.55107500 |
| Pd | 8.69157500 | 12.73505000 | 10.03135000 |
| Pd | 12.44825000 | 12.05655000 | 9.85515000 |
| Pd | 17.06677500 | 11.21810000 | 10.07635000 |
| Pd | 9.22295000 | 15.37575000 | 9.46475000 |
| Pd | 15.88885000 | 13.64375000 | 9.53417500 |
| Pd | 14.64657500 | 16.04837500 | 9.03272500 |
| Pd | 10.26987500 | 10.70572500 | 8.93670000 |
| Pd | 11.93520000 | 15.75440000 | 9.16712500 |
| Pd | 12.73032500 | 9.44832500 | 9.16302500 |
| Pd | 14.71392500 | 11.31017500 | 8.61587500 |
| Pd | 10.76022500 | 13.39257500 | 8.30867500 |
| Pd | 12.32145000 | 11.42285000 | 7.25425000 |
| Pd | 13.52217500 | 13.74930000 | 8.04580000 |
| O | 8.09220000 | 11.03915000 | 17.32075000 |
| O | 13.29395000 | 10.36182500 | 17.22585000 |
| C | 8.98492500 | 11.24235000 | 18.44770000 |
| C | 10.23097500 | 10.41402500 | 18.26130000 |

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|---|-------------|-------------|-------------|
| C | 10.09667500 | 9.06552500 | 17.76207500 |
| H | 9.23730000 | 12.31097500 | 18.55027500 |
| H | 8.45962500 | 10.90980000 | 19.36607500 |
| H | 7.36047500 | 11.67977500 | 17.38767500 |
| H | 10.96835000 | 10.57190000 | 19.06085000 |
| H | 9.07025000 | 8.68352500 | 17.63937500 |
| H | 10.82905000 | 8.33777500 | 18.13332500 |

4_PdOH_2

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.38207500 | 11.34725000 | 16.86300000 |
| Pd | 12.88207500 | 13.81297500 | 17.47625000 |
| Pd | 14.40735000 | 11.75325000 | 16.52487500 |
| Pd | 10.34387500 | 14.05095000 | 16.21175000 |
| Pd | 10.51930000 | 9.05772500 | 15.77527500 |
| Pd | 14.88317500 | 14.43372500 | 15.80937500 |
| Pd | 12.48945000 | 15.81955000 | 15.60840000 |
| Pd | 13.18630000 | 9.42285000 | 15.66895000 |
| Pd | 9.08732500 | 11.57392500 | 15.27310000 |
| Pd | 15.88122500 | 9.77550000 | 15.32807500 |
| Pd | 8.04712500 | 14.06007500 | 14.65500000 |
| Pd | 12.68877500 | 13.09625000 | 14.97415000 |
| Pd | 16.42615000 | 12.39757500 | 14.70717500 |
| Pd | 10.02312500 | 15.86760000 | 14.22150000 |
| Pd | 11.54005000 | 10.82235000 | 14.08995000 |
| Pd | 16.90615000 | 15.00782500 | 13.94215000 |
| Pd | 14.53722500 | 16.40290000 | 13.83120000 |
| Pd | 12.06200000 | 17.61675000 | 13.59435000 |

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|----|-------------|-------------|-------------|
| Pd | 14.22442500 | 11.16737500 | 13.82597500 |
| Pd | 10.31620000 | 13.18385000 | 13.64032500 |
| Pd | 11.75827500 | 8.21665000 | 13.51752500 |
| Pd | 9.29087500 | 9.55595000 | 13.31512500 |
| Pd | 14.68325000 | 13.82620000 | 13.15425000 |
| Pd | 14.49215000 | 8.55882500 | 13.29500000 |
| Pd | 12.26292500 | 15.04427500 | 13.10037500 |
| Pd | 8.02760000 | 12.05405000 | 12.74650000 |
| Pd | 16.53722500 | 10.37247500 | 12.75220000 |
| Pd | 12.53977500 | 12.56045000 | 12.42607500 |
| Pd | 8.57055000 | 14.73520000 | 12.09437500 |
| Pd | 17.07442500 | 13.04907500 | 12.06027500 |
| Pd | 12.77430000 | 10.04790000 | 11.76702500 |
| Pd | 10.64362500 | 16.57747500 | 11.49162500 |
| Pd | 10.38560000 | 11.34702500 | 11.63820000 |
| Pd | 15.86700000 | 15.52485000 | 11.47940000 |
| Pd | 13.40930000 | 16.87040000 | 11.31832500 |
| Pd | 14.77165000 | 11.87615000 | 11.28792500 |
| Pd | 10.83025000 | 13.95825000 | 11.05757500 |
| Pd | 13.04000000 | 7.48247500 | 11.17630000 |
| Pd | 10.57992500 | 8.69042500 | 11.00515000 |
| Pd | 8.20692500 | 10.10407500 | 10.80607500 |
| Pd | 13.51677500 | 14.30262500 | 10.75572500 |
| Pd | 15.07815000 | 9.24300000 | 10.65755000 |
| Pd | 8.63067500 | 12.73180000 | 10.08917500 |
| Pd | 12.40600000 | 12.01175000 | 9.89685000 |
| Pd | 17.05872500 | 11.10382500 | 10.15927500 |

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|----|-------------|-------------|-------------|
| Pd | 9.21477500 | 15.34670000 | 9.50087500 |
| Pd | 15.88342500 | 13.52295000 | 9.55240000 |
| Pd | 14.65355000 | 15.94775000 | 9.03397500 |
| Pd | 10.21332500 | 10.66715000 | 9.04780000 |
| Pd | 11.93335000 | 15.70242500 | 9.18502500 |
| Pd | 12.66430000 | 9.33792500 | 9.22897500 |
| Pd | 14.69182500 | 11.15982500 | 8.70002500 |
| Pd | 10.72557500 | 13.33932500 | 8.35460000 |
| Pd | 12.28120000 | 11.33130000 | 7.33200000 |
| Pd | 13.51905000 | 13.63657500 | 8.09050000 |
| O | 8.06340000 | 10.78285000 | 17.23525000 |
| O | 11.06150000 | 13.14790000 | 17.85192500 |
| C | 8.86950000 | 10.98492500 | 18.43315000 |
| C | 10.18925000 | 10.26785000 | 18.28567500 |
| C | 10.18080000 | 8.90235000 | 17.80562500 |
| H | 9.03080000 | 12.05892500 | 18.61220000 |
| H | 8.31395000 | 10.55182500 | 19.28837500 |
| H | 7.22875000 | 11.27492500 | 17.34235000 |
| H | 10.87802500 | 10.49395000 | 19.11327500 |
| H | 9.19297500 | 8.42425000 | 17.69037500 |
| H | 10.96747500 | 8.24367500 | 18.19097500 |

TS4_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.41170000 | 11.10505000 | 16.79245000 |
| Pd | 12.43652500 | 13.75117500 | 17.46620000 |
| Pd | 14.16617500 | 11.71770000 | 16.59830000 |

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|----|-------------|-------------|-------------|
| Pd | 9.95135000 | 13.98177500 | 16.07292500 |
| Pd | 10.23165000 | 8.98370000 | 15.62500000 |
| Pd | 14.58400000 | 14.36395000 | 15.94235000 |
| Pd | 12.17852500 | 15.71502500 | 15.56000000 |
| Pd | 13.02365000 | 9.27385000 | 15.52632500 |
| Pd | 8.99875000 | 11.48660000 | 15.10080000 |
| Pd | 15.73130000 | 9.74122500 | 15.44040000 |
| Pd | 7.83157500 | 13.95800000 | 14.41200000 |
| Pd | 12.39867500 | 13.07700000 | 14.96720000 |
| Pd | 16.27797500 | 12.37937500 | 14.88070000 |
| Pd | 9.80457500 | 15.84582500 | 14.07180000 |
| Pd | 11.35612500 | 10.79705000 | 14.04647500 |
| Pd | 16.68600000 | 15.01512500 | 14.21227500 |
| Pd | 14.31252500 | 16.38310000 | 13.96295000 |
| Pd | 11.85880000 | 17.59762500 | 13.56045000 |
| Pd | 14.08212500 | 11.20575000 | 13.98567500 |
| Pd | 10.16945000 | 13.21727500 | 13.45417500 |
| Pd | 11.61440000 | 8.15962500 | 13.38177500 |
| Pd | 9.15172500 | 9.47877500 | 13.12150000 |
| Pd | 14.51727500 | 13.83032500 | 13.30225000 |
| Pd | 14.48240000 | 8.52267500 | 13.28135000 |
| Pd | 12.10800000 | 15.03680000 | 12.95700000 |
| Pd | 7.98717500 | 11.97525000 | 12.51032500 |
| Pd | 16.46097500 | 10.40875000 | 12.89535000 |
| Pd | 12.45965000 | 12.52432500 | 12.42672500 |
| Pd | 8.48180000 | 14.66597500 | 11.87517500 |
| Pd | 16.97600000 | 13.10435000 | 12.28715000 |

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|----|-------------|-------------|-------------|
| Pd | 12.81122500 | 9.98977500 | 11.89607500 |
| Pd | 10.53282500 | 16.53177500 | 11.42855000 |
| Pd | 10.39772500 | 11.21165000 | 11.54700000 |
| Pd | 15.77220000 | 15.55172500 | 11.69497500 |
| Pd | 13.32937500 | 16.86152500 | 11.39392500 |
| Pd | 14.75562500 | 11.84445000 | 11.42855000 |
| Pd | 10.82310000 | 13.82635000 | 10.87215000 |
| Pd | 13.09917500 | 7.47097500 | 11.13497500 |
| Pd | 10.63665000 | 8.67580000 | 10.81965000 |
| Pd | 8.25947500 | 10.03315000 | 10.55522500 |
| Pd | 13.53325000 | 14.21242500 | 10.76927500 |
| Pd | 15.13787500 | 9.29127500 | 10.67655000 |
| Pd | 8.68122500 | 12.67560000 | 9.89367500 |
| Pd | 12.48077500 | 11.85420000 | 9.91560000 |
| Pd | 17.10010000 | 11.19660000 | 10.33905000 |
| Pd | 9.25950000 | 15.30122500 | 9.32887500 |
| Pd | 15.95417500 | 13.60245000 | 9.72187500 |
| Pd | 14.71395000 | 15.98915000 | 9.19525000 |
| Pd | 10.32162500 | 10.68362500 | 8.86615000 |
| Pd | 11.98897500 | 15.71482500 | 9.22065000 |
| Pd | 12.79020000 | 9.35460000 | 9.18202500 |
| Pd | 14.83490000 | 11.24800000 | 8.75522500 |
| Pd | 10.87155000 | 13.34462500 | 8.25970000 |
| Pd | 12.49375000 | 11.32767500 | 7.30582500 |
| Pd | 13.62865000 | 13.69205000 | 8.17212500 |
| O | 8.58862500 | 11.36757500 | 18.30785000 |
| O | 10.50537500 | 13.73252500 | 17.95717500 |

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|---|-------------|-------------|-------------|
| C | 9.94060000 | 11.19947500 | 18.65395000 |
| C | 10.49340000 | 9.89100000 | 18.29522500 |
| C | 9.73857500 | 8.85315000 | 17.63387500 |
| H | 10.50375000 | 12.27610000 | 18.16360000 |
| H | 10.16892500 | 11.48637500 | 19.69865000 |
| H | 8.42417500 | 12.32870000 | 18.22595000 |
| H | 11.37647500 | 9.58392500 | 18.86785000 |
| H | 8.65185000 | 9.00675000 | 17.58187500 |
| H | 10.05540000 | 7.82570000 | 17.85892500 |

5_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.34152500 | 11.18125000 | 16.68085000 |
| Pd | 12.29507500 | 13.67102500 | 17.48697500 |
| Pd | 14.08107500 | 11.67857500 | 16.58777500 |
| Pd | 9.94162500 | 13.82512500 | 16.02602500 |
| Pd | 10.13447500 | 9.00462500 | 15.60467500 |
| Pd | 14.51380000 | 14.31847500 | 15.96300000 |
| Pd | 12.10575000 | 15.66177500 | 15.58622500 |
| Pd | 12.95920000 | 9.25910000 | 15.50015000 |
| Pd | 8.88812500 | 11.38765000 | 14.97917500 |
| Pd | 15.66772500 | 9.70642500 | 15.43117500 |
| Pd | 7.78012500 | 13.87840000 | 14.36655000 |
| Pd | 12.38475000 | 12.98880000 | 14.96200000 |
| Pd | 16.20277500 | 12.34635000 | 14.95560000 |
| Pd | 9.73392500 | 15.80895000 | 14.00200000 |
| Pd | 11.31687500 | 10.72487500 | 13.94617500 |
| Pd | 16.64050000 | 14.98440000 | 14.27507500 |

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|----|-------------|-------------|-------------|
| Pd | 14.27632500 | 16.34727500 | 14.01367500 |
| Pd | 11.81342500 | 17.55942500 | 13.61380000 |
| Pd | 14.06435000 | 11.14860000 | 13.89055000 |
| Pd | 10.15170000 | 13.17940000 | 13.49960000 |
| Pd | 11.59310000 | 8.13900000 | 13.32982500 |
| Pd | 9.14622500 | 9.41775000 | 13.00425000 |
| Pd | 14.49187500 | 13.78460000 | 13.33097500 |
| Pd | 14.37862500 | 8.50167500 | 13.29777500 |
| Pd | 12.09162500 | 15.00250000 | 13.03675000 |
| Pd | 7.96165000 | 11.92865000 | 12.40142500 |
| Pd | 16.41117500 | 10.38012500 | 12.92002500 |
| Pd | 12.42685000 | 12.51512500 | 12.39882500 |
| Pd | 8.45522500 | 14.60740000 | 11.81070000 |
| Pd | 16.93305000 | 13.05555000 | 12.36470000 |
| Pd | 12.76650000 | 10.01660000 | 11.76152500 |
| Pd | 10.52350000 | 16.52582500 | 11.40872500 |
| Pd | 10.33085000 | 11.27640000 | 11.48770000 |
| Pd | 15.75702500 | 15.54130000 | 11.75755000 |
| Pd | 13.31092500 | 16.85912500 | 11.42542500 |
| Pd | 14.71347500 | 11.88712500 | 11.33380000 |
| Pd | 10.80065000 | 13.89917500 | 10.91327500 |
| Pd | 13.09120000 | 7.47345000 | 11.07175000 |
| Pd | 10.65442500 | 8.68310000 | 10.74930000 |
| Pd | 8.26822500 | 10.02527500 | 10.43142500 |
| Pd | 13.50337500 | 14.27240000 | 10.81740000 |
| Pd | 15.13897500 | 9.26072500 | 10.72362500 |
| Pd | 8.71360000 | 12.66255000 | 9.77190000 |

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|----|-------------|-------------|-------------|
| Pd | 12.41057500 | 11.95480000 | 9.85925000 |
| Pd | 17.08717500 | 11.17532500 | 10.37660000 |
| Pd | 9.27067500 | 15.31315000 | 9.29077500 |
| Pd | 15.98705000 | 13.60207500 | 9.77227500 |
| Pd | 14.73547500 | 16.00425000 | 9.24297500 |
| Pd | 10.36457500 | 10.65675000 | 8.78250000 |
| Pd | 12.00680000 | 15.70815000 | 9.19010000 |
| Pd | 12.83522500 | 9.36195000 | 9.13782500 |
| Pd | 14.86680000 | 11.22602500 | 8.77190000 |
| Pd | 10.90577500 | 13.34662500 | 8.20037500 |
| Pd | 12.55255000 | 11.35680000 | 7.27355000 |
| Pd | 13.68700000 | 13.68440000 | 8.19795000 |
| O | 9.33610000 | 11.62930000 | 18.70705000 |
| O | 10.21532500 | 13.99912500 | 18.17245000 |
| C | 10.54837500 | 11.04060000 | 18.68092500 |
| C | 10.71450000 | 9.69502500 | 18.24155000 |
| C | 9.69347500 | 8.88300000 | 17.62957500 |
| H | 10.04385000 | 14.91095000 | 18.46997500 |
| H | 11.32392500 | 11.48982500 | 19.31655000 |
| H | 9.50250000 | 12.63612500 | 18.68807500 |
| H | 11.65260000 | 9.21590000 | 18.53360000 |
| H | 8.66310000 | 9.24997500 | 17.71565000 |
| H | 9.81172500 | 7.79715000 | 17.75585000 |

TS5_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.44287500 | 11.15215000 | 16.67487500 |
| Pd | 12.42062500 | 13.66487500 | 17.48935000 |

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|----|-------------|-------------|-------------|
| Pd | 14.18522500 | 11.66832500 | 16.57105000 |
| Pd | 10.01855000 | 13.78710000 | 16.03090000 |
| Pd | 10.22185000 | 8.98797500 | 15.59460000 |
| Pd | 14.57925000 | 14.32072500 | 15.93472500 |
| Pd | 12.14525000 | 15.64087500 | 15.59787500 |
| Pd | 13.04640000 | 9.25552500 | 15.47882500 |
| Pd | 8.96960000 | 11.35557500 | 14.98777500 |
| Pd | 15.76095000 | 9.71325000 | 15.39665000 |
| Pd | 7.83162500 | 13.81797500 | 14.39192500 |
| Pd | 12.45550000 | 12.95857500 | 14.96967500 |
| Pd | 16.30087500 | 12.36465000 | 14.93755000 |
| Pd | 9.77942500 | 15.77267500 | 14.02547500 |
| Pd | 11.39590000 | 10.70802500 | 13.93227500 |
| Pd | 16.68770000 | 15.02057500 | 14.27785000 |
| Pd | 14.32042500 | 16.36945000 | 14.02287500 |
| Pd | 11.86200000 | 17.54825000 | 13.64492500 |
| Pd | 14.14717500 | 11.16122500 | 13.87742500 |
| Pd | 10.22382500 | 13.17690000 | 13.51365000 |
| Pd | 11.66677500 | 8.11455000 | 13.32222500 |
| Pd | 9.21485000 | 9.39352500 | 13.00155000 |
| Pd | 14.57140000 | 13.77460000 | 13.30430000 |
| Pd | 14.45472500 | 8.55015000 | 13.25937500 |
| Pd | 12.18447500 | 14.99485000 | 13.04912500 |
| Pd | 8.01027500 | 11.89082500 | 12.42445000 |
| Pd | 16.51300000 | 10.42425000 | 12.89760000 |
| Pd | 12.48897500 | 12.51117500 | 12.39635000 |
| Pd | 8.48795000 | 14.57860000 | 11.84890000 |

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|----|-------------|-------------|-------------|
| Pd | 16.97385000 | 13.10817500 | 12.34585000 |
| Pd | 12.77180000 | 10.01245000 | 11.72345000 |
| Pd | 10.55700000 | 16.50442500 | 11.45067500 |
| Pd | 10.37712500 | 11.27727500 | 11.49640000 |
| Pd | 15.79340000 | 15.59480000 | 11.76405000 |
| Pd | 13.33882500 | 16.86787500 | 11.44250000 |
| Pd | 14.74735000 | 11.82302500 | 11.31997500 |
| Pd | 10.83605000 | 13.89087500 | 10.93882500 |
| Pd | 13.15927500 | 7.47727500 | 11.05525000 |
| Pd | 10.70325000 | 8.65620000 | 10.73907500 |
| Pd | 8.32020000 | 10.00267500 | 10.44170000 |
| Pd | 13.57170000 | 14.25850000 | 10.82132500 |
| Pd | 15.21850000 | 9.28162500 | 10.68910000 |
| Pd | 8.74590000 | 12.64827500 | 9.79550000 |
| Pd | 12.45367500 | 11.98967500 | 9.84365000 |
| Pd | 17.14082500 | 11.21077500 | 10.34540000 |
| Pd | 9.28782500 | 15.30442500 | 9.33272500 |
| Pd | 16.00980000 | 13.64070000 | 9.78335000 |
| Pd | 14.75617500 | 16.02775000 | 9.24522500 |
| Pd | 10.41722500 | 10.65427500 | 8.80067500 |
| Pd | 12.02897500 | 15.70140000 | 9.23087500 |
| Pd | 12.89922500 | 9.38602500 | 9.12955000 |
| Pd | 14.90780000 | 11.27150000 | 8.74785000 |
| Pd | 10.91740000 | 13.35722500 | 8.20892500 |
| Pd | 12.57637500 | 11.39075000 | 7.26147500 |
| Pd | 13.71352500 | 13.71685000 | 8.18020000 |
| O | 9.52987500 | 11.63777500 | 18.78605000 |

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|---|-------------|-------------|-------------|
| O | 10.22282500 | 13.88475000 | 18.26857500 |
| C | 10.66897500 | 11.00635000 | 18.74685000 |
| C | 10.83860000 | 9.67475000 | 18.22415000 |
| C | 9.79385000 | 8.88787500 | 17.62290000 |
| H | 9.87877500 | 14.67347500 | 18.72282500 |
| H | 11.51595000 | 11.42427500 | 19.32415000 |
| H | 9.79397500 | 12.86525000 | 18.65385000 |
| H | 11.77465000 | 9.17650000 | 18.49305000 |
| H | 8.77432500 | 9.27967500 | 17.72772500 |
| H | 9.89055000 | 7.79717500 | 17.73242500 |

6_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.59875000 | 11.17987500 | 16.72420000 |
| Pd | 12.72565000 | 13.58362500 | 17.50575000 |
| Pd | 14.39162500 | 11.60657500 | 16.47497500 |
| Pd | 10.26225000 | 13.74155000 | 16.19050000 |
| Pd | 10.42760000 | 8.97982500 | 15.66305000 |
| Pd | 14.82820000 | 14.30262500 | 15.86172500 |
| Pd | 12.36902500 | 15.60390000 | 15.66142500 |
| Pd | 13.20630000 | 9.24790000 | 15.47172500 |
| Pd | 9.15687500 | 11.36022500 | 15.11005000 |
| Pd | 15.94525000 | 9.65177500 | 15.26327500 |
| Pd | 8.03505000 | 13.83865000 | 14.57297500 |
| Pd | 12.65072500 | 12.94007500 | 14.99435000 |
| Pd | 16.49170000 | 12.30942500 | 14.79732500 |
| Pd | 9.98407500 | 15.76290000 | 14.16910000 |
| Pd | 11.52872500 | 10.71842500 | 13.96322500 |

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|----|-------------|-------------|-------------|
| Pd | 16.89212500 | 14.95472500 | 14.14145000 |
| Pd | 14.50932500 | 16.33575000 | 13.97600000 |
| Pd | 12.05855000 | 17.53207500 | 13.72755000 |
| Pd | 14.27245000 | 11.06727500 | 13.77550000 |
| Pd | 10.39082500 | 13.20732500 | 13.60587500 |
| Pd | 11.78430000 | 8.11502500 | 13.33190000 |
| Pd | 9.32940000 | 9.42497500 | 13.10502500 |
| Pd | 14.76087500 | 13.66042500 | 13.28040000 |
| Pd | 14.55975000 | 8.49830000 | 13.18437500 |
| Pd | 12.40385000 | 14.99652500 | 13.09302500 |
| Pd | 8.10205000 | 11.92370000 | 12.60007500 |
| Pd | 16.62235000 | 10.39712500 | 12.74037500 |
| Pd | 12.59977500 | 12.51005000 | 12.41715000 |
| Pd | 8.59357500 | 14.60470000 | 12.01910000 |
| Pd | 17.08350000 | 13.08490000 | 12.15422500 |
| Pd | 12.80025000 | 10.00585000 | 11.69167500 |
| Pd | 10.63967500 | 16.53360000 | 11.58287500 |
| Pd | 10.42692500 | 11.34682500 | 11.56735000 |
| Pd | 15.87422500 | 15.57275000 | 11.67255000 |
| Pd | 13.40985000 | 16.86887500 | 11.43772500 |
| Pd | 14.80625000 | 11.78757500 | 11.23305000 |
| Pd | 10.94650000 | 13.95647500 | 11.03052500 |
| Pd | 13.17462500 | 7.47885000 | 11.00522500 |
| Pd | 10.71412500 | 8.69327500 | 10.78967500 |
| Pd | 8.33333333 | 10.07710000 | 10.57205000 |
| Pd | 13.69147500 | 14.23005000 | 10.81892500 |
| Pd | 15.23470000 | 9.26882500 | 10.58322500 |

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|----|-------------|-------------|-------------|
| Pd | 8.76450000 | 12.70527500 | 9.94645000 |
| Pd | 12.45390000 | 12.00192500 | 9.86242500 |
| Pd | 17.15902500 | 11.18775000 | 10.15642500 |
| Pd | 9.30215000 | 15.35615000 | 9.50095000 |
| Pd | 16.04175000 | 13.64132500 | 9.64067500 |
| Pd | 14.78665000 | 16.03332500 | 9.20375000 |
| Pd | 10.38122500 | 10.70220000 | 8.87055000 |
| Pd | 12.03875000 | 15.72875000 | 9.29837500 |
| Pd | 12.87252500 | 9.40852500 | 9.09157500 |
| Pd | 14.86850000 | 11.29295000 | 8.64900000 |
| Pd | 10.87890000 | 13.41270000 | 8.29147500 |
| Pd | 12.49020000 | 11.43367500 | 7.26935000 |
| Pd | 13.65742500 | 13.75685000 | 8.16117500 |
| O | 9.39862500 | 11.46927500 | 18.78417500 |
| O | 9.37245000 | 13.95610000 | 18.18825000 |
| C | 10.60097500 | 11.06002500 | 18.83717500 |
| C | 11.05395000 | 9.78225000 | 18.31165000 |
| C | 10.15657500 | 8.82795000 | 17.71037500 |
| H | 8.46092500 | 14.28697500 | 18.09917500 |
| H | 11.35087500 | 11.64077500 | 19.41880000 |
| H | 9.30462500 | 12.97937500 | 18.52802500 |
| H | 12.03650000 | 9.43725000 | 18.64997500 |
| H | 9.08680000 | 9.05217500 | 17.82372500 |
| H | 10.43182500 | 7.76900000 | 17.82385000 |

TS1_Pd_S

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|----|-------------|-------------|-------------|
| Pd | 11.89762500 | 11.18910000 | 17.27220000 |
|----|-------------|-------------|-------------|

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|----|-------------|-------------|-------------|
| Pd | 13.08720000 | 13.63532500 | 17.57472500 |
| Pd | 14.76547500 | 11.73450000 | 16.40942500 |
| Pd | 10.48510000 | 13.62377500 | 16.41307500 |
| Pd | 10.72355000 | 8.99025000 | 15.84627500 |
| Pd | 14.95207500 | 14.42667500 | 15.78850000 |
| Pd | 12.35500000 | 15.55122500 | 15.77197500 |
| Pd | 13.52422500 | 9.18092500 | 15.39312500 |
| Pd | 9.20330000 | 11.17915000 | 15.25590000 |
| Pd | 16.20622500 | 9.81352500 | 15.03140000 |
| Pd | 8.04687500 | 13.68350000 | 14.81842500 |
| Pd | 12.73845000 | 12.93262500 | 15.06647500 |
| Pd | 16.61565000 | 12.48920000 | 14.53470000 |
| Pd | 9.90215000 | 15.66675000 | 14.42160000 |
| Pd | 11.66190000 | 10.73387500 | 14.16145000 |
| Pd | 16.82925000 | 15.14395000 | 13.91312500 |
| Pd | 14.40220000 | 16.45057500 | 13.83912500 |
| Pd | 11.87262500 | 17.48402500 | 13.84567500 |
| Pd | 14.37892500 | 11.15500000 | 13.71612500 |
| Pd | 10.33142500 | 13.10505000 | 13.65415000 |
| Pd | 11.96285000 | 8.14102500 | 13.40025000 |
| Pd | 9.43725000 | 9.32992500 | 13.36870000 |
| Pd | 14.66802500 | 13.81102500 | 13.25362500 |
| Pd | 14.73040000 | 8.55880000 | 13.04090000 |
| Pd | 12.24967500 | 14.97355000 | 13.22680000 |
| Pd | 8.02640000 | 11.76300000 | 12.79990000 |
| Pd | 16.67082500 | 10.56357500 | 12.45442500 |
| Pd | 12.55940000 | 12.51320000 | 12.48572500 |

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|----|-------------|-------------|-------------|
| Pd | 8.42237500 | 14.47632500 | 12.30110000 |
| Pd | 16.95402500 | 13.28185000 | 11.84677500 |
| Pd | 12.84762500 | 10.02980000 | 11.74680000 |
| Pd | 10.38025000 | 16.42962500 | 11.77482500 |
| Pd | 10.41727500 | 11.20490000 | 11.75087500 |
| Pd | 15.66225000 | 15.69005000 | 11.47870000 |
| Pd | 13.10222500 | 16.88105000 | 11.43302500 |
| Pd | 14.72752500 | 11.93477500 | 11.16277500 |
| Pd | 10.82747500 | 13.92172500 | 11.13680000 |
| Pd | 13.24110000 | 7.52950000 | 10.98600000 |
| Pd | 10.72837500 | 8.63180000 | 10.87435000 |
| Pd | 8.31290000 | 9.87050000 | 10.85910000 |
| Pd | 13.49537500 | 14.30735000 | 10.84652500 |
| Pd | 15.17957500 | 9.40665000 | 10.40175000 |
| Pd | 8.65452500 | 12.55805000 | 10.25155000 |
| Pd | 12.28245000 | 12.00797500 | 9.93945000 |
| Pd | 17.00670000 | 11.39477500 | 9.85932500 |
| Pd | 9.02145000 | 15.23897500 | 9.71085000 |
| Pd | 15.75250000 | 13.78767500 | 9.41152500 |
| Pd | 14.36712500 | 16.11965000 | 9.11090000 |
| Pd | 10.20850000 | 10.61555000 | 9.03592500 |
| Pd | 11.67050000 | 15.71540000 | 9.33010000 |
| Pd | 12.73985000 | 9.44452500 | 9.10957500 |
| Pd | 14.62000000 | 11.40020000 | 8.54692500 |
| Pd | 10.56662500 | 13.34760000 | 8.41580000 |
| Pd | 12.18357500 | 11.42615000 | 7.31402500 |
| Pd | 13.29045000 | 13.77830000 | 8.16880000 |

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|---|-------------|-------------|-------------|
| O | 8.65235000 | 12.71277500 | 16.44242500 |
| O | 13.70455000 | 10.19400000 | 17.08052500 |
| C | 10.26127500 | 11.23347500 | 18.77422500 |
| C | 10.64902500 | 9.85962500 | 18.52230000 |
| C | 9.85087500 | 8.95582500 | 17.73112500 |
| H | 10.61347500 | 11.68822500 | 19.70400000 |
| H | 9.23335000 | 11.50550000 | 18.50362500 |
| H | 10.72005000 | 12.29905000 | 17.82585000 |
| H | 11.43917500 | 9.42657500 | 19.14365000 |
| H | 8.80847500 | 9.25595000 | 17.55512500 |
| H | 9.98077500 | 7.88435000 | 17.94320000 |

3_Pd_S

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|----|-------------|-------------|-------------|
| Pd | 11.73762500 | 11.38902500 | 17.00002500 |
| Pd | 12.95320000 | 13.89440000 | 17.55367500 |
| Pd | 14.63867500 | 11.92852500 | 16.52662500 |
| Pd | 10.39325000 | 13.81897500 | 16.40180000 |
| Pd | 10.66497500 | 9.10245000 | 15.87310000 |
| Pd | 14.90345000 | 14.57895000 | 15.77037500 |
| Pd | 12.31947500 | 15.76202500 | 15.66960000 |
| Pd | 13.43195000 | 9.36300000 | 15.59102500 |
| Pd | 9.25482500 | 11.42407500 | 15.43267500 |
| Pd | 16.10682500 | 9.96027500 | 15.23015000 |
| Pd | 8.04465000 | 13.90407500 | 14.73760000 |
| Pd | 12.67695000 | 13.11505000 | 15.04027500 |
| Pd | 16.54525000 | 12.60232500 | 14.64000000 |
| Pd | 9.89332500 | 15.84330000 | 14.26860000 |

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|----|-------------|-------------|-------------|
| Pd | 11.60052500 | 10.85545000 | 14.17895000 |
| Pd | 16.82247500 | 15.23087500 | 13.88365000 |
| Pd | 14.41737500 | 16.56467500 | 13.76512500 |
| Pd | 11.88785000 | 17.61647500 | 13.66682500 |
| Pd | 14.32727500 | 11.27997500 | 13.81727500 |
| Pd | 10.30442500 | 13.24110000 | 13.60542500 |
| Pd | 11.89565000 | 8.23350000 | 13.56715000 |
| Pd | 9.35995000 | 9.48577500 | 13.45945000 |
| Pd | 14.64932500 | 13.92070000 | 13.23265000 |
| Pd | 14.65477500 | 8.65110000 | 13.25277500 |
| Pd | 12.24265000 | 15.08372500 | 13.14892500 |
| Pd | 8.03560000 | 11.88335000 | 12.85747500 |
| Pd | 16.62307500 | 10.60115000 | 12.63667500 |
| Pd | 12.54507500 | 12.59857500 | 12.47722500 |
| Pd | 8.42220000 | 14.58945000 | 12.20060000 |
| Pd | 16.95862500 | 13.29135000 | 11.91972500 |
| Pd | 12.82882500 | 10.07917500 | 11.83907500 |
| Pd | 10.42730000 | 16.52557500 | 11.60027500 |
| Pd | 10.41420000 | 11.26345000 | 11.76140000 |
| Pd | 15.71292500 | 15.72265000 | 11.42950000 |
| Pd | 13.16412500 | 16.91155000 | 11.31357500 |
| Pd | 14.72135000 | 11.93490000 | 11.23555000 |
| Pd | 10.83880000 | 13.99347500 | 11.08107500 |
| Pd | 13.17925000 | 7.54210000 | 11.21200000 |
| Pd | 10.66987500 | 8.64912500 | 11.04207500 |
| Pd | 8.28342500 | 9.95725000 | 10.92707500 |
| Pd | 13.53265000 | 14.32357500 | 10.79942500 |

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|----|-------------|-------------|-------------|
| Pd | 15.16932500 | 9.35670000 | 10.58897500 |
| Pd | 8.66810000 | 12.60577500 | 10.23605000 |
| Pd | 12.28745000 | 12.03400000 | 9.95630000 |
| Pd | 17.00850000 | 11.32795000 | 10.01840000 |
| Pd | 9.09377500 | 15.25825000 | 9.56837500 |
| Pd | 15.80607500 | 13.72092500 | 9.44210000 |
| Pd | 14.44982500 | 16.04957500 | 9.02305000 |
| Pd | 10.19990000 | 10.58662500 | 9.09617500 |
| Pd | 11.74807500 | 15.70180000 | 9.20900000 |
| Pd | 12.71965000 | 9.39575000 | 9.27665000 |
| Pd | 14.64632500 | 11.30862500 | 8.65202500 |
| Pd | 10.60280000 | 13.30120000 | 8.36905000 |
| Pd | 12.21562500 | 11.32445000 | 7.38957500 |
| Pd | 13.35762500 | 13.70002500 | 8.12462500 |
| O | 8.50487500 | 13.01887500 | 16.43822500 |
| O | 13.60807500 | 10.40415000 | 17.26887500 |
| C | 10.73227500 | 10.35367500 | 18.55145000 |
| C | 10.63185000 | 8.98500000 | 18.08680000 |
| C | 9.47972500 | 8.40807500 | 17.49502500 |
| H | 11.44917500 | 10.53067500 | 19.36105000 |
| H | 9.78790000 | 10.90230000 | 18.65120000 |
| H | 11.35492500 | 13.10332500 | 17.70517500 |
| H | 11.47487500 | 8.32912500 | 18.32957500 |
| H | 8.53380000 | 8.95812500 | 17.49637500 |
| H | 9.39790000 | 7.32067500 | 17.42472500 |

TS2_Pd_S

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|----|-------------|-------------|-------------|
| Pd | 11.76607500 | 11.37027500 | 16.97290000 |
| Pd | 12.94090000 | 13.84770000 | 17.53570000 |
| Pd | 14.66960000 | 11.90802500 | 16.52767500 |
| Pd | 10.47647500 | 13.78670000 | 16.43795000 |
| Pd | 10.67367500 | 9.09827500 | 15.88520000 |
| Pd | 14.89227500 | 14.55747500 | 15.76427500 |
| Pd | 12.34205000 | 15.75132500 | 15.68417500 |
| Pd | 13.46005000 | 9.33940000 | 15.61167500 |
| Pd | 9.26885000 | 11.40215000 | 15.43430000 |
| Pd | 16.12870000 | 9.94760000 | 15.23505000 |
| Pd | 8.04882500 | 13.89650000 | 14.70640000 |
| Pd | 12.71302500 | 13.09002500 | 15.04030000 |
| Pd | 16.55045000 | 12.59715000 | 14.65565000 |
| Pd | 9.89450000 | 15.82537500 | 14.24397500 |
| Pd | 11.62815000 | 10.82617500 | 14.17635000 |
| Pd | 16.83407500 | 15.22005000 | 13.90052500 |
| Pd | 14.43132500 | 16.54662500 | 13.77982500 |
| Pd | 11.90297500 | 17.59377500 | 13.68117500 |
| Pd | 14.33632500 | 11.25162500 | 13.81815000 |
| Pd | 10.32137500 | 13.23175000 | 13.63545000 |
| Pd | 11.91655000 | 8.20970000 | 13.58325000 |
| Pd | 9.38277500 | 9.47347500 | 13.46567500 |
| Pd | 14.68877500 | 13.88595000 | 13.18285000 |
| Pd | 14.66040000 | 8.64362500 | 13.26552500 |
| Pd | 12.27532500 | 15.06532500 | 13.16832500 |
| Pd | 8.03810000 | 11.87040000 | 12.85145000 |

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|----|-------------|-------------|-------------|
| Pd | 16.63107500 | 10.60910000 | 12.63912500 |
| Pd | 12.55510000 | 12.58340000 | 12.48485000 |
| Pd | 8.43390000 | 14.55980000 | 12.17845000 |
| Pd | 16.99137500 | 13.28507500 | 11.93917500 |
| Pd | 12.82450000 | 10.06492500 | 11.82110000 |
| Pd | 10.45067500 | 16.50872500 | 11.59967500 |
| Pd | 10.40350000 | 11.27685000 | 11.78102500 |
| Pd | 15.72130000 | 15.71862500 | 11.44365000 |
| Pd | 13.17535000 | 16.88942500 | 11.31912500 |
| Pd | 14.72455000 | 11.91270000 | 11.22387500 |
| Pd | 10.84892500 | 13.97570000 | 11.09225000 |
| Pd | 13.20455000 | 7.52727500 | 11.20732500 |
| Pd | 10.69825000 | 8.64180000 | 11.05905000 |
| Pd | 8.30012500 | 9.93907500 | 10.93177500 |
| Pd | 13.51720000 | 14.30610000 | 10.79050000 |
| Pd | 15.18725000 | 9.34815000 | 10.59852500 |
| Pd | 8.67527500 | 12.58117500 | 10.21652500 |
| Pd | 12.29002500 | 12.00680000 | 9.95875000 |
| Pd | 17.02205000 | 11.31617500 | 10.01615000 |
| Pd | 9.10840000 | 15.23537500 | 9.56740000 |
| Pd | 15.81900000 | 13.71730000 | 9.47622500 |
| Pd | 14.46537500 | 16.04080000 | 9.02875000 |
| Pd | 10.22080000 | 10.56947500 | 9.10215000 |
| Pd | 11.76140000 | 15.69925000 | 9.20680000 |
| Pd | 12.74872500 | 9.37775000 | 9.26300000 |
| Pd | 14.65995000 | 11.30280000 | 8.65132500 |
| Pd | 10.62312500 | 13.29380000 | 8.37097500 |

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|----|-------------|-------------|-------------|
| Pd | 12.22685000 | 11.31205000 | 7.38582500 |
| Pd | 13.37232500 | 13.69085000 | 8.13315000 |
| O | 8.50745000 | 13.06130000 | 16.50367500 |
| O | 13.59502500 | 10.42050000 | 17.28630000 |
| C | 10.79422500 | 10.35277500 | 18.54677500 |
| C | 10.65887500 | 8.98070000 | 18.09160000 |
| C | 9.48812500 | 8.42317500 | 17.51825000 |
| H | 11.53082500 | 10.51622500 | 19.34152500 |
| H | 9.86060000 | 10.91515000 | 18.66810000 |
| H | 9.38237500 | 13.71945000 | 17.57980000 |
| H | 11.48995000 | 8.30817500 | 18.32955000 |
| H | 8.55340000 | 8.99202500 | 17.52645000 |
| H | 9.38322500 | 7.33750000 | 17.45380000 |

TS2_Pd_O

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|----|-------------|-------------|-------------|
| Pd | 11.44345000 | 11.65830000 | 16.81572500 |
| Pd | 12.71847500 | 13.98095000 | 17.53020000 |
| Pd | 14.34130000 | 11.90385000 | 16.69225000 |
| Pd | 10.30620000 | 14.01742500 | 16.27210000 |
| Pd | 10.45992500 | 9.17552500 | 15.91055000 |
| Pd | 14.74745000 | 14.54195000 | 15.83542500 |
| Pd | 12.21922500 | 15.85680000 | 15.60065000 |
| Pd | 13.21957500 | 9.32880000 | 15.59900000 |
| Pd | 9.05632500 | 11.47872500 | 15.31187500 |
| Pd | 15.85272500 | 9.91080000 | 15.44697500 |

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|----|-------------|-------------|-------------|
| Pd | 7.92027500 | 14.07487500 | 14.48492500 |
| Pd | 12.60182500 | 13.26327500 | 14.97777500 |
| Pd | 16.37315000 | 12.55152500 | 14.83080000 |
| Pd | 9.86860000 | 15.96057500 | 14.08067500 |
| Pd | 11.45865000 | 10.93197500 | 14.18610000 |
| Pd | 16.76882500 | 15.16807500 | 14.06200000 |
| Pd | 14.38640000 | 16.51367500 | 13.83645000 |
| Pd | 11.94020000 | 17.68832500 | 13.55350000 |
| Pd | 14.16735000 | 11.31380000 | 13.98320000 |
| Pd | 10.24777500 | 13.32260000 | 13.55492500 |
| Pd | 11.70055000 | 8.27712500 | 13.56472500 |
| Pd | 9.23827500 | 9.57185000 | 13.41685000 |
| Pd | 14.66530000 | 13.88677500 | 13.16370000 |
| Pd | 14.53432500 | 8.62052500 | 13.38202500 |
| Pd | 12.23407500 | 15.10752500 | 13.04792500 |
| Pd | 8.00315000 | 12.01227500 | 12.68885000 |
| Pd | 16.46495000 | 10.57495000 | 12.84587500 |
| Pd | 12.51107500 | 12.59995000 | 12.47090000 |
| Pd | 8.46040000 | 14.70155000 | 12.01215000 |
| Pd | 17.01702500 | 13.21330000 | 12.14285000 |
| Pd | 12.83632500 | 10.07002500 | 11.95332500 |
| Pd | 10.54462500 | 16.51937500 | 11.47165000 |
| Pd | 10.39565000 | 11.26237500 | 11.73825000 |
| Pd | 15.76045000 | 15.65845000 | 11.54722500 |
| Pd | 13.28940000 | 16.90267500 | 11.28710000 |
| Pd | 14.71585000 | 11.88830000 | 11.30682500 |
| Pd | 10.82675000 | 13.89535000 | 10.96830000 |

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|----|-------------|-------------|-------------|
| Pd | 13.11210000 | 7.52755000 | 11.30765000 |
| Pd | 10.63510000 | 8.70510000 | 11.00390000 |
| Pd | 8.26480000 | 10.00170000 | 10.82827500 |
| Pd | 13.48852500 | 14.28470000 | 10.74505000 |
| Pd | 15.15907500 | 9.31042500 | 10.70725000 |
| Pd | 8.67362500 | 12.65512500 | 10.09715000 |
| Pd | 12.35785000 | 11.92160000 | 9.96317500 |
| Pd | 17.05002500 | 11.24550000 | 10.21535000 |
| Pd | 9.17507500 | 15.28540000 | 9.42250000 |
| Pd | 15.88812500 | 13.66317500 | 9.63787500 |
| Pd | 14.59492500 | 16.01910000 | 9.03915000 |
| Pd | 10.24505000 | 10.64707500 | 9.03562500 |
| Pd | 11.88020000 | 15.71110000 | 9.16147500 |
| Pd | 12.75957500 | 9.37935000 | 9.31460000 |
| Pd | 14.74387500 | 11.25107500 | 8.72497500 |
| Pd | 10.75530000 | 13.32562500 | 8.31650000 |
| Pd | 12.35050000 | 11.29345000 | 7.37470000 |
| Pd | 13.52300000 | 13.65662500 | 8.16045000 |
| O | 8.26682500 | 13.23267500 | 16.41197500 |
| O | 12.98775000 | 10.42057500 | 17.32097500 |
| C | 12.29885000 | 9.11735000 | 18.72085000 |
| C | 11.41550000 | 8.24585000 | 18.05700000 |
| C | 10.03347500 | 8.50872500 | 17.85212500 |
| H | 13.29807500 | 8.77152500 | 18.98302500 |
| H | 11.89765000 | 9.93777500 | 19.31867500 |
| H | 7.69617500 | 13.24592500 | 17.20237500 |
| H | 11.81815000 | 7.29462500 | 17.69685000 |

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|---|------------|------------|-------------|
| H | 9.57302500 | 9.33897500 | 18.40105000 |
| H | 9.36127500 | 7.66687500 | 17.64440000 |

4_Pd₀

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.95295000 | 11.57292500 | 16.95865000 |
| Pd | 13.05505000 | 14.08960000 | 17.51242500 |
| Pd | 14.67557500 | 12.09890000 | 16.47630000 |
| Pd | 10.57120000 | 13.95432500 | 16.41307500 |
| Pd | 10.61342500 | 9.15455000 | 15.89955000 |
| Pd | 14.96165000 | 14.74900000 | 15.71080000 |
| Pd | 12.37927500 | 15.91037500 | 15.60032500 |
| Pd | 13.49132500 | 9.52805000 | 15.86362500 |
| Pd | 9.26935000 | 11.49360000 | 15.47200000 |
| Pd | 16.15660000 | 10.04850000 | 15.31445000 |
| Pd | 8.06442500 | 14.03807500 | 14.69200000 |
| Pd | 12.73007500 | 13.27475000 | 15.02685000 |
| Pd | 16.61072500 | 12.66165000 | 14.58442500 |
| Pd | 9.96095000 | 15.92987500 | 14.19732500 |
| Pd | 11.61427500 | 10.91367500 | 14.28567500 |
| Pd | 16.88070000 | 15.28137500 | 13.85145000 |
| Pd | 14.45562500 | 16.59965000 | 13.68907500 |
| Pd | 11.97107500 | 17.69932500 | 13.54810000 |
| Pd | 14.28022500 | 11.30872500 | 13.97967500 |
| Pd | 10.36232500 | 13.30567500 | 13.68187500 |
| Pd | 11.87550000 | 8.30260000 | 13.66040000 |
| Pd | 9.33602500 | 9.55927500 | 13.53190000 |

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|----|-------------|-------------|-------------|
| Pd | 14.71902500 | 13.91787500 | 13.21775000 |
| Pd | 14.62975000 | 8.68780000 | 13.47185000 |
| Pd | 12.29545000 | 15.13067500 | 13.07397500 |
| Pd | 8.07595000 | 11.97572500 | 12.90210000 |
| Pd | 16.60777500 | 10.60990000 | 12.69962500 |
| Pd | 12.58522500 | 12.61947500 | 12.51312500 |
| Pd | 8.49637500 | 14.63315000 | 12.19062500 |
| Pd | 17.07402500 | 13.30662500 | 11.91422500 |
| Pd | 12.93472500 | 10.09800000 | 11.96145000 |
| Pd | 10.50955000 | 16.47905000 | 11.53790000 |
| Pd | 10.45080000 | 11.27592500 | 11.86587500 |
| Pd | 15.70320000 | 15.65342500 | 11.37617500 |
| Pd | 13.22665000 | 16.93692500 | 11.21792500 |
| Pd | 14.81605000 | 11.99540000 | 11.34637500 |
| Pd | 10.84097500 | 13.86135000 | 11.03625000 |
| Pd | 13.22190000 | 7.53862500 | 11.38342500 |
| Pd | 10.72317500 | 8.70747500 | 11.16777500 |
| Pd | 8.29337500 | 9.98687500 | 11.00885000 |
| Pd | 13.46545000 | 14.30812500 | 10.74025000 |
| Pd | 15.14812500 | 9.34527500 | 10.68640000 |
| Pd | 8.62892500 | 12.58687500 | 10.26030000 |
| Pd | 12.41015000 | 11.86737500 | 10.02027500 |
| Pd | 17.03032500 | 11.26320000 | 10.07950000 |
| Pd | 9.07285000 | 15.19522500 | 9.57212500 |
| Pd | 15.79337500 | 13.64947500 | 9.45865000 |
| Pd | 14.44635000 | 16.00470000 | 8.94920000 |
| Pd | 10.21415000 | 10.61170000 | 9.18830000 |

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|----|-------------|-------------|-------------|
| Pd | 11.74517500 | 15.68322500 | 9.18000000 |
| Pd | 12.71350000 | 9.31097500 | 9.33412500 |
| Pd | 14.64135000 | 11.23182500 | 8.70035000 |
| Pd | 10.64570000 | 13.26320000 | 8.43265000 |
| Pd | 12.21572500 | 11.22342500 | 7.43412500 |
| Pd | 13.36710000 | 13.62542500 | 8.13775000 |
| O | 8.51032500 | 13.25390000 | 16.61817500 |
| O | 12.80557500 | 9.83232500 | 17.88495000 |
| C | 11.93257500 | 8.89415000 | 18.52852500 |
| C | 11.20312500 | 7.97390000 | 17.58007500 |
| C | 9.80575000 | 7.92020000 | 17.46785000 |
| H | 12.56220000 | 8.28835000 | 19.21090000 |
| H | 11.20800000 | 9.45087500 | 19.14972500 |
| H | 7.94277500 | 13.26220000 | 17.41112500 |
| H | 11.80300000 | 7.15675000 | 17.16210000 |
| H | 9.17672500 | 8.54307500 | 18.11165000 |
| H | 9.31392500 | 7.06557500 | 16.99797500 |

TS3_Pd_S

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|----|-------------|-------------|-------------|
| Pd | 11.29317500 | 11.42545000 | 16.85605000 |
| Pd | 12.89262500 | 13.90492500 | 17.46870000 |
| Pd | 14.30527500 | 11.75310000 | 16.55555000 |
| Pd | 10.30672500 | 14.05490000 | 16.18255000 |
| Pd | 10.47457500 | 9.05837500 | 15.78357500 |
| Pd | 14.87300000 | 14.42520000 | 15.80722500 |
| Pd | 12.47552500 | 15.82962500 | 15.58417500 |

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|----|-------------|-------------|-------------|
| Pd | 13.13912500 | 9.42497500 | 15.66107500 |
| Pd | 9.03340000 | 11.53922500 | 15.22172500 |
| Pd | 15.83577500 | 9.78620000 | 15.38512500 |
| Pd | 8.02822500 | 14.03840000 | 14.61562500 |
| Pd | 12.65025000 | 13.08270000 | 14.98100000 |
| Pd | 16.41047500 | 12.39110000 | 14.76057500 |
| Pd | 10.00392500 | 15.88595000 | 14.17027500 |
| Pd | 11.48905000 | 10.83390000 | 14.09400000 |
| Pd | 16.89627500 | 14.98847500 | 13.98557500 |
| Pd | 14.53527500 | 16.38797500 | 13.80787500 |
| Pd | 12.06592500 | 17.61392500 | 13.55710000 |
| Pd | 14.20885000 | 11.16107500 | 13.84222500 |
| Pd | 10.30815000 | 13.24897500 | 13.57550000 |
| Pd | 11.73325000 | 8.22060000 | 13.51410000 |
| Pd | 9.26492500 | 9.53390000 | 13.28282500 |
| Pd | 14.67815000 | 13.77817500 | 13.16777500 |
| Pd | 14.48337500 | 8.55442500 | 13.32985000 |
| Pd | 12.27695000 | 15.04200000 | 13.08192500 |
| Pd | 8.02970000 | 12.04975000 | 12.66737500 |
| Pd | 16.53235000 | 10.37317500 | 12.82052500 |
| Pd | 12.52347500 | 12.55055000 | 12.42642500 |
| Pd | 8.57400000 | 14.72502500 | 12.02715000 |
| Pd | 17.05130000 | 13.01342500 | 12.10772500 |
| Pd | 12.75440000 | 10.03215000 | 11.79510000 |
| Pd | 10.65677500 | 16.55827500 | 11.44270000 |
| Pd | 10.38220000 | 11.32745000 | 11.63015000 |
| Pd | 15.88882500 | 15.49512500 | 11.50500000 |

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|----|-------------|-------------|-------------|
| Pd | 13.42190000 | 16.84990000 | 11.29425000 |
| Pd | 14.74625000 | 11.82120000 | 11.27552500 |
| Pd | 10.85105000 | 13.94847500 | 11.00840000 |
| Pd | 13.04970000 | 7.46357500 | 11.20567500 |
| Pd | 10.59772500 | 8.66100000 | 10.96945000 |
| Pd | 8.22825000 | 10.07590000 | 10.76005000 |
| Pd | 13.55232500 | 14.27277500 | 10.76307500 |
| Pd | 15.11122500 | 9.21520000 | 10.71432500 |
| Pd | 8.67290000 | 12.71392500 | 10.02297500 |
| Pd | 12.40977500 | 11.98572500 | 9.89565000 |
| Pd | 17.07357500 | 11.05407500 | 10.19640000 |
| Pd | 9.26357500 | 15.32607500 | 9.42132500 |
| Pd | 15.92565000 | 13.48992500 | 9.59107500 |
| Pd | 14.69707500 | 15.92275000 | 9.04875000 |
| Pd | 10.25645000 | 10.64007500 | 9.01747500 |
| Pd | 11.97860000 | 15.66045000 | 9.14475000 |
| Pd | 12.71780000 | 9.31640000 | 9.24802500 |
| Pd | 14.74987500 | 11.12802500 | 8.71327500 |
| Pd | 10.77777500 | 13.29792500 | 8.30097500 |
| Pd | 12.35837500 | 11.28375000 | 7.33152500 |
| Pd | 13.58142500 | 13.59740000 | 8.10917500 |
| O | 7.96442500 | 10.24990000 | 18.26822500 |
| O | 11.07735000 | 13.26277500 | 17.86085000 |
| C | 9.17712500 | 10.88180000 | 18.33765000 |
| C | 10.34592500 | 10.04010000 | 18.34420000 |
| C | 10.31045000 | 8.69400000 | 17.82637500 |
| H | 9.22352500 | 11.57785000 | 16.88480000 |

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|---|-------------|-------------|-------------|
| H | 9.21952500 | 11.83865000 | 18.87230000 |
| H | 7.25860000 | 10.91250000 | 18.14460000 |
| H | 11.16322500 | 10.34637500 | 19.00802500 |
| H | 9.32332500 | 8.20912500 | 17.78220000 |
| H | 11.12715000 | 8.03790000 | 18.14317500 |

5_Pd_S

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.52542500 | 11.40795000 | 16.87960000 |
| Pd | 12.75437500 | 13.95805000 | 17.43350000 |
| Pd | 14.37252500 | 11.89550000 | 16.58992500 |
| Pd | 10.16897500 | 13.93890000 | 16.20020000 |
| Pd | 10.43630000 | 9.12687500 | 15.84225000 |
| Pd | 14.78167500 | 14.54845000 | 15.81542500 |
| Pd | 12.32845000 | 15.84852500 | 15.52417500 |
| Pd | 13.21780000 | 9.49610000 | 15.74695000 |
| Pd | 9.07825000 | 11.48822500 | 15.22465000 |
| Pd | 15.92190000 | 9.90870000 | 15.47627500 |
| Pd | 7.92295000 | 13.96710000 | 14.52575000 |
| Pd | 12.64812500 | 13.17502500 | 14.94867500 |
| Pd | 16.41082500 | 12.52232500 | 14.81952500 |
| Pd | 9.93990000 | 15.80195000 | 14.11035000 |
| Pd | 11.50612500 | 10.83815000 | 14.16075000 |
| Pd | 16.83042500 | 15.09665000 | 13.98627500 |
| Pd | 14.42555000 | 16.41157500 | 13.77787500 |
| Pd | 11.93795000 | 17.59170000 | 13.45637500 |

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|----|-------------|-------------|-------------|
| Pd | 14.22325000 | 11.21530000 | 13.93380000 |
| Pd | 10.30072500 | 13.20437500 | 13.56455000 |
| Pd | 11.81485000 | 8.19382500 | 13.65022500 |
| Pd | 9.32690000 | 9.43115000 | 13.33972500 |
| Pd | 14.69095000 | 13.80672500 | 13.13920000 |
| Pd | 14.60357500 | 8.59382500 | 13.45445000 |
| Pd | 12.23855000 | 15.01865000 | 12.98010000 |
| Pd | 8.07272500 | 11.92280000 | 12.64022500 |
| Pd | 16.59645000 | 10.48565000 | 12.91055000 |
| Pd | 12.54990000 | 12.51470000 | 12.43110000 |
| Pd | 8.55180000 | 14.59582500 | 11.94217500 |
| Pd | 17.07190000 | 13.11395000 | 12.14212500 |
| Pd | 12.81927500 | 9.97212500 | 11.93050000 |
| Pd | 10.58792500 | 16.45422500 | 11.35832500 |
| Pd | 10.42805000 | 11.20495000 | 11.68550000 |
| Pd | 15.83222500 | 15.55527500 | 11.49380000 |
| Pd | 13.35200000 | 16.81672500 | 11.23772500 |
| Pd | 14.78057500 | 11.77220000 | 11.32640000 |
| Pd | 10.84067500 | 13.81740000 | 10.96417500 |
| Pd | 13.19327500 | 7.42210000 | 11.37947500 |
| Pd | 10.73027500 | 8.56855000 | 11.04077500 |
| Pd | 8.32990000 | 9.90757500 | 10.76357500 |
| Pd | 13.54675000 | 14.19337500 | 10.71407500 |
| Pd | 15.22102500 | 9.21172500 | 10.80712500 |
| Pd | 8.73092500 | 12.53415000 | 9.98292500 |
| Pd | 12.43795000 | 11.84557500 | 9.93017500 |
| Pd | 17.14785000 | 11.08680000 | 10.29280000 |

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|----|-------------|-------------|-------------|
| Pd | 9.26232500 | 15.15537500 | 9.32572500 |
| Pd | 15.94830000 | 13.48820000 | 9.63497500 |
| Pd | 14.66487500 | 15.86897500 | 9.01500000 |
| Pd | 10.35650000 | 10.49392500 | 9.02702500 |
| Pd | 11.96075000 | 15.55135000 | 9.09700000 |
| Pd | 12.85345000 | 9.22865000 | 9.34995000 |
| Pd | 14.84837500 | 11.08852500 | 8.77487500 |
| Pd | 10.85080000 | 13.15377500 | 8.26920000 |
| Pd | 12.46025000 | 11.11935000 | 7.37095000 |
| Pd | 13.62647500 | 13.49272500 | 8.11057500 |
| O | 9.60490000 | 10.98717500 | 18.90137500 |
| O | 10.99122500 | 13.19317500 | 17.90747500 |
| C | 10.77222500 | 10.35892500 | 18.53847500 |
| C | 10.63807500 | 8.99667500 | 18.03602500 |
| C | 9.43022500 | 8.42485000 | 17.57197500 |
| H | 8.56847500 | 13.07582500 | 15.94385000 |
| H | 11.63722500 | 10.54807500 | 19.19630000 |
| H | 9.81047500 | 11.95160000 | 18.96122500 |
| H | 11.51217500 | 8.36010000 | 18.19960000 |
| H | 8.49512500 | 8.97945000 | 17.68072500 |
| H | 9.34650000 | 7.33812500 | 17.50037500 |

TS5_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.71017500 | 11.22555000 | 16.71320000 |
| Pd | 12.61152500 | 13.74955000 | 17.48952500 |
| Pd | 14.41875000 | 11.80952500 | 16.56532500 |

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|----|-------------|-------------|-------------|
| Pd | 10.12697500 | 13.86182500 | 16.21135000 |
| Pd | 10.39735000 | 9.05277500 | 15.81507500 |
| Pd | 14.73680000 | 14.45982500 | 15.89267500 |
| Pd | 12.28600000 | 15.71432500 | 15.54225000 |
| Pd | 13.26942500 | 9.28760000 | 15.58325000 |
| Pd | 9.07727500 | 11.41145000 | 15.21010000 |
| Pd | 15.97292500 | 9.83537500 | 15.39532500 |
| Pd | 7.90897500 | 13.88070000 | 14.54117500 |
| Pd | 12.55592500 | 13.09272500 | 14.96472500 |
| Pd | 16.45755000 | 12.45410000 | 14.76595000 |
| Pd | 9.88982500 | 15.75432500 | 14.09925000 |
| Pd | 11.47335000 | 10.73952500 | 14.05905000 |
| Pd | 16.78717500 | 15.07375000 | 14.06900000 |
| Pd | 14.37205000 | 16.39262500 | 13.81470000 |
| Pd | 11.88610000 | 17.56585000 | 13.49085000 |
| Pd | 14.19302500 | 11.18350000 | 13.98682500 |
| Pd | 10.28485000 | 13.13855000 | 13.56657500 |
| Pd | 11.78397500 | 8.12045000 | 13.55220000 |
| Pd | 9.30217500 | 9.38820000 | 13.27932500 |
| Pd | 14.61472500 | 13.79180000 | 13.33250000 |
| Pd | 14.64097500 | 8.52982500 | 13.33310000 |
| Pd | 12.17147500 | 14.99582500 | 12.96567500 |
| Pd | 8.11677500 | 11.84525000 | 12.62132500 |
| Pd | 16.58482500 | 10.44600000 | 12.82517500 |
| Pd | 12.55240000 | 12.48390000 | 12.43680000 |
| Pd | 8.54327500 | 14.51947500 | 11.94960000 |
| Pd | 17.03680000 | 13.15225000 | 12.12292500 |

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|----|-------------|-------------|-------------|
| Pd | 12.91620000 | 9.95147500 | 11.92500000 |
| Pd | 10.52837500 | 16.42300000 | 11.40810000 |
| Pd | 10.48650000 | 11.16462500 | 11.55652500 |
| Pd | 15.76877500 | 15.54527500 | 11.54037500 |
| Pd | 13.28610000 | 16.84695000 | 11.27632500 |
| Pd | 14.84620000 | 11.84492500 | 11.40665000 |
| Pd | 10.85862500 | 13.74145000 | 10.92792500 |
| Pd | 13.20462500 | 7.41867500 | 11.27650000 |
| Pd | 10.73235000 | 8.56517500 | 10.99542500 |
| Pd | 8.34947500 | 9.87290000 | 10.69187500 |
| Pd | 13.58760000 | 14.21935000 | 10.81275000 |
| Pd | 15.20117500 | 9.26220000 | 10.67725000 |
| Pd | 8.67277500 | 12.51120000 | 9.98127500 |
| Pd | 12.58720000 | 11.83552500 | 9.92565000 |
| Pd | 17.14270000 | 11.17760000 | 10.23605000 |
| Pd | 9.22672500 | 15.13997500 | 9.36665000 |
| Pd | 15.90627500 | 13.53887500 | 9.58130000 |
| Pd | 14.62415000 | 15.92842500 | 9.07822500 |
| Pd | 10.34012500 | 10.53005000 | 8.97400000 |
| Pd | 11.92560000 | 15.56182500 | 9.16637500 |
| Pd | 12.80260000 | 9.26530000 | 9.27097500 |
| Pd | 14.83277500 | 11.14570000 | 8.70750000 |
| Pd | 10.80962500 | 13.16852500 | 8.30730000 |
| Pd | 12.45787500 | 11.18440000 | 7.33687500 |
| Pd | 13.55015000 | 13.56807500 | 8.12685000 |
| O | 9.83005000 | 11.52410000 | 18.72207500 |
| O | 10.74105000 | 13.75747500 | 18.11360000 |

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|---|-------------|-------------|-------------|
| C | 10.84137500 | 10.66985000 | 18.55565000 |
| C | 10.58037500 | 9.30357500 | 18.13252500 |
| C | 9.34115000 | 8.83905000 | 17.62847500 |
| H | 8.54077500 | 12.98997500 | 15.96285000 |
| H | 11.75060000 | 10.83515000 | 19.16282500 |
| H | 10.21170000 | 12.54260000 | 18.58910000 |
| H | 11.36395000 | 8.58397500 | 18.38402500 |
| H | 8.48180000 | 9.51635000 | 17.64690000 |
| H | 9.11387500 | 7.76970000 | 17.67675000 |

7_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.53632500 | 11.42997500 | 16.80365000 |
| Pd | 12.63817500 | 13.95905000 | 17.42572500 |
| Pd | 14.32925000 | 11.87430000 | 16.56315000 |
| Pd | 10.12467500 | 13.88310000 | 16.18077500 |
| Pd | 10.38912500 | 9.08052500 | 15.78777500 |
| Pd | 14.72232500 | 14.52095000 | 15.85625000 |
| Pd | 12.24245000 | 15.78910000 | 15.48237500 |
| Pd | 13.22460000 | 9.42222500 | 15.67597500 |
| Pd | 9.02267500 | 11.43182500 | 15.17817500 |
| Pd | 15.93172500 | 9.89977500 | 15.43432500 |
| Pd | 7.86785000 | 13.90025000 | 14.52455000 |
| Pd | 12.59627500 | 13.13257500 | 14.94230000 |
| Pd | 16.38152500 | 12.52230000 | 14.83247500 |
| Pd | 9.83515000 | 15.80685000 | 14.03115000 |
| Pd | 11.48902500 | 10.81142500 | 14.15010000 |

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|----|-------------|-------------|-------------|
| Pd | 16.75402500 | 15.11092500 | 14.06647500 |
| Pd | 14.35735000 | 16.42052500 | 13.79835000 |
| Pd | 11.86490000 | 17.59472500 | 13.45587500 |
| Pd | 14.20410000 | 11.19137500 | 13.90730000 |
| Pd | 10.27550000 | 13.21415000 | 13.61002500 |
| Pd | 11.79555000 | 8.17207500 | 13.59345000 |
| Pd | 9.29802500 | 9.38727500 | 13.28660000 |
| Pd | 14.60842500 | 13.82320000 | 13.19827500 |
| Pd | 14.59585000 | 8.58192500 | 13.41427500 |
| Pd | 12.18262500 | 15.01200000 | 12.93197500 |
| Pd | 8.03067500 | 11.88645000 | 12.61075000 |
| Pd | 16.58807500 | 10.50975000 | 12.88977500 |
| Pd | 12.50930000 | 12.49730000 | 12.42672500 |
| Pd | 8.49965000 | 14.53645000 | 11.92845000 |
| Pd | 16.98990000 | 13.16785000 | 12.17480000 |
| Pd | 12.79265000 | 9.97347500 | 11.90002500 |
| Pd | 10.50365000 | 16.44450000 | 11.37255000 |
| Pd | 10.37765000 | 11.20805000 | 11.69937500 |
| Pd | 15.75387500 | 15.57700000 | 11.54165000 |
| Pd | 13.28537500 | 16.81777500 | 11.26457500 |
| Pd | 14.74735000 | 11.79515000 | 11.31357500 |
| Pd | 10.80345000 | 13.78502500 | 10.94920000 |
| Pd | 13.19962500 | 7.43470000 | 11.32360000 |
| Pd | 10.73500000 | 8.57492500 | 10.99077500 |
| Pd | 8.32657500 | 9.89362500 | 10.71795000 |
| Pd | 13.53017500 | 14.16867500 | 10.71587500 |
| Pd | 15.22090000 | 9.24125000 | 10.78547500 |

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|----|-------------|-------------|-------------|
| Pd | 8.70742500 | 12.51212500 | 9.94165000 |
| Pd | 12.39435000 | 11.83115000 | 9.92130000 |
| Pd | 17.11685000 | 11.15722500 | 10.28657500 |
| Pd | 9.21830000 | 15.13827500 | 9.32527500 |
| Pd | 15.93775000 | 13.56605000 | 9.64055000 |
| Pd | 14.61295000 | 15.91665000 | 9.03177500 |
| Pd | 10.34957500 | 10.49455000 | 8.98710000 |
| Pd | 11.91757500 | 15.56522500 | 9.13110000 |
| Pd | 12.87410000 | 9.24720000 | 9.29317500 |
| Pd | 14.84380000 | 11.14857500 | 8.76522500 |
| Pd | 10.83332500 | 13.17232500 | 8.24147500 |
| Pd | 12.46872500 | 11.15632500 | 7.35567500 |
| Pd | 13.59587500 | 13.54720000 | 8.11957500 |
| O | 10.46510000 | 11.11755000 | 18.70167500 |
| O | 10.73720000 | 14.15070000 | 18.20165000 |
| C | 11.13182500 | 10.03997500 | 18.48367500 |
| C | 10.52787500 | 8.80952500 | 17.92737500 |
| C | 9.18287500 | 8.71982500 | 17.50490000 |
| H | 8.55517500 | 13.01642500 | 15.95965000 |
| H | 12.13547500 | 9.92135000 | 18.94085000 |
| H | 10.52942500 | 13.30117500 | 18.65327500 |
| H | 11.11900000 | 7.90080000 | 18.08342500 |
| H | 8.51640000 | 9.57327500 | 17.65760000 |
| H | 8.70805000 | 7.74192500 | 17.40032500 |

TS6_Pd

| | | | |
|----|-------------|-------------|-------------|
| Pd | 11.55070000 | 11.10227500 | 16.72010000 |
| Pd | 12.50825000 | 13.63610000 | 17.48615000 |
| Pd | 14.27437500 | 11.66550000 | 16.57022500 |
| Pd | 9.96332500 | 13.78220000 | 16.09970000 |
| Pd | 10.29647500 | 8.96620000 | 15.63180000 |
| Pd | 14.65060000 | 14.32040000 | 15.96820000 |
| Pd | 12.20612500 | 15.60190000 | 15.55985000 |
| Pd | 13.10865000 | 9.19930000 | 15.47885000 |
| Pd | 9.02687500 | 11.33932500 | 15.04655000 |
| Pd | 15.82482500 | 9.70992500 | 15.37010000 |
| Pd | 7.87255000 | 13.81720000 | 14.43047500 |
| Pd | 12.40800000 | 12.99525000 | 14.98737500 |
| Pd | 16.35090000 | 12.35887500 | 14.84595000 |
| Pd | 9.81157500 | 15.76235000 | 14.09675000 |
| Pd | 11.38515000 | 10.72445000 | 13.96270000 |
| Pd | 16.69872500 | 15.00750000 | 14.23290000 |
| Pd | 14.33110000 | 16.35587500 | 13.94592500 |
| Pd | 11.86125000 | 17.52530000 | 13.57545000 |
| Pd | 14.10512500 | 11.14725000 | 13.97800000 |
| Pd | 10.21860000 | 13.18235000 | 13.42217500 |
| Pd | 11.71030000 | 8.10490000 | 13.35095000 |
| Pd | 9.25230000 | 9.35390000 | 13.06832500 |
| Pd | 14.53827500 | 13.76927500 | 13.40122500 |
| Pd | 14.53232500 | 8.50295000 | 13.24760000 |
| Pd | 12.13800000 | 14.99380000 | 12.95170000 |
| Pd | 8.05982500 | 11.84535000 | 12.49570000 |
| Pd | 16.53632500 | 10.40327500 | 12.85437500 |

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|----|-------------|-------------|-------------|
| Pd | 12.51357500 | 12.49247500 | 12.41982500 |
| Pd | 8.53900000 | 14.54315000 | 11.89475000 |
| Pd | 16.98997500 | 13.13950000 | 12.24117500 |
| Pd | 12.87975000 | 9.98007500 | 11.81850000 |
| Pd | 10.52107500 | 16.46312500 | 11.45257500 |
| Pd | 10.46115000 | 11.20357500 | 11.47495000 |
| Pd | 15.78832500 | 15.57135000 | 11.68380000 |
| Pd | 13.31382500 | 16.86257500 | 11.38380000 |
| Pd | 14.83847500 | 11.82222500 | 11.44965000 |
| Pd | 10.94120000 | 13.79092500 | 10.80847500 |
| Pd | 13.18790000 | 7.44687500 | 11.08857500 |
| Pd | 10.71835000 | 8.62042500 | 10.80462500 |
| Pd | 8.34120000 | 9.94275000 | 10.50477500 |
| Pd | 13.67200000 | 14.21475000 | 10.85975000 |
| Pd | 15.21590000 | 9.27235000 | 10.62882500 |
| Pd | 8.71425000 | 12.61142500 | 9.89100000 |
| Pd | 12.62225000 | 11.88472500 | 9.88402500 |
| Pd | 17.15562500 | 11.19757500 | 10.29667500 |
| Pd | 9.27880000 | 15.24437500 | 9.33542500 |
| Pd | 15.96945000 | 13.60445000 | 9.67750000 |
| Pd | 14.71792500 | 15.99812500 | 9.19482500 |
| Pd | 10.39377500 | 10.64582500 | 8.87215000 |
| Pd | 11.98850000 | 15.67247500 | 9.22790000 |
| Pd | 12.84812500 | 9.33022500 | 9.14872500 |
| Pd | 14.89027500 | 11.23960000 | 8.71795000 |
| Pd | 10.86945000 | 13.29710000 | 8.22860000 |
| Pd | 12.55137500 | 11.31040000 | 7.28115000 |

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|----|-------------|-------------|-------------|
| Pd | 13.61515000 | 13.68590000 | 8.16965000 |
| O | 9.71542500 | 11.53240000 | 18.93197500 |
| O | 10.54177500 | 13.98487500 | 18.22860000 |
| C | 10.81867500 | 10.91145000 | 18.89450000 |
| C | 11.03080000 | 9.61490000 | 18.25982500 |
| C | 9.97780000 | 8.82812500 | 17.67710000 |
| H | 9.35722500 | 14.53957500 | 17.32197500 |
| H | 11.69047500 | 11.30742500 | 19.46325000 |
| H | 10.14310000 | 13.12987500 | 18.60072500 |
| H | 11.97702500 | 9.11890000 | 18.50000000 |
| H | 8.95877500 | 9.20822500 | 17.82982500 |
| H | 10.09047500 | 7.73527500 | 17.75002500 |

Rh₅₅(Ih)

| | | | |
|----|-------------|-------------|-------------|
| Rh | 12.50000000 | 12.50000000 | 12.50000000 |
| Rh | 12.50000000 | 12.50990000 | 15.02585000 |
| Rh | 10.34540000 | 11.79545000 | 13.63957500 |
| Rh | 10.34540000 | 13.20455000 | 11.36042500 |
| Rh | 12.50000000 | 14.76302500 | 11.37825000 |
| Rh | 13.83457500 | 14.33457500 | 13.63425000 |
| Rh | 12.50000000 | 10.23697500 | 13.62175000 |
| Rh | 11.16542500 | 10.66542500 | 11.36575000 |
| Rh | 12.50000000 | 12.49010000 | 9.97415000 |
| Rh | 14.65460000 | 13.20452500 | 11.36042500 |
| Rh | 14.65457500 | 11.79545000 | 13.63957500 |
| Rh | 11.16542500 | 14.33457500 | 13.63425000 |
| Rh | 13.83457500 | 10.66542500 | 11.36575000 |

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|----|-------------|-------------|-------------|
| Rh | 12.50000000 | 10.18822500 | 16.24345000 |
| Rh | 10.32347500 | 9.47282500 | 14.81887500 |
| Rh | 8.95320000 | 9.91037500 | 12.49615000 |
| Rh | 8.95252500 | 11.33955000 | 10.18537500 |
| Rh | 10.32350000 | 13.21975000 | 8.75532500 |
| Rh | 12.50000000 | 14.81177500 | 8.75655000 |
| Rh | 14.67652500 | 15.52717500 | 10.18112500 |
| Rh | 16.04680000 | 15.08962500 | 12.50385000 |
| Rh | 16.04747500 | 13.66045000 | 14.81462500 |
| Rh | 14.67647500 | 11.78025000 | 16.24467500 |
| Rh | 12.50000000 | 12.51495000 | 17.53977500 |
| Rh | 10.32352500 | 11.78025000 | 16.24467500 |
| Rh | 8.23762500 | 11.10887500 | 14.74915000 |
| Rh | 8.12877500 | 12.50000000 | 12.50000000 |
| Rh | 8.23760000 | 13.89112500 | 10.25085000 |
| Rh | 10.32347500 | 15.52717500 | 10.18112500 |
| Rh | 12.50000000 | 17.01247500 | 10.25690000 |
| Rh | 13.85655000 | 16.67560000 | 12.51305000 |
| Rh | 15.15740000 | 16.14252500 | 14.75265000 |
| Rh | 13.85745000 | 14.37925000 | 16.22970000 |
| Rh | 14.67652500 | 9.47282500 | 14.81887500 |
| Rh | 12.50000000 | 7.98752500 | 14.74310000 |
| Rh | 11.14345000 | 8.32440000 | 12.48695000 |
| Rh | 9.84260000 | 8.85747500 | 10.24737500 |
| Rh | 11.14255000 | 10.62075000 | 8.77030000 |
| Rh | 12.50000000 | 12.48505000 | 7.46022500 |
| Rh | 14.67647500 | 13.21975000 | 8.75532500 |

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|----|-------------|-------------|-------------|
| Rh | 16.76240000 | 13.89112500 | 10.25085000 |
| Rh | 16.87122500 | 12.50000000 | 12.50000000 |
| Rh | 16.76237500 | 11.10887500 | 14.74915000 |
| Rh | 11.14255000 | 14.37925000 | 16.22970000 |
| Rh | 8.95252500 | 13.66045000 | 14.81462500 |
| Rh | 8.95320000 | 15.08962500 | 12.50385000 |
| Rh | 11.14345000 | 16.67560000 | 12.51305000 |
| Rh | 12.50000000 | 16.25362500 | 14.81950000 |
| Rh | 13.85655000 | 8.32440000 | 12.48695000 |
| Rh | 12.50000000 | 8.74637500 | 10.18050000 |
| Rh | 13.85745000 | 10.62075000 | 8.77030000 |
| Rh | 16.04747500 | 11.33955000 | 10.18537500 |
| Rh | 16.04680000 | 9.91037500 | 12.49615000 |
| Rh | 9.84260000 | 16.14252500 | 14.75265000 |
| Rh | 15.15740000 | 8.85747500 | 10.24737500 |

1_Rh_a

| | | | |
|----|-------------|-------------|-------------|
| Rh | 12.39077500 | 15.64465000 | 15.75680000 |
| Rh | 12.94670000 | 13.48237500 | 17.42135000 |
| Rh | 14.84087500 | 14.35245000 | 15.69445000 |
| Rh | 10.52297500 | 13.65545000 | 16.22537500 |
| Rh | 14.30650000 | 16.24565000 | 13.85155000 |
| Rh | 11.84962500 | 17.36702500 | 13.63560000 |
| Rh | 9.98905000 | 15.54567500 | 14.38035000 |
| Rh | 12.18710000 | 14.87172500 | 13.09607500 |
| Rh | 12.71185000 | 13.02195000 | 14.89907500 |
| Rh | 14.21367500 | 11.15930000 | 13.77952500 |

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|----|-------------|-------------|-------------|
| Rh | 11.62870000 | 10.74095000 | 14.09520000 |
| Rh | 10.35992500 | 13.01537500 | 13.64822500 |
| Rh | 8.15737500 | 13.55847500 | 14.84232500 |
| Rh | 9.41575000 | 11.35217500 | 15.40957500 |
| Rh | 10.76077500 | 9.06660000 | 15.73195000 |
| Rh | 11.81422500 | 11.32945000 | 16.64782500 |
| Rh | 13.36055000 | 9.38762500 | 15.47910000 |
| Rh | 14.46965000 | 11.75667500 | 16.32202500 |
| Rh | 15.91270000 | 9.89427500 | 15.10292500 |
| Rh | 16.38120000 | 12.47035000 | 14.54987500 |
| Rh | 16.72080000 | 14.94537500 | 13.79007500 |
| Rh | 14.58067500 | 13.70027500 | 13.12900000 |
| Rh | 16.42240000 | 10.55582500 | 12.57330000 |
| Rh | 15.01235000 | 9.40002500 | 10.57992500 |
| Rh | 13.12782500 | 7.64867500 | 11.19725000 |
| Rh | 14.59150000 | 8.67682500 | 13.17395000 |
| Rh | 11.91542500 | 8.24695000 | 13.49730000 |
| Rh | 9.50662500 | 9.43062500 | 13.42102500 |
| Rh | 10.69825000 | 8.69735000 | 11.10937500 |
| Rh | 12.81912500 | 10.04677500 | 11.83017500 |
| Rh | 12.50000000 | 12.46875000 | 12.46657500 |
| Rh | 16.80130000 | 13.17247500 | 11.95320000 |
| Rh | 14.61827500 | 11.88252500 | 11.24777500 |
| Rh | 15.51852500 | 15.55085000 | 11.56245000 |
| Rh | 13.08037500 | 16.70962500 | 11.49870000 |
| Rh | 13.37412500 | 14.18665000 | 10.82885000 |
| Rh | 10.42395000 | 16.27952500 | 11.82210000 |

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|----|-------------|-------------|-------------|
| Rh | 10.78815000 | 13.76947500 | 11.14602500 |
| Rh | 8.55307500 | 14.41875000 | 12.40902500 |
| Rh | 8.20080000 | 11.78510000 | 13.00392500 |
| Rh | 10.44840000 | 11.20050000 | 11.76555000 |
| Rh | 8.37630000 | 9.96400000 | 11.09450000 |
| Rh | 8.64390000 | 12.51240000 | 10.42545000 |
| Rh | 9.08730000 | 15.08025000 | 9.87077500 |
| Rh | 11.64077500 | 15.55965000 | 9.46612500 |
| Rh | 14.24032500 | 15.91197500 | 9.24462500 |
| Rh | 15.56150000 | 13.63197500 | 9.57070000 |
| Rh | 16.75325000 | 11.32592500 | 10.06097500 |
| Rh | 14.47565000 | 11.31047500 | 8.71520000 |
| Rh | 13.19282500 | 13.67062500 | 8.30685000 |
| Rh | 12.28660000 | 11.91062500 | 10.01442500 |
| Rh | 10.51500000 | 13.24167500 | 8.63235000 |
| Rh | 10.16077500 | 10.61155000 | 9.24875000 |
| Rh | 12.60722500 | 9.42755000 | 9.31452500 |
| Rh | 12.08090000 | 11.35522500 | 7.58627500 |
| O | 10.49695000 | 15.66125000 | 16.31970000 |
| O | 14.26247500 | 16.26887500 | 15.85867500 |

2_Rh

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.65177500 | 11.35392500 | 17.01220000 |
| Rh | 12.91947500 | 13.87425000 | 17.26432500 |
| Rh | 14.46655000 | 11.88362500 | 16.30762500 |
| Rh | 10.49935000 | 13.89620000 | 16.07017500 |
| Rh | 10.64327500 | 9.24650000 | 15.77547500 |

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|----|-------------|-------------|-------------|
| Rh | 14.81907500 | 14.44362500 | 15.62080000 |
| Rh | 12.42265000 | 15.66282500 | 15.47862500 |
| Rh | 13.32632500 | 9.56625000 | 15.55485000 |
| Rh | 9.36040000 | 11.57892500 | 15.31270000 |
| Rh | 15.99042500 | 9.96042500 | 15.07677500 |
| Rh | 8.17407500 | 13.93897500 | 14.60817500 |
| Rh | 12.69422500 | 13.15030000 | 14.85265000 |
| Rh | 16.37145000 | 12.48017500 | 14.57062500 |
| Rh | 10.03240000 | 15.70560000 | 14.19352500 |
| Rh | 11.60122500 | 10.91697500 | 14.08235000 |
| Rh | 16.66195000 | 15.02150000 | 13.79055000 |
| Rh | 14.37652500 | 16.31780000 | 13.66510000 |
| Rh | 11.98505000 | 17.40170000 | 13.51092500 |
| Rh | 14.21765000 | 11.26747500 | 13.73780000 |
| Rh | 10.39020000 | 13.21562500 | 13.50857500 |
| Rh | 11.83637500 | 8.37840000 | 13.64165000 |
| Rh | 9.45785000 | 9.58860000 | 13.49477500 |
| Rh | 14.60932500 | 13.79732500 | 13.09387500 |
| Rh | 14.50990000 | 8.71677500 | 13.32817500 |
| Rh | 12.26287500 | 14.99197500 | 12.95447500 |
| Rh | 8.19972500 | 11.92850000 | 12.94800000 |
| Rh | 16.43027500 | 10.55287500 | 12.63847500 |
| Rh | 12.53902500 | 12.55970000 | 12.40112500 |
| Rh | 8.62590000 | 14.52535000 | 12.17015000 |
| Rh | 16.81742500 | 13.14242500 | 11.92202500 |
| Rh | 12.79097500 | 10.09527500 | 11.86797500 |
| Rh | 10.55525000 | 16.32972500 | 11.54957500 |

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|----|-------------|-------------|-------------|
| Rh | 10.45492500 | 11.28505000 | 11.72747500 |
| Rh | 15.62845000 | 15.48587500 | 11.41287500 |
| Rh | 13.18745000 | 16.72730000 | 11.26720000 |
| Rh | 14.64820000 | 11.89042500 | 11.23862500 |
| Rh | 10.87847500 | 13.81002500 | 11.01360000 |
| Rh | 13.07452500 | 7.67280000 | 11.34732500 |
| Rh | 10.67715000 | 8.75992500 | 11.18642500 |
| Rh | 8.38455000 | 10.06080000 | 11.06175000 |
| Rh | 13.46637500 | 14.18442500 | 10.73110000 |
| Rh | 14.97400000 | 9.37500000 | 10.67557500 |
| Rh | 8.71225000 | 12.56300000 | 10.29890000 |
| Rh | 12.34265000 | 11.88975000 | 9.97667500 |
| Rh | 16.79362500 | 11.21240000 | 10.11457500 |
| Rh | 9.18500000 | 15.08792500 | 9.65980000 |
| Rh | 15.68097500 | 13.54070000 | 9.50885000 |
| Rh | 14.39127500 | 15.80952500 | 9.08190000 |
| Rh | 10.20182500 | 10.59787500 | 9.24077500 |
| Rh | 11.76830000 | 15.53220000 | 9.27527500 |
| Rh | 12.62157500 | 9.36622500 | 9.38700000 |
| Rh | 14.53407500 | 11.19455000 | 8.73605000 |
| Rh | 10.62002500 | 13.18720000 | 8.50160000 |
| Rh | 12.16045000 | 11.24802500 | 7.56367500 |
| Rh | 13.29380000 | 13.55272500 | 8.21822500 |
| O | 9.88230000 | 12.32020000 | 17.09210000 |
| O | 13.46120000 | 10.50872500 | 17.31342500 |
| C | 10.07947500 | 10.78487500 | 19.52602500 |
| C | 10.96805000 | 10.01865000 | 18.57490000 |

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|---|-------------|-------------|-------------|
| C | 10.38640000 | 8.90822500 | 17.81715000 |
| H | 10.54095000 | 11.72447500 | 19.86137500 |
| H | 9.90272500 | 10.16497500 | 20.42452500 |
| H | 9.10620000 | 11.02262500 | 19.07705000 |
| H | 11.96150000 | 9.79785000 | 18.98622500 |
| H | 9.29260000 | 8.79587500 | 17.89657500 |
| H | 10.92692500 | 7.94800000 | 17.87677500 |

TS1_Rh_{C1}

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|----|-------------|-------------|-------------|
| Rh | 11.29537500 | 11.48790000 | 16.90880000 |
| Rh | 12.77102500 | 13.83482500 | 17.26637500 |
| Rh | 14.23145000 | 11.75687500 | 16.35507500 |
| Rh | 10.36102500 | 13.99035000 | 15.98357500 |
| Rh | 10.23522500 | 9.25560000 | 15.55362500 |
| Rh | 14.73470000 | 14.30047500 | 15.69880000 |
| Rh | 12.39877500 | 15.65867500 | 15.49580000 |
| Rh | 12.93272500 | 9.40532500 | 15.46832500 |
| Rh | 9.09790000 | 11.71260000 | 15.12177500 |
| Rh | 15.63292500 | 9.74177500 | 15.14567500 |
| Rh | 8.10832500 | 14.17742500 | 14.42785000 |
| Rh | 12.56332500 | 13.11045000 | 14.85850000 |
| Rh | 16.20087500 | 12.24650000 | 14.67037500 |
| Rh | 10.08062500 | 15.84617500 | 14.10680000 |
| Rh | 11.36962500 | 10.95850000 | 14.05565000 |
| Rh | 16.67755000 | 14.77232500 | 13.96805000 |
| Rh | 14.46500000 | 16.19962500 | 13.78132500 |

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|----|-------------|-------------|-------------|
| Rh | 12.14167500 | 17.43015000 | 13.53350000 |
| Rh | 14.00672500 | 11.15187500 | 13.78417500 |
| Rh | 10.30637500 | 13.33965000 | 13.42377500 |
| Rh | 11.47190000 | 8.40805000 | 13.47582500 |
| Rh | 9.14530000 | 9.78057500 | 13.27887500 |
| Rh | 14.57977500 | 13.66562500 | 13.17385000 |
| Rh | 14.18705000 | 8.60105000 | 13.29182500 |
| Rh | 12.31055000 | 14.99415000 | 12.96712500 |
| Rh | 8.06150000 | 12.20700000 | 12.72975000 |
| Rh | 16.21580000 | 10.33867500 | 12.71807500 |
| Rh | 12.45085000 | 12.53960000 | 12.40220000 |
| Rh | 8.67745000 | 14.77292500 | 12.01820000 |
| Rh | 16.79585000 | 12.92795000 | 12.06312500 |
| Rh | 12.59357500 | 10.08200000 | 11.82272500 |
| Rh | 10.73422500 | 16.46420000 | 11.52102500 |
| Rh | 10.33065000 | 11.41875000 | 11.61980000 |
| Rh | 15.73407500 | 15.33087500 | 11.56745000 |
| Rh | 13.39150000 | 16.70320000 | 11.34420000 |
| Rh | 14.59102500 | 11.77552500 | 11.29025000 |
| Rh | 10.92402500 | 13.92932500 | 10.96482500 |
| Rh | 12.73215000 | 7.64747500 | 11.27205000 |
| Rh | 10.41842500 | 8.89207500 | 11.02450000 |
| Rh | 8.21000000 | 10.32495000 | 10.85030000 |
| Rh | 13.53925000 | 14.14565000 | 10.79152500 |
| Rh | 14.76377500 | 9.25542500 | 10.67575000 |
| Rh | 8.71810000 | 12.82005000 | 10.14457500 |
| Rh | 12.31542500 | 11.93785000 | 9.95647500 |

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|----|-------------|-------------|-------------|
| Rh | 16.70257500 | 11.01690000 | 10.20872500 |
| Rh | 9.37500000 | 15.32115000 | 9.54757500 |
| Rh | 15.75165000 | 13.40527500 | 9.62657500 |
| Rh | 14.61232500 | 15.74867500 | 9.19380000 |
| Rh | 10.11697500 | 10.79242500 | 9.11072500 |
| Rh | 11.98077500 | 15.61445000 | 9.28947500 |
| Rh | 12.45747500 | 9.40895000 | 9.32847500 |
| Rh | 14.49702500 | 11.14367500 | 8.76845000 |
| Rh | 10.72985000 | 13.35297500 | 8.43367500 |
| Rh | 12.17195000 | 11.34070000 | 7.53162500 |
| Rh | 13.42182500 | 13.57177500 | 8.25510000 |
| O | 9.55420000 | 12.42797500 | 16.92235000 |
| O | 13.02255000 | 10.38017500 | 17.25620000 |
| C | 9.72340000 | 10.00240000 | 19.04642500 |
| C | 10.96860000 | 10.85502500 | 18.94767500 |
| C | 12.26040000 | 10.26682500 | 19.03027500 |
| H | 8.85272500 | 10.51975000 | 18.62142500 |
| H | 9.49282500 | 9.77757500 | 20.10362500 |
| H | 9.84717500 | 9.03927500 | 18.52362500 |
| H | 10.87990000 | 11.84845000 | 19.40820000 |
| H | 12.35707500 | 9.17867500 | 19.06205000 |
| H | 13.08755000 | 10.82760000 | 19.46732500 |

3_Rh_{C1}

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|----|-------------|-------------|-------------|
| Rh | 12.49115000 | 13.87860000 | 17.27522500 |
| Rh | 12.05752500 | 15.83192500 | 15.33447500 |

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|----|-------------|-------------|-------------|
| Rh | 10.21985000 | 14.01852500 | 15.92402500 |
| Rh | 11.54425000 | 11.62692500 | 16.61525000 |
| Rh | 14.21740000 | 12.15135000 | 16.48020000 |
| Rh | 14.55325000 | 14.66627500 | 15.65957500 |
| Rh | 12.51685000 | 13.19240000 | 14.80580000 |
| Rh | 11.60815000 | 17.36895000 | 13.07242500 |
| Rh | 9.77500000 | 15.63620000 | 13.72650000 |
| Rh | 8.02725000 | 13.72412500 | 14.32680000 |
| Rh | 9.25380000 | 11.58092500 | 15.19442500 |
| Rh | 10.55550000 | 9.32787500 | 15.80990000 |
| Rh | 13.19097500 | 9.69225000 | 15.74742500 |
| Rh | 15.80357500 | 10.18635000 | 15.47990000 |
| Rh | 16.20827500 | 12.72057500 | 14.78487500 |
| Rh | 16.53872500 | 15.12397500 | 13.84572500 |
| Rh | 14.06320000 | 16.35412500 | 13.61370000 |
| Rh | 13.09675000 | 16.59890000 | 11.08210000 |
| Rh | 10.44497500 | 16.10407500 | 11.18902500 |
| Rh | 8.55150000 | 14.22150000 | 11.80317500 |
| Rh | 8.20050000 | 11.70832500 | 12.66025000 |
| Rh | 9.48375000 | 9.45102500 | 13.42830000 |
| Rh | 11.93492500 | 8.31557500 | 13.77967500 |
| Rh | 14.61705000 | 8.78730000 | 13.62825000 |
| Rh | 16.46090000 | 10.64295000 | 12.99545000 |
| Rh | 16.82300000 | 13.20127500 | 12.18057500 |
| Rh | 15.53292500 | 15.50395000 | 11.49452500 |
| Rh | 12.08135000 | 14.88035000 | 12.79335000 |
| Rh | 14.48965000 | 13.77540000 | 13.13485000 |

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|----|-------------|-------------|-------------|
| Rh | 14.13960000 | 11.30105000 | 13.96047500 |
| Rh | 12.50000000 | 12.43825000 | 12.38487500 |
| Rh | 10.26910000 | 13.09497500 | 13.39982500 |
| Rh | 11.53700000 | 10.85442500 | 14.09830000 |
| Rh | 12.91932500 | 9.97997500 | 12.02485000 |
| Rh | 10.86972500 | 13.56227500 | 10.82172500 |
| Rh | 10.51985000 | 11.07450000 | 11.65610000 |
| Rh | 8.54672500 | 9.71362500 | 10.95697500 |
| Rh | 8.80942500 | 12.18555000 | 10.04110000 |
| Rh | 9.26757500 | 14.67815000 | 9.27897500 |
| Rh | 10.88952500 | 8.53112500 | 11.29215000 |
| Rh | 13.32375000 | 7.53957500 | 11.66390000 |
| Rh | 15.22197500 | 9.26892500 | 11.02217500 |
| Rh | 12.93697500 | 9.12305000 | 9.57337500 |
| Rh | 10.48892500 | 10.22482500 | 9.20510000 |
| Rh | 12.52412500 | 10.89047500 | 7.63422500 |
| Rh | 10.84337500 | 12.79662500 | 8.35002500 |
| Rh | 11.84900000 | 15.20842500 | 9.04937500 |
| Rh | 13.53960000 | 13.28057500 | 8.22795000 |
| Rh | 12.50960000 | 11.65830000 | 10.00660000 |
| Rh | 14.80617500 | 10.99480000 | 8.96160000 |
| Rh | 16.96737500 | 11.19625000 | 10.47387500 |
| Rh | 14.74017500 | 11.79440000 | 11.42330000 |
| Rh | 15.78365000 | 13.42997500 | 9.69255000 |
| Rh | 13.48185000 | 14.03942500 | 10.70492500 |
| Rh | 14.45467500 | 15.62075000 | 9.04085000 |
| O | 10.41057500 | 15.94635000 | 16.66666667 |

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|---|-------------|-------------|-------------|
| O | 13.92512500 | 16.58515000 | 15.57707500 |
| C | 12.69515000 | 15.61300000 | 19.59157500 |
| C | 11.58962500 | 15.05387500 | 18.70832500 |
| C | 10.70132500 | 16.12405000 | 18.07177500 |
| H | 13.31507500 | 14.81927500 | 20.03442500 |
| H | 12.26650000 | 16.18920000 | 20.43547500 |
| H | 13.35230000 | 16.29780000 | 19.03365000 |
| H | 10.97895000 | 14.30187500 | 19.23997500 |
| H | 11.17675000 | 17.11747500 | 18.15515000 |
| H | 9.72010000 | 16.17377500 | 18.57927500 |

TS1_RhC2

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|----|-------------|-------------|-------------|
| Rh | 11.91905000 | 11.42380000 | 16.79972500 |
| Rh | 13.10417500 | 13.87525000 | 17.28570000 |
| Rh | 14.56922500 | 11.83715000 | 16.28172500 |
| Rh | 10.65357500 | 13.83760000 | 16.22085000 |
| Rh | 10.66697500 | 9.23372500 | 15.80607500 |
| Rh | 14.96697500 | 14.42282500 | 15.59897500 |
| Rh | 12.53535000 | 15.63240000 | 15.52767500 |
| Rh | 13.41155000 | 9.49480000 | 15.52325000 |
| Rh | 9.46040000 | 11.53860000 | 15.38967500 |
| Rh | 16.06552500 | 9.92777500 | 15.00332500 |
| Rh | 8.30642500 | 13.90855000 | 14.82472500 |
| Rh | 12.79987500 | 13.15847500 | 14.84445000 |
| Rh | 16.45955000 | 12.44670000 | 14.49015000 |
| Rh | 10.13410000 | 15.67667500 | 14.30437500 |

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|----|-------------|-------------|-------------|
| Rh | 11.67627500 | 10.89215000 | 14.10185000 |
| Rh | 16.74867500 | 14.99397500 | 13.72435000 |
| Rh | 14.44487500 | 16.29367500 | 13.67930000 |
| Rh | 12.04160000 | 17.39515000 | 13.59697500 |
| Rh | 14.27902500 | 11.24307500 | 13.71630000 |
| Rh | 10.45565000 | 13.19895000 | 13.63372500 |
| Rh | 11.90262500 | 8.34272500 | 13.66742500 |
| Rh | 9.52007500 | 9.57182500 | 13.52777500 |
| Rh | 14.67037500 | 13.77582500 | 13.07600000 |
| Rh | 14.57410000 | 8.69915000 | 13.24620000 |
| Rh | 12.30797500 | 14.98772500 | 12.99710000 |
| Rh | 8.23277500 | 11.94412500 | 13.08875000 |
| Rh | 16.46102500 | 10.53660000 | 12.55772500 |
| Rh | 12.56400000 | 12.54515000 | 12.42420000 |
| Rh | 8.65060000 | 14.52682500 | 12.34870000 |
| Rh | 16.84600000 | 13.12465000 | 11.84092500 |
| Rh | 12.80790000 | 10.07370000 | 11.86597500 |
| Rh | 10.54552500 | 16.35015000 | 11.68227500 |
| Rh | 10.45065000 | 11.29620000 | 11.79522500 |
| Rh | 15.62905000 | 15.48792500 | 11.39170000 |
| Rh | 13.19685000 | 16.73100000 | 11.31482500 |
| Rh | 14.64692500 | 11.88172500 | 11.20312500 |
| Rh | 10.85942500 | 13.82980000 | 11.10105000 |
| Rh | 13.09992500 | 7.66402500 | 11.28322500 |
| Rh | 10.68692500 | 8.76610000 | 11.22277500 |
| Rh | 8.36380000 | 10.05882500 | 11.20695000 |
| Rh | 13.45212500 | 14.19117500 | 10.75022500 |

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|----|-------------|-------------|-------------|
| Rh | 14.96780000 | 9.38042500 | 10.59550000 |
| Rh | 8.66440000 | 12.57825000 | 10.45365000 |
| Rh | 12.30000000 | 11.90282500 | 10.00340000 |
| Rh | 16.75937500 | 11.22027500 | 10.02137500 |
| Rh | 9.13777500 | 15.11735000 | 9.82077500 |
| Rh | 15.62917500 | 13.55330000 | 9.46992500 |
| Rh | 14.33490000 | 15.83387500 | 9.09695000 |
| Rh | 10.13665000 | 10.61497500 | 9.32507500 |
| Rh | 11.71067500 | 15.55702500 | 9.36595000 |
| Rh | 12.58382500 | 9.38562500 | 9.38147500 |
| Rh | 14.46227500 | 11.23690000 | 8.69222500 |
| Rh | 10.54195000 | 13.21810000 | 8.60215000 |
| Rh | 12.04650000 | 11.28320000 | 7.59742500 |
| Rh | 13.20372500 | 13.58767500 | 8.23312500 |
| O | 10.04837500 | 11.99182500 | 17.29085000 |
| O | 13.57342500 | 10.43062500 | 17.28845000 |
| C | 7.95305000 | 11.11030000 | 18.51932500 |
| C | 9.33312500 | 10.56725000 | 18.32530000 |
| C | 9.53685000 | 9.31887500 | 17.61887500 |
| H | 7.97312500 | 12.16627500 | 18.81905000 |
| H | 7.45535000 | 10.53797500 | 19.32165000 |
| H | 7.35207500 | 11.00475000 | 17.60370000 |
| H | 10.03087500 | 10.77372500 | 19.14355000 |
| H | 8.60225000 | 8.84732500 | 17.27697500 |
| H | 10.20867500 | 8.62145000 | 18.14987500 |

3_RhC2

| | | | |
|----|-------------|-------------|-------------|
| Rh | 12.62605000 | 13.94767500 | 17.25317500 |
| Rh | 12.17410000 | 15.88307500 | 15.30490000 |
| Rh | 10.32765000 | 14.08412500 | 15.93715000 |
| Rh | 11.63887500 | 11.70302500 | 16.65872500 |
| Rh | 14.30022500 | 12.16097500 | 16.44035000 |
| Rh | 14.65480000 | 14.68767500 | 15.59257500 |
| Rh | 12.57360000 | 13.23305000 | 14.79847500 |
| Rh | 11.69712500 | 17.39105000 | 13.01815000 |
| Rh | 9.85297500 | 15.68337500 | 13.72955000 |
| Rh | 8.09247500 | 13.80522500 | 14.38395000 |
| Rh | 9.31190000 | 11.66037500 | 15.27147500 |
| Rh | 10.60307500 | 9.40810000 | 15.90380000 |
| Rh | 13.23550000 | 9.72220000 | 15.77062500 |
| Rh | 15.84575000 | 10.17070000 | 15.44495000 |
| Rh | 16.26660000 | 12.68692500 | 14.71407500 |
| Rh | 16.61107500 | 15.07227500 | 13.73595000 |
| Rh | 14.14105000 | 16.35072500 | 13.52627500 |
| Rh | 13.13040000 | 16.56857500 | 11.00277500 |
| Rh | 10.47575000 | 16.12252500 | 11.17980000 |
| Rh | 8.57050000 | 14.27570000 | 11.84892500 |
| Rh | 8.20730000 | 11.76732500 | 12.75292500 |
| Rh | 9.48055000 | 9.51252500 | 13.52622500 |
| Rh | 11.91415000 | 8.34962500 | 13.85095000 |
| Rh | 14.59677500 | 8.76552500 | 13.63077500 |
| Rh | 16.45370000 | 10.58477500 | 12.93812500 |
| Rh | 16.83862500 | 13.14390000 | 12.08680000 |

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|----|-------------|-------------|-------------|
| Rh | 15.54892500 | 15.44627500 | 11.38102500 |
| Rh | 12.13312500 | 14.89585000 | 12.76052500 |
| Rh | 14.54515000 | 13.76257500 | 13.08697500 |
| Rh | 14.16317500 | 11.29637500 | 13.93897500 |
| Rh | 12.51040000 | 12.44070000 | 12.38442500 |
| Rh | 10.31315000 | 13.12390000 | 13.41677500 |
| Rh | 11.56132500 | 10.89392500 | 14.15367500 |
| Rh | 12.88387500 | 9.96952500 | 12.05312500 |
| Rh | 10.86295000 | 13.56682500 | 10.85307500 |
| Rh | 10.49707500 | 11.07680000 | 11.70605000 |
| Rh | 8.50347500 | 9.75097500 | 11.05682500 |
| Rh | 8.77837500 | 12.20867500 | 10.10932500 |
| Rh | 9.23887500 | 14.69370000 | 9.32630000 |
| Rh | 10.82717500 | 8.52947500 | 11.37657500 |
| Rh | 13.23970000 | 7.51307500 | 11.71152500 |
| Rh | 15.16405000 | 9.21512500 | 11.01570000 |
| Rh | 12.84922500 | 9.07537500 | 9.61502500 |
| Rh | 10.40235000 | 10.21075000 | 9.26490000 |
| Rh | 12.41627500 | 10.81100000 | 7.65912500 |
| Rh | 10.76987500 | 12.75730000 | 8.38352500 |
| Rh | 11.81697500 | 15.15715000 | 9.01875000 |
| Rh | 13.46182500 | 13.19662500 | 8.18650000 |
| Rh | 12.46177500 | 11.62122500 | 10.01677500 |
| Rh | 14.72820000 | 10.90867500 | 8.94320000 |
| Rh | 16.92680000 | 11.12310000 | 10.40532500 |
| Rh | 14.71725000 | 11.76090000 | 11.39507500 |
| Rh | 15.74915000 | 13.34060000 | 9.60905000 |

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|----|-------------|-------------|-------------|
| Rh | 13.47717500 | 13.99322500 | 10.64832500 |
| Rh | 14.42290000 | 15.52855000 | 8.93572500 |
| O | 10.54675000 | 16.04415000 | 16.62042500 |
| O | 14.05547500 | 16.61517500 | 15.48222500 |
| C | 9.45655000 | 15.90810000 | 18.75465000 |
| C | 10.77582500 | 16.20122500 | 18.05437500 |
| C | 11.93835000 | 15.34985000 | 18.57910000 |
| H | 8.64227500 | 16.49370000 | 18.30597500 |
| H | 9.52892500 | 16.16477500 | 19.82220000 |
| H | 9.21325000 | 14.83690000 | 18.66680000 |
| H | 11.02207500 | 17.27420000 | 18.16405000 |
| H | 11.66582500 | 14.78830000 | 19.48895000 |
| H | 12.84712500 | 15.94860000 | 18.76920000 |

4_Rh_C

| | | | |
|----|-------------|-------------|-------------|
| Rh | 13.31187500 | 13.69420000 | 17.23867500 |
| Rh | 12.76092500 | 15.63885000 | 15.47755000 |
| Rh | 10.76125000 | 13.60177500 | 16.25907500 |
| Rh | 12.14565000 | 11.41315000 | 16.70392500 |
| Rh | 14.72790000 | 11.79510000 | 16.22702500 |
| Rh | 15.12075000 | 14.38515000 | 15.42862500 |
| Rh | 12.94067500 | 13.02515000 | 14.82207500 |
| Rh | 12.09950000 | 17.28630000 | 13.43352500 |
| Rh | 10.10725000 | 15.59792500 | 14.23072500 |
| Rh | 8.39910000 | 13.57490000 | 14.93105000 |
| Rh | 9.66355000 | 11.35890000 | 15.52640000 |

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|----|-------------|-------------|-------------|
| Rh | 11.00377500 | 9.10650000 | 15.90755000 |
| Rh | 13.60577500 | 9.42307500 | 15.52040000 |
| Rh | 16.15935000 | 9.87222500 | 14.97200000 |
| Rh | 16.57577500 | 12.39770000 | 14.30107500 |
| Rh | 16.83050000 | 14.92260000 | 13.51740000 |
| Rh | 14.49015000 | 16.19477500 | 13.53100000 |
| Rh | 13.14587500 | 16.53737500 | 11.18745000 |
| Rh | 10.53387500 | 16.14155000 | 11.68435000 |
| Rh | 8.67137500 | 14.30707500 | 12.44347500 |
| Rh | 8.33867500 | 11.71445000 | 13.17265000 |
| Rh | 9.66357500 | 9.35790000 | 13.63840000 |
| Rh | 12.07432500 | 8.20025000 | 13.66705000 |
| Rh | 14.71120000 | 8.59225000 | 13.17702500 |
| Rh | 16.55002500 | 10.42175000 | 12.42665000 |
| Rh | 16.89067500 | 13.03630000 | 11.66972500 |
| Rh | 15.59312500 | 15.36880000 | 11.20442500 |
| Rh | 12.33947500 | 14.83132500 | 13.04062500 |
| Rh | 14.75237500 | 13.64995000 | 12.96247500 |
| Rh | 14.40080000 | 11.11300000 | 13.71167500 |
| Rh | 12.61440000 | 12.38965000 | 12.42267500 |
| Rh | 10.54747500 | 13.01987500 | 13.70757500 |
| Rh | 11.81242500 | 10.73045000 | 14.18092500 |
| Rh | 12.88382500 | 9.94012500 | 11.88927500 |
| Rh | 10.83035000 | 13.62947500 | 11.13585000 |
| Rh | 10.50075000 | 11.09237500 | 11.88630000 |
| Rh | 8.41890000 | 9.82562500 | 11.33985000 |
| Rh | 8.66160000 | 12.31992500 | 10.51925000 |

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|----|-------------|-------------|-------------|
| Rh | 9.07237500 | 14.86895000 | 9.87025000 |
| Rh | 10.74875000 | 8.55937500 | 11.31475000 |
| Rh | 13.16285000 | 7.48737500 | 11.35092500 |
| Rh | 15.01822500 | 9.20487500 | 10.56122500 |
| Rh | 12.57825000 | 9.18415000 | 9.41225000 |
| Rh | 10.14035000 | 10.35765000 | 9.41202500 |
| Rh | 11.97610000 | 11.04060000 | 7.62225000 |
| Rh | 10.45362500 | 12.96780000 | 8.65507500 |
| Rh | 11.61655000 | 15.30390000 | 9.30065000 |
| Rh | 13.12375000 | 13.35297500 | 8.18575000 |
| Rh | 12.29317500 | 11.70800000 | 10.01552500 |
| Rh | 14.41475000 | 11.01542500 | 8.65297500 |
| Rh | 16.75825000 | 11.08362500 | 9.88035000 |
| Rh | 14.68980000 | 11.72937500 | 11.14360000 |
| Rh | 15.56432500 | 13.37897500 | 9.33712500 |
| Rh | 13.42770000 | 14.02265000 | 10.67560000 |
| Rh | 14.21380000 | 15.63085000 | 8.94705000 |
| O | 10.75077500 | 15.70745000 | 16.30527500 |
| O | 13.07825000 | 15.76147500 | 17.62322500 |
| C | 9.40002500 | 16.50370000 | 18.16097500 |
| C | 10.74857500 | 16.56452500 | 17.47140000 |
| C | 11.90907500 | 16.11140000 | 18.37185000 |
| H | 8.60615000 | 16.84672500 | 17.48307500 |
| H | 9.39272500 | 17.14290000 | 19.05685000 |
| H | 9.17942500 | 15.46872500 | 18.46580000 |
| H | 10.95645000 | 17.58130000 | 17.09450000 |
| H | 11.57622500 | 15.24927500 | 18.98145000 |

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|---|-------------|-------------|-------------|
| H | 12.17252500 | 16.93700000 | 19.05872500 |
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5_Rh_C

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|----|-------------|-------------|-------------|
| Rh | 13.04245000 | 13.88742500 | 17.27347500 |
| Rh | 12.39217500 | 15.78430000 | 15.46982500 |
| Rh | 10.58182500 | 13.75680000 | 16.21965000 |
| Rh | 11.98067500 | 11.49962500 | 16.69402500 |
| Rh | 14.56947500 | 12.00232500 | 16.25720000 |
| Rh | 14.86512500 | 14.58512500 | 15.45587500 |
| Rh | 12.73440000 | 13.21582500 | 14.89405000 |
| Rh | 11.81572500 | 17.40895000 | 13.34140000 |
| Rh | 9.96447500 | 15.67780000 | 14.34802500 |
| Rh | 8.24240000 | 13.66407500 | 14.96657500 |
| Rh | 9.49517500 | 11.42597500 | 15.52977500 |
| Rh | 10.89142500 | 9.20605000 | 15.92427500 |
| Rh | 13.48995000 | 9.56835000 | 15.56707500 |
| Rh | 16.02272500 | 10.12960000 | 15.04595000 |
| Rh | 16.39915000 | 12.65860000 | 14.33340000 |
| Rh | 16.56375000 | 15.14922500 | 13.48600000 |
| Rh | 14.20312500 | 16.34790000 | 13.55005000 |
| Rh | 12.89677500 | 16.66232500 | 11.16787500 |
| Rh | 10.23800000 | 16.20147500 | 11.66957500 |
| Rh | 8.47972500 | 14.35340000 | 12.47315000 |
| Rh | 8.17532500 | 11.74582500 | 13.19760000 |
| Rh | 9.53385000 | 9.42690000 | 13.68017500 |
| Rh | 11.98060000 | 8.30437500 | 13.70040000 |

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|----|-------------|-------------|-------------|
| Rh | 14.63177500 | 8.78882500 | 13.24147500 |
| Rh | 16.40402500 | 10.66642500 | 12.50365000 |
| Rh | 16.68977500 | 13.23470000 | 11.69762500 |
| Rh | 15.32725000 | 15.52585000 | 11.20470000 |
| Rh | 12.10495000 | 14.93267500 | 12.93102500 |
| Rh | 14.50182500 | 13.80760000 | 12.98417500 |
| Rh | 14.22347500 | 11.30940000 | 13.77327500 |
| Rh | 12.42440000 | 12.47550000 | 12.42027500 |
| Rh | 10.35562500 | 13.09840000 | 13.72987500 |
| Rh | 11.66980000 | 10.85345000 | 14.21215000 |
| Rh | 12.76970000 | 10.03215000 | 11.93980000 |
| Rh | 10.62365000 | 13.65770000 | 11.13167500 |
| Rh | 10.34675000 | 11.14067500 | 11.92560000 |
| Rh | 8.28050000 | 9.83785000 | 11.39612500 |
| Rh | 8.46255000 | 12.35187500 | 10.58260000 |
| Rh | 8.83915000 | 14.85192500 | 9.85962500 |
| Rh | 10.65142500 | 8.62700000 | 11.33952500 |
| Rh | 13.10887500 | 7.60647500 | 11.42367500 |
| Rh | 14.90652500 | 9.36390000 | 10.60935000 |
| Rh | 12.46560000 | 9.27175000 | 9.45400000 |
| Rh | 9.98482500 | 10.42572500 | 9.44507500 |
| Rh | 11.83725000 | 11.09855000 | 7.65852500 |
| Rh | 10.27857500 | 13.00315000 | 8.64782500 |
| Rh | 11.37350000 | 15.38452500 | 9.33632500 |
| Rh | 12.91127500 | 13.46332500 | 8.19355000 |
| Rh | 12.12795000 | 11.77525000 | 10.02710000 |
| Rh | 14.26882500 | 11.18100000 | 8.67760000 |

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|----|-------------|-------------|-------------|
| Rh | 16.59945000 | 11.26157500 | 9.92580000 |
| Rh | 14.52212500 | 11.86742500 | 11.18002500 |
| Rh | 15.37187500 | 13.54537500 | 9.36920000 |
| Rh | 13.20350000 | 14.10885000 | 10.68300000 |
| Rh | 13.97085000 | 15.75015000 | 8.94517500 |
| O | 11.21342500 | 16.89542500 | 16.61160000 |
| O | 13.03535000 | 14.78970000 | 19.10910000 |
| C | 8.82392500 | 16.76057500 | 16.93545000 |
| C | 9.98935000 | 16.98250000 | 15.99815000 |
| C | 12.50000000 | 15.86747500 | 19.44272500 |
| H | 7.86757500 | 16.80855000 | 16.39472500 |
| H | 8.81597500 | 17.53792500 | 17.72207500 |
| H | 8.90865000 | 15.77592500 | 17.42640000 |
| H | 9.89170000 | 17.91637500 | 15.39215000 |
| H | 11.93182500 | 16.47565000 | 18.71562500 |
| H | 12.61042500 | 16.19587500 | 20.49142500 |

TS1_Rh_S

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|----|-------------|-------------|-------------|
| Rh | 11.73917500 | 11.22877500 | 16.89215000 |
| Rh | 12.82947500 | 13.73232500 | 17.31432500 |
| Rh | 14.45105000 | 11.81457500 | 16.32142500 |
| Rh | 10.46155000 | 13.66107500 | 16.24100000 |
| Rh | 10.56700000 | 9.09735000 | 15.63522500 |
| Rh | 14.77795000 | 14.39120000 | 15.74445000 |
| Rh | 12.32877500 | 15.53700000 | 15.59080000 |
| Rh | 13.33197500 | 9.46035000 | 15.47167500 |

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|----|-------------|-------------|-------------|
| Rh | 9.34455000 | 11.38915000 | 15.36617500 |
| Rh | 15.99720000 | 9.95637500 | 15.02675000 |
| Rh | 8.24155000 | 13.73015000 | 14.72302500 |
| Rh | 12.64197500 | 13.08092500 | 14.89592500 |
| Rh | 16.36390000 | 12.49720000 | 14.60517500 |
| Rh | 9.99717500 | 15.62500000 | 14.21867500 |
| Rh | 11.58425000 | 10.85045000 | 14.07727500 |
| Rh | 16.59915000 | 15.05250000 | 13.90347500 |
| Rh | 14.28267500 | 16.29432500 | 13.81852500 |
| Rh | 11.87940000 | 17.33930000 | 13.66427500 |
| Rh | 14.23447500 | 11.24875000 | 13.73292500 |
| Rh | 10.37605000 | 13.13825000 | 13.55075000 |
| Rh | 11.90200000 | 8.30515000 | 13.54095000 |
| Rh | 9.48777500 | 9.54265000 | 13.38410000 |
| Rh | 14.57765000 | 13.79852500 | 13.17790000 |
| Rh | 14.57807500 | 8.71742500 | 13.22275000 |
| Rh | 12.21192500 | 14.96475000 | 13.03070000 |
| Rh | 8.22155000 | 11.88602500 | 12.82700000 |
| Rh | 16.46962500 | 10.60890000 | 12.62905000 |
| Rh | 12.53435000 | 12.54260000 | 12.42965000 |
| Rh | 8.55982500 | 14.47895000 | 12.26945000 |
| Rh | 16.82030000 | 13.24265000 | 11.99715000 |
| Rh | 12.82972500 | 10.11247500 | 11.82750000 |
| Rh | 10.48827500 | 16.33775000 | 11.65100000 |
| Rh | 10.48010000 | 11.28305000 | 11.68155000 |
| Rh | 15.56842500 | 15.55785000 | 11.54257500 |
| Rh | 13.13007500 | 16.76705000 | 11.39987500 |

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|----|-------------|-------------|-------------|
| Rh | 14.69015000 | 11.94587500 | 11.25620000 |
| Rh | 10.81790000 | 13.84800000 | 11.05800000 |
| Rh | 13.15475000 | 7.71962500 | 11.20437500 |
| Rh | 10.74795000 | 8.79150000 | 11.05812500 |
| Rh | 8.42815000 | 10.05752500 | 10.95857500 |
| Rh | 13.44027500 | 14.23462500 | 10.81735000 |
| Rh | 15.02432500 | 9.45087500 | 10.61407500 |
| Rh | 8.71732500 | 12.57940000 | 10.27127500 |
| Rh | 12.37177500 | 11.97497500 | 9.99245000 |
| Rh | 16.81377500 | 11.34280000 | 10.14320000 |
| Rh | 9.20062500 | 15.10070000 | 9.68590000 |
| Rh | 15.67467500 | 13.67442500 | 9.58682500 |
| Rh | 14.36407500 | 15.92925000 | 9.21580000 |
| Rh | 10.25597500 | 10.66930000 | 9.16870000 |
| Rh | 11.75985000 | 15.58950000 | 9.35475000 |
| Rh | 12.69737500 | 9.47602500 | 9.30815000 |
| Rh | 14.57295000 | 11.34047500 | 8.72750000 |
| Rh | 10.67757500 | 13.28065000 | 8.50362500 |
| Rh | 12.22027500 | 11.38800000 | 7.54332500 |
| Rh | 13.32787500 | 13.68575000 | 8.25820000 |
| O | 8.65347500 | 12.85575000 | 16.55002500 |
| O | 13.63937500 | 10.27222500 | 17.22932500 |
| C | 10.68615000 | 11.08122500 | 18.82405000 |
| C | 10.93757500 | 9.75080000 | 18.29040000 |
| C | 9.96207500 | 8.90352500 | 17.63302500 |
| H | 11.19797500 | 11.30572500 | 19.76682500 |
| H | 9.65385000 | 11.44692500 | 18.78697500 |

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|---|-------------|-------------|-------------|
| H | 11.33127500 | 12.22642500 | 18.19905000 |
| H | 11.84265000 | 9.25192500 | 18.65242500 |
| H | 8.91330000 | 9.22747500 | 17.67925000 |
| H | 10.09722500 | 7.82265000 | 17.79080000 |

3_Rh_S

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.82102500 | 11.36517500 | 16.85607500 |
| Rh | 12.91490000 | 13.88617500 | 17.32180000 |
| Rh | 14.47415000 | 11.89927500 | 16.35127500 |
| Rh | 10.48177500 | 13.71185000 | 16.33407500 |
| Rh | 10.67912500 | 9.20420000 | 15.76260000 |
| Rh | 14.82957500 | 14.47080000 | 15.72150000 |
| Rh | 12.33382500 | 15.63450000 | 15.55740000 |
| Rh | 13.37275000 | 9.55805000 | 15.52595000 |
| Rh | 9.38200000 | 11.44795000 | 15.38895000 |
| Rh | 16.04792500 | 10.04940000 | 15.07375000 |
| Rh | 8.27685000 | 13.80387500 | 14.75637500 |
| Rh | 12.67322500 | 13.18957500 | 14.90700000 |
| Rh | 16.39092500 | 12.56935000 | 14.61297500 |
| Rh | 9.99445000 | 15.68937500 | 14.18010000 |
| Rh | 11.62195000 | 10.92477500 | 14.10400000 |
| Rh | 16.64497500 | 15.12210000 | 13.87597500 |
| Rh | 14.31060000 | 16.36500000 | 13.77005000 |
| Rh | 11.90280000 | 17.41525000 | 13.60840000 |
| Rh | 14.25450000 | 11.33152500 | 13.76265000 |
| Rh | 10.38942500 | 13.19935000 | 13.58677500 |

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|----|-------------|-------------|-------------|
| Rh | 11.89997500 | 8.38090000 | 13.62562500 |
| Rh | 9.49045000 | 9.61495000 | 13.45037500 |
| Rh | 14.61297500 | 13.86565000 | 13.17825000 |
| Rh | 14.60387500 | 8.78122500 | 13.30900000 |
| Rh | 12.22847500 | 15.03812500 | 13.01067500 |
| Rh | 8.23112500 | 11.93285000 | 12.86360000 |
| Rh | 16.48705000 | 10.67370000 | 12.65307500 |
| Rh | 12.54987500 | 12.60875000 | 12.44565000 |
| Rh | 8.55780000 | 14.50555000 | 12.27062500 |
| Rh | 16.83657500 | 13.29122500 | 11.98197500 |
| Rh | 12.85015000 | 10.14200000 | 11.89157500 |
| Rh | 10.49002500 | 16.36615000 | 11.62035000 |
| Rh | 10.47890000 | 11.31552500 | 11.71930000 |
| Rh | 15.58925000 | 15.60320000 | 11.51650000 |
| Rh | 13.14315000 | 16.80397500 | 11.35445000 |
| Rh | 14.69457500 | 11.98305000 | 11.26260000 |
| Rh | 10.82475000 | 13.87195000 | 11.07447500 |
| Rh | 13.14740000 | 7.73142500 | 11.33855000 |
| Rh | 10.74225000 | 8.81247500 | 11.13780000 |
| Rh | 8.42752500 | 10.09187500 | 10.99030000 |
| Rh | 13.45292500 | 14.26917500 | 10.80287500 |
| Rh | 15.03500000 | 9.46662500 | 10.68605000 |
| Rh | 8.71845000 | 12.60912500 | 10.29665000 |
| Rh | 12.37197500 | 11.98845000 | 10.01612500 |
| Rh | 16.83057500 | 11.37540000 | 10.15077500 |
| Rh | 9.19357500 | 15.13065000 | 9.67130000 |
| Rh | 15.68505000 | 13.69485000 | 9.58605000 |

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|----|-------------|-------------|-------------|
| Rh | 14.36265000 | 15.93937500 | 9.17907500 |
| Rh | 10.25660000 | 10.67152500 | 9.21602500 |
| Rh | 11.75840000 | 15.58990000 | 9.33882500 |
| Rh | 12.70020000 | 9.46905000 | 9.39792500 |
| Rh | 14.57670000 | 11.33050000 | 8.76680000 |
| Rh | 10.67280000 | 13.27817500 | 8.52600000 |
| Rh | 12.22045000 | 11.35652500 | 7.58695000 |
| Rh | 13.32752500 | 13.66962500 | 8.25622500 |
| O | 8.62905000 | 12.91292500 | 16.54400000 |
| O | 13.58842500 | 10.39040000 | 17.30117500 |
| C | 10.78502500 | 10.41865000 | 18.45457500 |
| C | 10.64807500 | 9.04920000 | 17.97685000 |
| C | 9.48110000 | 8.50050000 | 17.37702500 |
| H | 11.49747500 | 10.55680000 | 19.27575000 |
| H | 9.84712500 | 10.97050000 | 18.58997500 |
| H | 11.29865000 | 12.96835000 | 17.73502500 |
| H | 11.47382500 | 8.36980000 | 18.21530000 |
| H | 8.54050000 | 9.05972500 | 17.40582500 |
| H | 9.37500000 | 7.41435000 | 17.29977500 |

TS2_Rh_S

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.83270000 | 11.34830000 | 16.77687500 |
| Rh | 12.92862500 | 13.83915000 | 17.36410000 |
| Rh | 14.49657500 | 11.88285000 | 16.35712500 |
| Rh | 10.55530000 | 13.73022500 | 16.29360000 |
| Rh | 10.66725000 | 9.18365000 | 15.75827500 |

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|----|-------------|-------------|-------------|
| Rh | 14.83160000 | 14.46057500 | 15.72350000 |
| Rh | 12.35015000 | 15.60215000 | 15.59327500 |
| Rh | 13.38210000 | 9.52827500 | 15.51615000 |
| Rh | 9.39950000 | 11.43405000 | 15.37102500 |
| Rh | 16.04465000 | 10.01225000 | 15.08122500 |
| Rh | 8.24282500 | 13.75302500 | 14.71795000 |
| Rh | 12.70330000 | 13.16535000 | 14.91022500 |
| Rh | 16.39902500 | 12.55760000 | 14.61567500 |
| Rh | 10.00835000 | 15.66507500 | 14.21605000 |
| Rh | 11.62992500 | 10.90580000 | 14.09315000 |
| Rh | 16.64875000 | 15.12090000 | 13.88870000 |
| Rh | 14.31505000 | 16.34830000 | 13.79442500 |
| Rh | 11.91037500 | 17.39257500 | 13.63945000 |
| Rh | 14.26395000 | 11.30747500 | 13.77210000 |
| Rh | 10.39440000 | 13.17555000 | 13.57462500 |
| Rh | 11.90560000 | 8.35752500 | 13.60462500 |
| Rh | 9.50442500 | 9.58310000 | 13.44920000 |
| Rh | 14.61015000 | 13.85425000 | 13.17792500 |
| Rh | 14.62112500 | 8.75722500 | 13.29432500 |
| Rh | 12.23375000 | 15.00995000 | 13.03802500 |
| Rh | 8.23710000 | 11.90315000 | 12.85847500 |
| Rh | 16.49770000 | 10.64855000 | 12.67292500 |
| Rh | 12.56525000 | 12.58852500 | 12.43925000 |
| Rh | 8.58490000 | 14.49075000 | 12.27607500 |
| Rh | 16.84705000 | 13.25890000 | 12.00640000 |
| Rh | 12.86355000 | 10.13542500 | 11.88857500 |
| Rh | 10.50337500 | 16.34635000 | 11.64767500 |

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|----|-------------|-------------|-------------|
| Rh | 10.49920000 | 11.29010000 | 11.72897500 |
| Rh | 15.58675000 | 15.58890000 | 11.53457500 |
| Rh | 13.14367500 | 16.79152500 | 11.37557500 |
| Rh | 14.71495000 | 11.96107500 | 11.28017500 |
| Rh | 10.84822500 | 13.85102500 | 11.08392500 |
| Rh | 13.18235000 | 7.72925000 | 11.30527500 |
| Rh | 10.76870000 | 8.79765000 | 11.13380000 |
| Rh | 8.43852500 | 10.06772500 | 10.99530000 |
| Rh | 13.46760000 | 14.25767500 | 10.80985000 |
| Rh | 15.04422500 | 9.45510000 | 10.67742500 |
| Rh | 8.73322500 | 12.58752500 | 10.29857500 |
| Rh | 12.38065000 | 11.97525000 | 10.01032500 |
| Rh | 16.83922500 | 11.34457500 | 10.16082500 |
| Rh | 9.20357500 | 15.11590000 | 9.68520000 |
| Rh | 15.70140000 | 13.67267500 | 9.59447500 |
| Rh | 14.38232500 | 15.91572500 | 9.19055000 |
| Rh | 10.26372500 | 10.65050000 | 9.22332500 |
| Rh | 11.76690000 | 15.58195000 | 9.35805000 |
| Rh | 12.71282500 | 9.46797500 | 9.37500000 |
| Rh | 14.59100000 | 11.33230000 | 8.77275000 |
| Rh | 10.67055000 | 13.26415000 | 8.53882500 |
| Rh | 12.22982500 | 11.36837500 | 7.58462500 |
| Rh | 13.33340000 | 13.66747500 | 8.26635000 |
| O | 8.65112500 | 12.91537500 | 16.63355000 |
| O | 13.57257500 | 10.38960000 | 17.29522500 |
| C | 10.79102500 | 10.49835000 | 18.42140000 |
| C | 10.66115000 | 9.11095000 | 17.99462500 |

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|---|-------------|-------------|-------------|
| C | 9.50197500 | 8.52612500 | 17.41697500 |
| H | 11.50810000 | 10.66825000 | 19.23365000 |
| H | 9.84990000 | 11.04780000 | 18.54365000 |
| H | 9.61360000 | 13.32747500 | 17.57157500 |
| H | 11.49602500 | 8.44912500 | 18.24850000 |
| H | 8.55472500 | 9.07582500 | 17.42190000 |
| H | 9.40962500 | 7.43692500 | 17.38312500 |

3_Rh

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.75760000 | 11.24225000 | 16.78772500 |
| Rh | 12.87230000 | 13.67187500 | 17.34795000 |
| Rh | 14.48555000 | 11.75555000 | 16.33057500 |
| Rh | 10.52662500 | 13.65332500 | 16.24220000 |
| Rh | 10.59525000 | 9.10225000 | 15.63510000 |
| Rh | 14.79627500 | 14.34735000 | 15.75307500 |
| Rh | 12.34152500 | 15.49832500 | 15.59540000 |
| Rh | 13.32667500 | 9.43020000 | 15.44250000 |
| Rh | 9.37500000 | 11.35612500 | 15.28430000 |
| Rh | 16.00627500 | 9.90142500 | 15.02817500 |
| Rh | 8.22902500 | 13.75525000 | 14.65122500 |
| Rh | 12.66262500 | 13.03147500 | 14.92585000 |
| Rh | 16.39027500 | 12.45542500 | 14.62612500 |
| Rh | 10.00935000 | 15.62172500 | 14.22912500 |
| Rh | 11.59622500 | 10.83372500 | 14.02570000 |
| Rh | 16.64675000 | 15.03745000 | 13.96752500 |

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|----|-------------|-------------|-------------|
| Rh | 14.33245000 | 16.28280000 | 13.85937500 |
| Rh | 11.92552500 | 17.34572500 | 13.69337500 |
| Rh | 14.25342500 | 11.22575000 | 13.72927500 |
| Rh | 10.40155000 | 13.14412500 | 13.56350000 |
| Rh | 11.90840000 | 8.29217500 | 13.49620000 |
| Rh | 9.50457500 | 9.53282500 | 13.33242500 |
| Rh | 14.61037500 | 13.78755000 | 13.20995000 |
| Rh | 14.58867500 | 8.69255000 | 13.20800000 |
| Rh | 12.24640000 | 14.96680000 | 13.06297500 |
| Rh | 8.24300000 | 11.88230000 | 12.79172500 |
| Rh | 16.49082500 | 10.59775000 | 12.63777500 |
| Rh | 12.56872500 | 12.55702500 | 12.43075000 |
| Rh | 8.60842500 | 14.47635000 | 12.24475000 |
| Rh | 16.85392500 | 13.21592500 | 12.03552500 |
| Rh | 12.86255000 | 10.10942500 | 11.80397500 |
| Rh | 10.53820000 | 16.34977500 | 11.67887500 |
| Rh | 10.51077500 | 11.29755000 | 11.66587500 |
| Rh | 15.62500000 | 15.55547500 | 11.60532500 |
| Rh | 13.17680000 | 16.77412500 | 11.44240000 |
| Rh | 14.71247500 | 11.94860000 | 11.26472500 |
| Rh | 10.87805000 | 13.86445000 | 11.06957500 |
| Rh | 13.19115000 | 7.72035000 | 11.17150000 |
| Rh | 10.77965000 | 8.79467500 | 11.02002500 |
| Rh | 8.46250000 | 10.07365000 | 10.90340000 |
| Rh | 13.50167500 | 14.25340000 | 10.84095000 |
| Rh | 15.06545000 | 9.45670000 | 10.61595000 |
| Rh | 8.76482500 | 12.61177500 | 10.25295000 |

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|----|-------------|-------------|-------------|
| Rh | 12.40540000 | 11.99707500 | 9.98392500 |
| Rh | 16.86510000 | 11.34317500 | 10.14550000 |
| Rh | 9.25545000 | 15.16335000 | 9.68935000 |
| Rh | 15.74230000 | 13.68452500 | 9.62150000 |
| Rh | 14.43832500 | 15.94812500 | 9.26402500 |
| Rh | 10.30762500 | 10.68790000 | 9.15052500 |
| Rh | 11.81952500 | 15.61927500 | 9.38947500 |
| Rh | 12.74507500 | 9.50290000 | 9.27920000 |
| Rh | 14.62892500 | 11.36902500 | 8.74037500 |
| Rh | 10.72532500 | 13.32317500 | 8.51167500 |
| Rh | 12.27810000 | 11.44222500 | 7.53615000 |
| Rh | 13.39090000 | 13.72262500 | 8.28540000 |
| O | 8.48427500 | 12.88937500 | 16.61265000 |
| O | 13.56680000 | 10.24790000 | 17.21837500 |
| C | 10.70937500 | 11.01322500 | 18.61922500 |
| C | 10.86795000 | 9.65022500 | 18.22877500 |
| C | 9.87957500 | 8.81862500 | 17.58087500 |
| H | 11.33630000 | 11.38957500 | 19.43165000 |
| H | 9.71895000 | 11.47192500 | 18.55200000 |
| H | 7.91072500 | 12.83570000 | 17.39917500 |
| H | 11.78122500 | 9.14967500 | 18.56405000 |
| H | 8.83890000 | 9.16847500 | 17.59875000 |
| H | 9.99100000 | 7.73542500 | 17.72775000 |

TS2_RhOH

Rh 12.01530000 12.00747500 16.77347500

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|----|-------------|-------------|-------------|
| Rh | 13.22047500 | 14.45335000 | 17.16802500 |
| Rh | 14.66160000 | 12.27922500 | 16.34880000 |
| Rh | 10.82952500 | 14.36195000 | 16.14062500 |
| Rh | 10.69110000 | 9.69272500 | 16.06037500 |
| Rh | 15.14000000 | 14.77587500 | 15.44075000 |
| Rh | 12.74925000 | 16.06930000 | 15.27000000 |
| Rh | 13.44545000 | 9.92970000 | 15.79050000 |
| Rh | 9.58165000 | 12.00290000 | 15.65510000 |
| Rh | 16.09660000 | 10.24170000 | 15.19520000 |
| Rh | 8.50615000 | 14.33970000 | 14.81647500 |
| Rh | 12.91967500 | 13.53597500 | 14.80937500 |
| Rh | 16.55807500 | 12.68502500 | 14.47570000 |
| Rh | 10.33837500 | 16.07730000 | 14.04327500 |
| Rh | 11.68987500 | 11.21095000 | 14.27387500 |
| Rh | 16.91917500 | 15.14075000 | 13.49807500 |
| Rh | 14.64330000 | 16.49465000 | 13.37190000 |
| Rh | 12.27907500 | 17.66850000 | 13.21315000 |
| Rh | 14.32947500 | 11.48332500 | 13.84895000 |
| Rh | 10.55055000 | 13.52075000 | 13.65997500 |
| Rh | 11.93007500 | 8.62475000 | 14.00522500 |
| Rh | 9.52187500 | 9.91217500 | 13.80202500 |
| Rh | 14.78910000 | 13.92585000 | 12.97045000 |
| Rh | 14.56527500 | 8.89480000 | 13.57107500 |
| Rh | 12.44877500 | 15.19380000 | 12.81922500 |
| Rh | 8.33775000 | 12.29287500 | 13.16955000 |
| Rh | 16.48887500 | 10.61887500 | 12.70577500 |
| Rh | 12.64260000 | 12.72317500 | 12.43337500 |

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|----|-------------|-------------|-------------|
| Rh | 8.80105000 | 14.81640000 | 12.25375000 |
| Rh | 16.94660000 | 13.13522500 | 11.78812500 |
| Rh | 12.82322500 | 10.21177500 | 12.10055000 |
| Rh | 10.72050000 | 16.51457500 | 11.40027500 |
| Rh | 10.49745000 | 11.48910000 | 11.94965000 |
| Rh | 15.77167500 | 15.48665000 | 11.15477500 |
| Rh | 13.38842500 | 16.78672500 | 10.99967500 |
| Rh | 14.70835000 | 11.88860000 | 11.27132500 |
| Rh | 10.93320000 | 13.93487500 | 11.03385000 |
| Rh | 13.03120000 | 7.74410000 | 11.71002500 |
| Rh | 10.64302500 | 8.91965000 | 11.57117500 |
| Rh | 8.36262500 | 10.27895000 | 11.45867500 |
| Rh | 13.55237500 | 14.20915000 | 10.62252500 |
| Rh | 14.93617500 | 9.33305000 | 10.87162500 |
| Rh | 8.70227500 | 12.69805000 | 10.52252500 |
| Rh | 12.34065000 | 11.88610000 | 10.07922500 |
| Rh | 16.77155000 | 11.08672500 | 10.12207500 |
| Rh | 9.26162500 | 15.14257500 | 9.64427500 |
| Rh | 15.70360000 | 13.39372500 | 9.40695000 |
| Rh | 14.45692500 | 15.66705000 | 8.84902500 |
| Rh | 10.14415000 | 10.60347500 | 9.52540000 |
| Rh | 11.83582500 | 15.49767500 | 9.15987500 |
| Rh | 12.53177500 | 9.32160000 | 9.67915000 |
| Rh | 14.46632500 | 11.04542500 | 8.82855000 |
| Rh | 10.59655000 | 13.12312500 | 8.59880000 |
| Rh | 12.05552500 | 11.08167500 | 7.73570000 |
| Rh | 13.27007500 | 13.39085000 | 8.17727500 |

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|---|-------------|-------------|-------------|
| O | 8.32767500 | 11.74675000 | 17.18642500 |
| O | 13.59557500 | 11.00565000 | 17.48147500 |
| C | 8.45847500 | 9.86630000 | 18.10025000 |
| C | 9.68737500 | 9.18372500 | 18.02807500 |
| C | 9.94040000 | 8.08392500 | 17.12612500 |
| H | 8.18915000 | 10.38727500 | 19.01917500 |
| H | 7.62792500 | 9.54037500 | 17.47330000 |
| H | 8.71040000 | 12.30070000 | 17.89867500 |
| H | 10.42597500 | 9.39260000 | 18.80757500 |
| H | 9.09567500 | 7.62775000 | 16.59852500 |
| H | 10.73712500 | 7.38337500 | 17.39560000 |

4_RhoH

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|----|-------------|-------------|-------------|
| Rh | 11.62592500 | 11.34350000 | 16.65745000 |
| Rh | 12.77812500 | 13.81090000 | 17.30077500 |
| Rh | 14.31610000 | 11.78200000 | 16.35630000 |
| Rh | 10.49950000 | 13.84727500 | 16.08697500 |
| Rh | 10.51517500 | 9.20395000 | 15.57397500 |
| Rh | 14.81005000 | 14.35465000 | 15.74365000 |
| Rh | 12.43597500 | 15.61862500 | 15.53165000 |
| Rh | 13.22317500 | 9.47585000 | 15.47955000 |
| Rh | 9.33082500 | 11.56410000 | 15.27145000 |
| Rh | 15.88237500 | 9.87392500 | 15.08087500 |
| Rh | 8.26137500 | 13.89445000 | 14.62765000 |
| Rh | 12.66740000 | 13.13822500 | 14.85100000 |
| Rh | 16.31395000 | 12.39062500 | 14.66575000 |

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|----|-------------|-------------|-------------|
| Rh | 10.08445000 | 15.72372500 | 14.14652500 |
| Rh | 11.54010000 | 10.88490000 | 13.96965000 |
| Rh | 16.69970000 | 14.93972500 | 13.96152500 |
| Rh | 14.43042500 | 16.28917500 | 13.79180000 |
| Rh | 12.04240000 | 17.41107500 | 13.60577500 |
| Rh | 14.17885000 | 11.22725000 | 13.74945000 |
| Rh | 10.36177500 | 13.20492500 | 13.53902500 |
| Rh | 11.80305000 | 8.35085000 | 13.48387500 |
| Rh | 9.42617500 | 9.60125000 | 13.26732500 |
| Rh | 14.63575000 | 13.77697500 | 13.18442500 |
| Rh | 14.47785000 | 8.68807500 | 13.23887500 |
| Rh | 12.29337500 | 15.02322500 | 12.99717500 |
| Rh | 8.22682500 | 12.01500000 | 12.74410000 |
| Rh | 16.42390000 | 10.52017500 | 12.68190000 |
| Rh | 12.55275000 | 12.59372500 | 12.40070000 |
| Rh | 8.70490000 | 14.62162500 | 12.12700000 |
| Rh | 16.87330000 | 13.12067500 | 12.05660000 |
| Rh | 12.80792500 | 10.14127500 | 11.78010000 |
| Rh | 10.65495000 | 16.44262500 | 11.57662500 |
| Rh | 10.48052500 | 11.38290000 | 11.61367500 |
| Rh | 15.72712500 | 15.49827500 | 11.58047500 |
| Rh | 13.32035000 | 16.78177500 | 11.38300000 |
| Rh | 14.70115000 | 11.92232500 | 11.27900000 |
| Rh | 10.93432500 | 13.92390000 | 11.00040000 |
| Rh | 13.09882500 | 7.72470000 | 11.19082500 |
| Rh | 10.70782500 | 8.87162500 | 11.00172500 |
| Rh | 8.42352500 | 10.20212500 | 10.84192500 |

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|----|-------------|-------------|-------------|
| Rh | 13.55485000 | 14.25417500 | 10.79950000 |
| Rh | 15.02270000 | 9.41270000 | 10.63740000 |
| Rh | 8.77865000 | 12.70740000 | 10.17552500 |
| Rh | 12.43075000 | 12.00627500 | 9.94085000 |
| Rh | 16.86497500 | 11.26355000 | 10.19595000 |
| Rh | 9.32852500 | 15.24820000 | 9.61992500 |
| Rh | 15.79077500 | 13.61050000 | 9.62520000 |
| Rh | 14.55772500 | 15.90715000 | 9.21990000 |
| Rh | 10.31802500 | 10.75712500 | 9.08725000 |
| Rh | 11.92757500 | 15.65685000 | 9.31680000 |
| Rh | 12.71490000 | 9.48950000 | 9.28072500 |
| Rh | 14.64945000 | 11.31282500 | 8.74897500 |
| Rh | 10.78122500 | 13.36740000 | 8.46275000 |
| Rh | 12.31620000 | 11.43590000 | 7.50365000 |
| Rh | 13.47075000 | 13.69732500 | 8.25100000 |
| O | 8.19205000 | 11.12120000 | 17.10765000 |
| O | 13.32627500 | 10.34030000 | 17.27937500 |
| C | 9.03460000 | 11.25977500 | 18.30370000 |
| C | 10.29652500 | 10.45915000 | 18.10767500 |
| C | 10.12155000 | 9.08085000 | 17.62075000 |
| H | 9.26205000 | 12.32472500 | 18.47070000 |
| H | 8.44465000 | 10.86365000 | 19.15302500 |
| H | 7.46697500 | 11.77185000 | 17.15812500 |
| H | 10.97995000 | 10.57975000 | 18.96220000 |
| H | 9.08775000 | 8.69707500 | 17.59035000 |
| H | 10.84622500 | 8.35157500 | 18.00762500 |

4_RhonH_2

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|----|-------------|-------------|-------------|
| Rh | 11.49457500 | 11.38145000 | 16.81487500 |
| Rh | 12.87777500 | 13.72387500 | 17.29200000 |
| Rh | 14.39025000 | 11.81765000 | 16.34992500 |
| Rh | 10.47612500 | 13.88820000 | 16.14965000 |
| Rh | 10.59995000 | 9.19460000 | 15.67300000 |
| Rh | 14.84315000 | 14.39985000 | 15.74202500 |
| Rh | 12.53760000 | 15.68655000 | 15.51795000 |
| Rh | 13.16842500 | 9.55950000 | 15.57305000 |
| Rh | 9.27960000 | 11.56360000 | 15.26812500 |
| Rh | 15.78762500 | 9.90622500 | 15.21205000 |
| Rh | 8.24927500 | 13.91567500 | 14.67097500 |
| Rh | 12.70532500 | 13.13580000 | 14.87697500 |
| Rh | 16.34600000 | 12.41575000 | 14.61632500 |
| Rh | 10.13952500 | 15.70435000 | 14.23975000 |
| Rh | 11.55405000 | 10.90165000 | 14.08170000 |
| Rh | 16.77340000 | 14.91147500 | 13.84367500 |
| Rh | 14.48985000 | 16.26052500 | 13.78755000 |
| Rh | 12.10880000 | 17.41627500 | 13.60030000 |
| Rh | 14.19270000 | 11.21287500 | 13.82252500 |
| Rh | 10.39775000 | 13.20827500 | 13.61095000 |
| Rh | 11.76925000 | 8.34055000 | 13.52855000 |
| Rh | 9.42272500 | 9.61312500 | 13.35565000 |
| Rh | 14.67120000 | 13.75780000 | 13.19207500 |
| Rh | 14.44487500 | 8.69680000 | 13.30160000 |
| Rh | 12.33297500 | 15.02100000 | 13.01302500 |

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|----|-------------|-------------|-------------|
| Rh | 8.21560000 | 12.03572500 | 12.85162500 |
| Rh | 16.41192500 | 10.47050000 | 12.70172500 |
| Rh | 12.54867500 | 12.56452500 | 12.43322500 |
| Rh | 8.69152500 | 14.61490000 | 12.18362500 |
| Rh | 16.89410000 | 13.06760000 | 11.99990000 |
| Rh | 12.77752500 | 10.09350000 | 11.85370000 |
| Rh | 10.64642500 | 16.41080000 | 11.64090000 |
| Rh | 10.45970000 | 11.35292500 | 11.69185000 |
| Rh | 15.74260000 | 15.42752500 | 11.49135000 |
| Rh | 13.33710000 | 16.74227500 | 11.36780000 |
| Rh | 14.69560000 | 11.86450000 | 11.32007500 |
| Rh | 10.89790000 | 13.88487500 | 11.04945000 |
| Rh | 13.03830000 | 7.68072500 | 11.28160000 |
| Rh | 10.65747500 | 8.82610000 | 11.08980000 |
| Rh | 8.37625000 | 10.18682500 | 10.96145000 |
| Rh | 13.54632500 | 14.20217500 | 10.81350000 |
| Rh | 14.98210000 | 9.33827500 | 10.70985000 |
| Rh | 8.74037500 | 12.68112500 | 10.24810000 |
| Rh | 12.41485000 | 11.94727500 | 9.97972500 |
| Rh | 16.83682500 | 11.15617500 | 10.19070000 |
| Rh | 9.29862500 | 15.20715000 | 9.68587500 |
| Rh | 15.76575000 | 13.52040000 | 9.58772500 |
| Rh | 14.52025000 | 15.83797500 | 9.18397500 |
| Rh | 10.25427500 | 10.70787500 | 9.19335000 |
| Rh | 11.90112500 | 15.59710000 | 9.36765000 |
| Rh | 12.64260000 | 9.42840000 | 9.35030000 |
| Rh | 14.60995000 | 11.22272500 | 8.79470000 |

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|----|-------------|-------------|-------------|
| Rh | 10.73175000 | 13.30740000 | 8.52930000 |
| Rh | 12.25880000 | 11.35845000 | 7.57862500 |
| Rh | 13.42825000 | 13.61987500 | 8.27317500 |
| O | 8.10270000 | 10.89537500 | 17.02050000 |
| O | 11.06045000 | 13.09395000 | 17.88747500 |
| C | 8.84745000 | 11.03880000 | 18.28137500 |
| C | 10.17327500 | 10.32450000 | 18.16197500 |
| C | 10.13640000 | 8.94102500 | 17.67997500 |
| H | 8.99465000 | 12.10427500 | 18.50752500 |
| H | 8.22730000 | 10.56787500 | 19.06782500 |
| H | 7.29152500 | 11.43410000 | 17.07172500 |
| H | 10.79712500 | 10.50630000 | 19.05127500 |
| H | 9.13835000 | 8.48342500 | 17.56375000 |
| H | 10.88145000 | 8.26210000 | 18.11172500 |

TS3_Rh

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.20235000 | 11.35005000 | 16.68477500 |
| Rh | 12.32172500 | 13.77862500 | 17.28745000 |
| Rh | 13.92497500 | 11.83760000 | 16.49755000 |
| Rh | 10.01247500 | 13.89885000 | 15.99170000 |
| Rh | 10.17630000 | 9.21247500 | 15.50365000 |
| Rh | 14.41737500 | 14.35410000 | 15.87715000 |
| Rh | 12.16415000 | 15.70787500 | 15.44547500 |
| Rh | 12.85957500 | 9.45547500 | 15.53275000 |
| Rh | 9.01300000 | 11.55380000 | 14.98602500 |
| Rh | 15.45780000 | 9.88975000 | 15.43917500 |
| Rh | 7.97585000 | 13.87197500 | 14.30082500 |

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|----|-------------|-------------|-------------|
| Rh | 12.36545000 | 13.11322500 | 14.87247500 |
| Rh | 16.04050000 | 12.39425000 | 14.89175000 |
| Rh | 9.87552500 | 15.69400000 | 13.99552500 |
| Rh | 11.32377500 | 10.88382500 | 13.96532500 |
| Rh | 16.49267500 | 14.92840000 | 14.20745000 |
| Rh | 14.23337500 | 16.26647500 | 13.87755000 |
| Rh | 11.86262500 | 17.41980000 | 13.49172500 |
| Rh | 13.94635000 | 11.20505000 | 13.94307500 |
| Rh | 10.19760000 | 13.20992500 | 13.39967500 |
| Rh | 11.57560000 | 8.34120000 | 13.40797500 |
| Rh | 9.24020000 | 9.59912500 | 13.12045000 |
| Rh | 14.47152500 | 13.74090000 | 13.34132500 |
| Rh | 14.28577500 | 8.69315000 | 13.41417500 |
| Rh | 12.15382500 | 14.99870000 | 12.96455000 |
| Rh | 8.10415000 | 11.99267500 | 12.48165000 |
| Rh | 16.26395000 | 10.46567500 | 12.99312500 |
| Rh | 12.43667500 | 12.55650000 | 12.40987500 |
| Rh | 8.60487500 | 14.57982500 | 11.84337500 |
| Rh | 16.79322500 | 13.08840000 | 12.36380000 |
| Rh | 12.72595000 | 10.09807500 | 11.85875000 |
| Rh | 10.57547500 | 16.39102500 | 11.45450000 |
| Rh | 10.41012500 | 11.33815000 | 11.49530000 |
| Rh | 15.67840000 | 15.44220000 | 11.75000000 |
| Rh | 13.28155000 | 16.73550000 | 11.37787500 |
| Rh | 14.68420000 | 11.87577500 | 11.48147500 |
| Rh | 10.91357500 | 13.87337500 | 10.89257500 |
| Rh | 13.03182500 | 7.66735000 | 11.31110000 |

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|----|-------------|-------------|-------------|
| Rh | 10.65432500 | 8.80535000 | 10.93297500 |
| Rh | 8.39412500 | 10.15515000 | 10.61080000 |
| Rh | 13.56505000 | 14.19797500 | 10.87682500 |
| Rh | 15.01285000 | 9.34892500 | 10.88312500 |
| Rh | 8.80205000 | 12.65990000 | 9.93587500 |
| Rh | 12.49167500 | 11.93202500 | 9.95497500 |
| Rh | 16.89420000 | 11.18082500 | 10.52695000 |
| Rh | 9.41400000 | 15.19377500 | 9.39330000 |
| Rh | 15.86020000 | 13.51860000 | 9.84672500 |
| Rh | 14.65847500 | 15.81907500 | 9.32440000 |
| Rh | 10.40075000 | 10.69127500 | 8.99505000 |
| Rh | 12.03460000 | 15.58627500 | 9.29152500 |
| Rh | 12.76707500 | 9.40642500 | 9.36112500 |
| Rh | 14.76492500 | 11.21077500 | 8.94805000 |
| Rh | 10.91600000 | 13.28375000 | 8.37137500 |
| Rh | 12.54262500 | 11.33172500 | 7.55217500 |
| Rh | 13.61795000 | 13.60592500 | 8.33333333 |
| O | 8.87590000 | 11.25707500 | 18.56825000 |
| O | 10.37777500 | 14.08125000 | 17.89577500 |
| C | 10.22730000 | 10.96675000 | 18.58127500 |
| C | 10.63482500 | 9.68077500 | 18.11742500 |
| C | 9.74405000 | 8.73045000 | 17.47702500 |
| H | 10.76715000 | 12.65742500 | 17.69700000 |
| H | 10.79720000 | 11.42917500 | 19.39592500 |
| H | 8.77032500 | 12.22585000 | 18.66087500 |
| H | 11.60167500 | 9.32355000 | 18.48050000 |
| H | 8.66965000 | 8.91575000 | 17.60195000 |

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|---|-------------|------------|-------------|
| H | 10.03785000 | 7.67602500 | 17.56677500 |
|---|-------------|------------|-------------|

5_Rh

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.32545000 | 11.23917500 | 16.58715000 |
| Rh | 12.32397500 | 13.62940000 | 17.30032500 |
| Rh | 13.97942500 | 11.74362500 | 16.47080000 |
| Rh | 10.09900000 | 13.72195000 | 15.95562500 |
| Rh | 10.21200000 | 9.14672500 | 15.47072500 |
| Rh | 14.45412500 | 14.27935000 | 15.87527500 |
| Rh | 12.14290000 | 15.58755000 | 15.49335000 |
| Rh | 12.91002500 | 9.38397500 | 15.44500000 |
| Rh | 9.02797500 | 11.43357500 | 14.95947500 |
| Rh | 15.50757500 | 9.80832500 | 15.34780000 |
| Rh | 8.00352500 | 13.80212500 | 14.36480000 |
| Rh | 12.39352500 | 13.01687500 | 14.88967500 |
| Rh | 16.05970000 | 12.33107500 | 14.85277500 |
| Rh | 9.85140000 | 15.65202500 | 14.02912500 |
| Rh | 11.32697500 | 10.80787500 | 13.90452500 |
| Rh | 16.46910000 | 14.90357500 | 14.22025000 |
| Rh | 14.21017500 | 16.22472500 | 13.93772500 |
| Rh | 11.84507500 | 17.35982500 | 13.59830000 |
| Rh | 13.96135000 | 11.16605000 | 13.88965000 |
| Rh | 10.20345000 | 13.17317500 | 13.42617500 |
| Rh | 11.62282500 | 8.28165000 | 13.33572500 |
| Rh | 9.26000000 | 9.52735000 | 13.06520000 |
| Rh | 14.46827500 | 13.72307500 | 13.32830000 |

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|----|-------------|-------------|-------------|
| Rh | 14.31947500 | 8.64160000 | 13.31937500 |
| Rh | 12.14190000 | 14.94855000 | 13.01195000 |
| Rh | 8.12472500 | 11.94125000 | 12.47247500 |
| Rh | 16.28367500 | 10.45497500 | 12.92290000 |
| Rh | 12.43732500 | 12.52465000 | 12.39522500 |
| Rh | 8.59412500 | 14.53550000 | 11.88607500 |
| Rh | 16.79102500 | 13.06975000 | 12.34240000 |
| Rh | 12.75340000 | 10.07962500 | 11.79152500 |
| Rh | 10.56337500 | 16.36987500 | 11.51260000 |
| Rh | 10.41665000 | 11.28660000 | 11.46665000 |
| Rh | 15.65252500 | 15.43897500 | 11.77517500 |
| Rh | 13.24232500 | 16.72545000 | 11.43975000 |
| Rh | 14.68245000 | 11.86185000 | 11.43670000 |
| Rh | 10.89580000 | 13.85842500 | 10.91282500 |
| Rh | 13.07347500 | 7.66982500 | 11.18742500 |
| Rh | 10.69882500 | 8.79700000 | 10.84827500 |
| Rh | 8.41540000 | 10.12087500 | 10.56420000 |
| Rh | 13.54282500 | 14.20237500 | 10.88702500 |
| Rh | 15.02500000 | 9.36060000 | 10.77620000 |
| Rh | 8.79532500 | 12.64237500 | 9.94282500 |
| Rh | 12.46455000 | 11.96612500 | 9.93232500 |
| Rh | 16.88882500 | 11.20382500 | 10.46605000 |
| Rh | 9.37500000 | 15.19590000 | 9.44932500 |
| Rh | 15.85297500 | 13.54972500 | 9.84142500 |
| Rh | 14.64000000 | 15.86360000 | 9.37152500 |
| Rh | 10.40022500 | 10.70540000 | 8.93950000 |
| Rh | 12.00635000 | 15.61052500 | 9.32380000 |

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|----|-------------|-------------|-------------|
| Rh | 12.78900000 | 9.46465000 | 9.25980000 |
| Rh | 14.76175000 | 11.27207500 | 8.89092500 |
| Rh | 10.89790000 | 13.33225000 | 8.37715000 |
| Rh | 12.51470000 | 11.42100000 | 7.49932500 |
| Rh | 13.60880000 | 13.66325000 | 8.33740000 |
| O | 9.27195000 | 11.57515000 | 18.64787500 |
| O | 10.29287500 | 14.06100000 | 18.02987500 |
| C | 10.53772500 | 11.05985000 | 18.54977500 |
| C | 10.74647500 | 9.71810000 | 18.10822500 |
| C | 9.73782500 | 8.87022500 | 17.49437500 |
| H | 10.15412500 | 15.00787500 | 18.22215000 |
| H | 11.27962500 | 11.49880000 | 19.23197500 |
| H | 9.37500000 | 12.56375000 | 18.63565000 |
| H | 11.68067500 | 9.25050000 | 18.43040000 |
| H | 8.69787500 | 9.19697500 | 17.62092500 |
| H | 9.88855000 | 7.78947500 | 17.62797500 |

6_Rh

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.77762500 | 11.21312500 | 16.64150000 |
| Rh | 12.94370000 | 13.58875000 | 17.32640000 |
| Rh | 14.39697500 | 11.66602500 | 16.32445000 |
| Rh | 10.60990000 | 13.77462500 | 16.13455000 |
| Rh | 10.72427500 | 9.04525000 | 15.60222500 |
| Rh | 14.88285000 | 14.28017500 | 15.71090000 |
| Rh | 12.49657500 | 15.53097500 | 15.59000000 |
| Rh | 13.33630000 | 9.35807500 | 15.39057500 |

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|----|-------------|-------------|-------------|
| Rh | 9.42835000 | 11.40672500 | 15.32487500 |
| Rh | 15.90942500 | 9.82337500 | 15.09340000 |
| Rh | 8.29925000 | 13.74922500 | 14.72122500 |
| Rh | 12.74550000 | 13.02287500 | 14.87700000 |
| Rh | 16.41105000 | 12.34672500 | 14.57155000 |
| Rh | 10.11962500 | 15.62217500 | 14.26560000 |
| Rh | 11.63677500 | 10.78965000 | 13.99910000 |
| Rh | 16.73987500 | 14.90812500 | 13.94520000 |
| Rh | 14.43407500 | 16.22707500 | 13.84220000 |
| Rh | 12.05775000 | 17.35240000 | 13.69395000 |
| Rh | 14.26877500 | 11.16170000 | 13.75992500 |
| Rh | 10.41762500 | 13.13037500 | 13.60602500 |
| Rh | 11.91202500 | 8.25372500 | 13.40550000 |
| Rh | 9.52692500 | 9.48915000 | 13.28840000 |
| Rh | 14.68212500 | 13.72507500 | 13.18932500 |
| Rh | 14.58590000 | 8.64432500 | 13.13057500 |
| Rh | 12.31450000 | 14.93452500 | 13.04750000 |
| Rh | 8.29345000 | 11.86447500 | 12.84995000 |
| Rh | 16.49160000 | 10.47867500 | 12.60517500 |
| Rh | 12.62005000 | 12.50987500 | 12.40702500 |
| Rh | 8.71262500 | 14.52212500 | 12.25075000 |
| Rh | 16.91935000 | 13.10412500 | 12.01407500 |
| Rh | 12.88987500 | 10.07822500 | 11.77992500 |
| Rh | 10.62182500 | 16.35930000 | 11.68665000 |
| Rh | 10.52832500 | 11.28887500 | 11.65052500 |
| Rh | 15.70830000 | 15.47792500 | 11.56765000 |
| Rh | 13.28315000 | 16.74480000 | 11.44912500 |

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|----|-------------|-------------|-------------|
| Rh | 14.76980000 | 11.87287500 | 11.24997500 |
| Rh | 10.93335000 | 13.84495000 | 11.06782500 |
| Rh | 13.18275000 | 7.66840000 | 11.10507500 |
| Rh | 10.77160000 | 8.77202500 | 10.99040000 |
| Rh | 8.47215000 | 10.09102500 | 10.90372500 |
| Rh | 13.55482500 | 14.22762500 | 10.83017500 |
| Rh | 15.06050000 | 9.37757500 | 10.53462500 |
| Rh | 8.77307500 | 12.63052500 | 10.29050000 |
| Rh | 12.44722500 | 11.98505000 | 9.95472500 |
| Rh | 16.86982500 | 11.27167500 | 10.10267500 |
| Rh | 9.27390000 | 15.15835000 | 9.73327500 |
| Rh | 15.76247500 | 13.61630000 | 9.59620000 |
| Rh | 14.52035000 | 15.91050000 | 9.25242500 |
| Rh | 10.32610000 | 10.71207500 | 9.13247500 |
| Rh | 11.87657500 | 15.62185000 | 9.41052500 |
| Rh | 12.71325000 | 9.48005000 | 9.24507500 |
| Rh | 14.61980000 | 11.31505000 | 8.69742500 |
| Rh | 10.73625000 | 13.33370000 | 8.53100000 |
| Rh | 12.27837500 | 11.44330000 | 7.50272500 |
| Rh | 13.40965000 | 13.71142500 | 8.26985000 |
| O | 8.01270000 | 11.02862500 | 16.85827500 |
| O | 6.73097500 | 13.21780000 | 16.14827500 |
| C | 9.12707500 | 11.42210000 | 17.48230000 |
| C | 10.16680000 | 10.48847500 | 17.91940000 |
| C | 10.03127500 | 9.07117500 | 17.58067500 |
| H | 9.12015000 | 12.41770000 | 17.96060000 |
| H | 10.71467500 | 10.77937500 | 18.83042500 |

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|---|-------------|-------------|-------------|
| H | 9.00050000 | 8.72705000 | 17.38825000 |
| H | 10.62470000 | 8.38227500 | 18.19235000 |
| H | 7.09760000 | 12.33240000 | 16.51872500 |
| H | 6.62065000 | 13.82945000 | 16.89850000 |

TS1_Rh

| | | | |
|----|-------------|-------------|-------------|
| Rh | 12.11727500 | 11.60797500 | 16.84657500 |
| Rh | 13.26265000 | 14.10627500 | 17.21555000 |
| Rh | 14.74960000 | 12.06495000 | 16.24265000 |
| Rh | 10.77880000 | 14.08290000 | 16.20730000 |
| Rh | 10.86702500 | 9.34035000 | 15.95830000 |
| Rh | 15.07577500 | 14.62965000 | 15.47017500 |
| Rh | 12.65402500 | 15.81820000 | 15.40822500 |
| Rh | 13.57740000 | 9.71010000 | 15.61162500 |
| Rh | 9.61502500 | 11.64942500 | 15.51217500 |
| Rh | 16.22252500 | 10.13107500 | 14.98202500 |
| Rh | 8.41505000 | 14.00010000 | 14.88715000 |
| Rh | 12.91125000 | 13.31727500 | 14.81885000 |
| Rh | 16.57307500 | 12.64795000 | 14.37827500 |
| Rh | 10.21457500 | 15.80120000 | 14.26195000 |
| Rh | 11.79737500 | 11.02375000 | 14.17607500 |
| Rh | 16.80792500 | 15.17852500 | 13.52217500 |
| Rh | 14.50245000 | 16.44727500 | 13.49027500 |
| Rh | 12.09897500 | 17.52165000 | 13.42432500 |
| Rh | 14.38757500 | 11.39395000 | 13.70187500 |
| Rh | 10.55575000 | 13.29820000 | 13.66747500 |

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|----|-------------|-------------|-------------|
| Rh | 12.03407500 | 8.46647500 | 13.81935000 |
| Rh | 9.64292500 | 9.67287500 | 13.72122500 |
| Rh | 14.72137500 | 13.91060000 | 12.97487500 |
| Rh | 14.68895000 | 8.83187500 | 13.33597500 |
| Rh | 12.35532500 | 15.09547500 | 12.91372500 |
| Rh | 8.34090000 | 11.99507500 | 13.21942500 |
| Rh | 16.54482500 | 10.66907500 | 12.51135000 |
| Rh | 12.62962500 | 12.64760000 | 12.40725000 |
| Rh | 8.69360000 | 14.56017500 | 12.39097500 |
| Rh | 16.87892500 | 13.22927500 | 11.70662500 |
| Rh | 12.87290000 | 10.15862500 | 11.94770000 |
| Rh | 10.55257500 | 16.39167500 | 11.59145000 |
| Rh | 10.52722500 | 11.33995000 | 11.89170000 |
| Rh | 15.63335000 | 15.55545000 | 11.19880000 |
| Rh | 13.18530000 | 16.78242500 | 11.14522500 |
| Rh | 14.68002500 | 11.94522500 | 11.16472500 |
| Rh | 10.86127500 | 13.85532500 | 11.10992500 |
| Rh | 13.15190000 | 7.71872500 | 11.46952500 |
| Rh | 10.74355000 | 8.78465000 | 11.39517500 |
| Rh | 8.42495000 | 10.06297500 | 11.39020000 |
| Rh | 13.44925000 | 14.22952500 | 10.65917500 |
| Rh | 14.99505000 | 9.42040000 | 10.65855000 |
| Rh | 8.67370000 | 12.55632500 | 10.55382500 |
| Rh | 12.29990000 | 11.90820000 | 10.02292500 |
| Rh | 16.76077500 | 11.25322500 | 9.93885000 |
| Rh | 9.09935000 | 15.06980000 | 9.82417500 |
| Rh | 15.60440000 | 13.55657500 | 9.35002500 |

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|----|-------------|-------------|-------------|
| Rh | 14.26665000 | 15.80097500 | 8.92557500 |
| Rh | 10.13917500 | 10.56690000 | 9.45715000 |
| Rh | 11.65760000 | 15.51877500 | 9.27957500 |
| Rh | 12.58082500 | 9.36987500 | 9.49432500 |
| Rh | 14.43335000 | 11.19550000 | 8.69157500 |
| Rh | 10.48697500 | 13.14860000 | 8.63402500 |
| Rh | 11.99527500 | 11.20980000 | 7.65015000 |
| Rh | 13.14165000 | 13.52795000 | 8.17337500 |
| O | 10.26767500 | 12.28832500 | 17.37310000 |
| O | 13.81085000 | 10.68360000 | 17.33925000 |
| C | 9.25635000 | 10.49695000 | 18.98545000 |
| C | 10.05162500 | 9.41527500 | 18.59235000 |
| C | 9.77085000 | 8.48277500 | 17.54422500 |
| H | 9.46050000 | 10.96180000 | 19.95432500 |
| H | 8.21812500 | 10.54155000 | 18.63880000 |
| H | 9.81040000 | 11.57790000 | 18.16130000 |
| H | 11.00502500 | 9.28352500 | 19.11735000 |
| H | 8.73172500 | 8.42637500 | 17.19335000 |
| H | 10.27105000 | 7.50660000 | 17.61795000 |

TS2_Rh_O

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|----|-------------|-------------|-------------|
| Rh | 11.65612500 | 11.63230000 | 16.68095000 |
| Rh | 12.77892500 | 14.05495000 | 17.31115000 |
| Rh | 14.33530000 | 12.06605000 | 16.46317500 |
| Rh | 10.45097500 | 13.95560000 | 16.15792500 |
| Rh | 10.49367500 | 9.32355000 | 15.83302500 |

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|----|-------------|-------------|-------------|
| Rh | 14.72957500 | 14.61515000 | 15.70000000 |
| Rh | 12.28847500 | 15.79147500 | 15.47112500 |
| Rh | 13.20735000 | 9.68410000 | 15.63565000 |
| Rh | 9.26137500 | 11.58762500 | 15.32130000 |
| Rh | 15.87205000 | 10.15680000 | 15.32255000 |
| Rh | 8.18650000 | 13.99740000 | 14.55495000 |
| Rh | 12.60715000 | 13.29407500 | 14.89422500 |
| Rh | 16.30897500 | 12.64985000 | 14.70095000 |
| Rh | 9.97267500 | 15.82967500 | 14.04272500 |
| Rh | 11.51812500 | 11.01720000 | 14.11545000 |
| Rh | 16.63370000 | 15.15590000 | 13.91737500 |
| Rh | 14.31747500 | 16.43132500 | 13.71667500 |
| Rh | 11.92045000 | 17.49827500 | 13.45377500 |
| Rh | 14.18007500 | 11.37485000 | 13.90872500 |
| Rh | 10.35072500 | 13.30485000 | 13.52437500 |
| Rh | 11.81227500 | 8.44080000 | 13.68525000 |
| Rh | 9.40220000 | 9.70762500 | 13.52337500 |
| Rh | 14.59590000 | 13.89680000 | 13.19220000 |
| Rh | 14.50720000 | 8.81342500 | 13.50250000 |
| Rh | 12.23340000 | 15.08045000 | 12.96705000 |
| Rh | 8.19325000 | 12.01117500 | 12.78195000 |
| Rh | 16.43762500 | 10.67497500 | 12.86802500 |
| Rh | 12.54507500 | 12.64210000 | 12.45040000 |
| Rh | 8.59542500 | 14.57930000 | 12.11240000 |
| Rh | 16.85975000 | 13.25307500 | 12.09097500 |
| Rh | 12.83097500 | 10.16285000 | 11.98647500 |
| Rh | 10.54472500 | 16.37992500 | 11.47435000 |

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|----|-------------|-------------|-------------|
| Rh | 10.47457500 | 11.35450000 | 11.74662500 |
| Rh | 15.62500000 | 15.57842500 | 11.50565000 |
| Rh | 13.20527500 | 16.79032500 | 11.27092500 |
| Rh | 14.71420000 | 11.95162500 | 11.38470000 |
| Rh | 10.87870000 | 13.87100000 | 10.99550000 |
| Rh | 13.13900000 | 7.73745000 | 11.48020000 |
| Rh | 10.71250000 | 8.83202500 | 11.25260000 |
| Rh | 8.43032500 | 10.12235000 | 10.99660000 |
| Rh | 13.51517500 | 14.24342500 | 10.79362500 |
| Rh | 15.04850000 | 9.41805000 | 10.88405000 |
| Rh | 8.76245000 | 12.60927500 | 10.22462500 |
| Rh | 12.42602500 | 11.94292500 | 10.04052500 |
| Rh | 16.86757500 | 11.26475000 | 10.33200000 |
| Rh | 9.29237500 | 15.10745000 | 9.51985000 |
| Rh | 15.76902500 | 13.58005000 | 9.64910000 |
| Rh | 14.47672500 | 15.84847500 | 9.14122500 |
| Rh | 10.31500000 | 10.63802500 | 9.24015000 |
| Rh | 11.86110000 | 15.54587500 | 9.24965000 |
| Rh | 12.71420000 | 9.41610000 | 9.50502500 |
| Rh | 14.65847500 | 11.23697500 | 8.89677500 |
| Rh | 10.77617500 | 13.20850000 | 8.47455000 |
| Rh | 12.33737500 | 11.25257500 | 7.63812500 |
| Rh | 13.44550000 | 13.58070000 | 8.27375000 |
| O | 8.43305000 | 13.14665000 | 16.55920000 |
| O | 13.01860000 | 10.40912500 | 17.50725000 |
| C | 12.13067500 | 9.01257500 | 18.51457500 |
| C | 11.22732500 | 8.24725000 | 17.72085000 |

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|---|-------------|-------------|-------------|
| C | 9.81685000 | 8.50482500 | 17.62822500 |
| H | 13.08090000 | 8.55935000 | 18.79932500 |
| H | 11.71972500 | 9.72622500 | 19.23182500 |
| H | 7.95292500 | 13.04850000 | 17.40162500 |
| H | 11.61552500 | 7.30657500 | 17.31607500 |
| H | 9.38002500 | 9.27072500 | 18.27797500 |
| H | 9.14567500 | 7.67290000 | 17.38832500 |

4_Rho

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.88070000 | 11.51792500 | 16.77080000 |
| Rh | 12.94332500 | 13.96120000 | 17.32305000 |
| Rh | 14.50085000 | 12.09732500 | 16.36412500 |
| Rh | 10.58992500 | 13.81077500 | 16.24172500 |
| Rh | 10.64202500 | 9.29360000 | 15.82030000 |
| Rh | 14.83990000 | 14.62117500 | 15.65262500 |
| Rh | 12.35662500 | 15.74567500 | 15.50032500 |
| Rh | 13.32512500 | 9.62450000 | 15.70657500 |
| Rh | 9.32827500 | 11.52685000 | 15.36027500 |
| Rh | 15.96460000 | 10.15482500 | 15.27342500 |
| Rh | 8.26432500 | 13.96440000 | 14.67042500 |
| Rh | 12.71202500 | 13.26057500 | 14.91342500 |
| Rh | 16.43077500 | 12.65660000 | 14.59997500 |
| Rh | 10.03035000 | 15.80652500 | 14.13947500 |
| Rh | 11.61430000 | 10.98550000 | 14.17787500 |
| Rh | 16.70052500 | 15.18042500 | 13.82047500 |
| Rh | 14.35332500 | 16.42932500 | 13.71037500 |

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|----|-------------|-------------|-------------|
| Rh | 11.94575000 | 17.48820000 | 13.50475000 |
| Rh | 14.26205000 | 11.37202500 | 13.89202500 |
| Rh | 10.41835000 | 13.28132500 | 13.59470000 |
| Rh | 11.87815000 | 8.43240000 | 13.66782500 |
| Rh | 9.45787500 | 9.67767500 | 13.54047500 |
| Rh | 14.65805000 | 13.90542500 | 13.16710000 |
| Rh | 14.55610000 | 8.82897500 | 13.49322500 |
| Rh | 12.26367500 | 15.08015000 | 12.98910000 |
| Rh | 8.23427500 | 11.98287500 | 12.89162500 |
| Rh | 16.48435000 | 10.66395000 | 12.77540000 |
| Rh | 12.59325000 | 12.64415000 | 12.46847500 |
| Rh | 8.62477500 | 14.54937500 | 12.22935000 |
| Rh | 16.88245000 | 13.26315000 | 12.00177500 |
| Rh | 12.87512500 | 10.17630000 | 12.00005000 |
| Rh | 10.53292500 | 16.36035000 | 11.55655000 |
| Rh | 10.51847500 | 11.34427500 | 11.80802500 |
| Rh | 15.63080000 | 15.59905000 | 11.45577500 |
| Rh | 13.19480000 | 16.79390000 | 11.26695000 |
| Rh | 14.73095000 | 11.96312500 | 11.34277500 |
| Rh | 10.88320000 | 13.85210000 | 11.05172500 |
| Rh | 13.16352500 | 7.73315000 | 11.47882500 |
| Rh | 10.74230000 | 8.81420000 | 11.28150000 |
| Rh | 8.44375000 | 10.10257500 | 11.07060000 |
| Rh | 13.50965000 | 14.25967500 | 10.79217500 |
| Rh | 15.05130000 | 9.41690000 | 10.84672500 |
| Rh | 8.75282500 | 12.59525000 | 10.33300000 |
| Rh | 12.40917500 | 11.95260000 | 10.06082500 |

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|----|-------------|-------------|-------------|
| Rh | 16.85030000 | 11.28002500 | 10.23485000 |
| Rh | 9.24865000 | 15.09142500 | 9.61637500 |
| Rh | 15.72615000 | 13.59705000 | 9.58355000 |
| Rh | 14.42772500 | 15.86180000 | 9.12432500 |
| Rh | 10.28965000 | 10.62657500 | 9.30742500 |
| Rh | 11.80730000 | 15.53815000 | 9.29035000 |
| Rh | 12.69492500 | 9.41972500 | 9.51192500 |
| Rh | 14.60845000 | 11.24182500 | 8.86190000 |
| Rh | 10.71065000 | 13.20627500 | 8.52997500 |
| Rh | 12.26925000 | 11.24922500 | 7.65565000 |
| Rh | 13.37212500 | 13.58745000 | 8.26655000 |
| O | 8.59220000 | 13.07817500 | 16.67055000 |
| O | 12.87972500 | 9.91910000 | 17.72330000 |
| C | 12.06525000 | 8.92065000 | 18.39677500 |
| C | 11.20930000 | 8.08175000 | 17.47260000 |
| C | 9.79530000 | 8.17415000 | 17.43140000 |
| H | 12.77235000 | 8.27897500 | 18.95265000 |
| H | 11.44025000 | 9.45867500 | 19.12872500 |
| H | 8.18080000 | 12.94135000 | 17.54377500 |
| H | 11.69272500 | 7.18090000 | 17.07800000 |
| H | 9.26692500 | 8.84672500 | 18.11390000 |
| H | 9.19970000 | 7.34970000 | 17.03110000 |

TS3_Rh_S

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|----|-------------|-------------|-------------|
| Rh | 11.28032500 | 11.44385000 | 16.80920000 |
| Rh | 12.77837500 | 13.93262500 | 17.24445000 |

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|----|-------------|-------------|-------------|
| Rh | 14.17320000 | 11.84152500 | 16.42322500 |
| Rh | 10.39552500 | 13.95700000 | 16.07170000 |
| Rh | 10.46045000 | 9.19880000 | 15.60635000 |
| Rh | 14.75892500 | 14.42557500 | 15.72152500 |
| Rh | 12.49420000 | 15.77072500 | 15.43272500 |
| Rh | 13.03722500 | 9.58832500 | 15.60612500 |
| Rh | 9.11047500 | 11.59555000 | 15.12930000 |
| Rh | 15.64665000 | 9.92085000 | 15.35015000 |
| Rh | 8.19712500 | 14.00852500 | 14.52647500 |
| Rh | 12.62100000 | 13.17705000 | 14.85742500 |
| Rh | 16.25787500 | 12.41320000 | 14.71680000 |
| Rh | 10.10000000 | 15.76010000 | 14.12367500 |
| Rh | 11.45472500 | 10.92222500 | 14.05587500 |
| Rh | 16.73670000 | 14.90877500 | 13.92552500 |
| Rh | 14.46682500 | 16.28897500 | 13.74625000 |
| Rh | 12.07172500 | 17.45472500 | 13.48662500 |
| Rh | 14.11320000 | 11.22932500 | 13.88995000 |
| Rh | 10.38057500 | 13.27462500 | 13.52622500 |
| Rh | 11.66687500 | 8.34455000 | 13.51905000 |
| Rh | 9.34735000 | 9.64892500 | 13.29590000 |
| Rh | 14.63895000 | 13.74955000 | 13.21032500 |
| Rh | 14.35460000 | 8.69787500 | 13.41510000 |
| Rh | 12.31427500 | 15.02055000 | 12.94800000 |
| Rh | 8.19627500 | 12.08372500 | 12.72357500 |
| Rh | 16.35887500 | 10.44205000 | 12.83575000 |
| Rh | 12.54355000 | 12.56252500 | 12.41612500 |
| Rh | 8.70372500 | 14.65050000 | 12.04105000 |

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|----|-------------|-------------|-------------|
| Rh | 16.90360000 | 13.01242500 | 12.13730000 |
| Rh | 12.77045000 | 10.09812500 | 11.90120000 |
| Rh | 10.69432500 | 16.42387500 | 11.51425000 |
| Rh | 10.45127500 | 11.37542500 | 11.64517500 |
| Rh | 15.76615000 | 15.39622500 | 11.54665000 |
| Rh | 13.39377500 | 16.73655000 | 11.32295000 |
| Rh | 14.72030000 | 11.82277500 | 11.36200000 |
| Rh | 10.93610000 | 13.87852500 | 10.98565000 |
| Rh | 13.02342500 | 7.64765000 | 11.37015000 |
| Rh | 10.63895000 | 8.83420000 | 11.06560000 |
| Rh | 8.35665000 | 10.21672500 | 10.85717500 |
| Rh | 13.59600000 | 14.17087500 | 10.79487500 |
| Rh | 14.96122500 | 9.27742500 | 10.81732500 |
| Rh | 8.77162500 | 12.70287500 | 10.13900000 |
| Rh | 12.43092500 | 11.89735000 | 9.97190000 |
| Rh | 16.84802500 | 11.08887500 | 10.30867500 |
| Rh | 9.38992500 | 15.20682500 | 9.54737500 |
| Rh | 15.84867500 | 13.43872500 | 9.68045000 |
| Rh | 14.63807500 | 15.74755000 | 9.17852500 |
| Rh | 10.27690000 | 10.68982500 | 9.14630000 |
| Rh | 11.99970000 | 15.56432500 | 9.31197500 |
| Rh | 12.64327500 | 9.36832500 | 9.39090000 |
| Rh | 14.64277500 | 11.13965000 | 8.86105000 |
| Rh | 10.81997500 | 13.27442500 | 8.46592500 |
| Rh | 12.34557500 | 11.30207500 | 7.57720000 |
| Rh | 13.51697500 | 13.55427500 | 8.27995000 |
| O | 8.10642500 | 10.24180000 | 18.11480000 |

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|---|-------------|-------------|-------------|
| O | 11.01117500 | 13.21410000 | 17.83745000 |
| C | 9.33255000 | 10.90275000 | 18.18517500 |
| C | 10.49982500 | 10.01475000 | 18.24065000 |
| C | 10.39350000 | 8.68720000 | 17.64120000 |
| H | 9.32735000 | 11.55277500 | 16.97742500 |
| H | 9.35800000 | 11.78060000 | 18.84670000 |
| H | 7.40620000 | 10.89117500 | 17.90977500 |
| H | 11.21535000 | 10.18340000 | 19.05205000 |
| H | 9.38807500 | 8.23410000 | 17.63965000 |
| H | 11.18452500 | 7.98297500 | 17.91975000 |

5_Rh_S

| | | | |
|----|-------------|-------------|-------------|
| Rh | 11.48510000 | 11.45955000 | 16.75747500 |
| Rh | 12.68835000 | 13.88730000 | 17.25170000 |
| Rh | 14.27392500 | 11.92552500 | 16.43295000 |
| Rh | 10.27885000 | 13.84760000 | 16.08920000 |
| Rh | 10.49827500 | 9.23550000 | 15.73285000 |
| Rh | 14.71217500 | 14.48012500 | 15.76807500 |
| Rh | 12.37345000 | 15.72585000 | 15.42270000 |
| Rh | 13.14390000 | 9.60882500 | 15.65962500 |
| Rh | 9.17035000 | 11.50440000 | 15.11947500 |
| Rh | 15.76087500 | 10.01415000 | 15.38775000 |
| Rh | 8.15552500 | 13.88112500 | 14.43817500 |
| Rh | 12.63040000 | 13.18407500 | 14.85492500 |

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|----|-------------|-------------|-------------|
| Rh | 16.27597500 | 12.52975000 | 14.74620000 |
| Rh | 10.02617500 | 15.65125000 | 14.07272500 |
| Rh | 11.52907500 | 10.90260000 | 14.10282500 |
| Rh | 16.68462500 | 15.00997500 | 13.91057500 |
| Rh | 14.37027500 | 16.29217500 | 13.73937500 |
| Rh | 11.97067500 | 17.39067500 | 13.43750000 |
| Rh | 14.18645000 | 11.25347500 | 13.90730000 |
| Rh | 10.37667500 | 13.17765000 | 13.50030000 |
| Rh | 11.79660000 | 8.35040000 | 13.63567500 |
| Rh | 9.44462500 | 9.54765000 | 13.33462500 |
| Rh | 14.63170000 | 13.78327500 | 13.21092500 |
| Rh | 14.49530000 | 8.72402500 | 13.48057500 |
| Rh | 12.27075000 | 14.98607500 | 12.91862500 |
| Rh | 8.23222500 | 11.92412500 | 12.68290000 |
| Rh | 16.45865000 | 10.53175000 | 12.89760000 |
| Rh | 12.56425000 | 12.52947500 | 12.41685000 |
| Rh | 8.66585000 | 14.48437500 | 11.98460000 |
| Rh | 16.91025000 | 13.09920000 | 12.12607500 |
| Rh | 12.85650000 | 10.04715000 | 11.94985000 |
| Rh | 10.62212500 | 16.30425000 | 11.44897500 |
| Rh | 10.51067500 | 11.24557500 | 11.65370000 |
| Rh | 15.71985000 | 15.43007500 | 11.51655000 |
| Rh | 13.30845000 | 16.67980000 | 11.25970000 |
| Rh | 14.76362500 | 11.82930000 | 11.39590000 |
| Rh | 10.92402500 | 13.77110000 | 10.94932500 |
| Rh | 13.15642500 | 7.61937500 | 11.47100000 |
| Rh | 10.76347500 | 8.71635000 | 11.11367500 |

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|----|-------------|-------------|-------------|
| Rh | 8.46995000 | 10.03910000 | 10.84042500 |
| Rh | 13.59295000 | 14.12875000 | 10.78502500 |
| Rh | 15.09512500 | 9.30115000 | 10.88562500 |
| Rh | 8.83612500 | 12.51387500 | 10.07847500 |
| Rh | 12.51635000 | 11.83010000 | 9.99635000 |
| Rh | 16.94115000 | 11.12147500 | 10.37007500 |
| Rh | 9.36810000 | 15.03147500 | 9.47277500 |
| Rh | 15.87090000 | 13.44785000 | 9.67352500 |
| Rh | 14.59757500 | 15.72375000 | 9.14880000 |
| Rh | 10.40460000 | 10.52885000 | 9.15517500 |
| Rh | 11.96567500 | 15.45697500 | 9.25317500 |
| Rh | 12.79982500 | 9.30787500 | 9.45602500 |
| Rh | 14.75717500 | 11.12112500 | 8.88897500 |
| Rh | 10.88135000 | 13.12692500 | 8.42830000 |
| Rh | 12.45057500 | 11.16905000 | 7.59632500 |
| Rh | 13.55295000 | 13.47257500 | 8.27020000 |
| O | 9.61250000 | 10.97812500 | 18.90437500 |
| O | 10.91737500 | 13.14040000 | 17.85950000 |
| C | 10.80035000 | 10.40860000 | 18.48530000 |
| C | 10.68457500 | 9.05632500 | 17.95762500 |
| C | 9.48272500 | 8.49485000 | 17.45152500 |
| H | 8.64747500 | 12.96465000 | 16.09007500 |
| H | 11.66487500 | 10.59182500 | 19.14435000 |
| H | 9.76970000 | 11.95087500 | 18.93642500 |
| H | 11.55637500 | 8.41545000 | 18.11715000 |
| H | 8.54500000 | 9.04077500 | 17.58290000 |
| H | 9.39865000 | 7.40852500 | 17.35965000 |