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Electronic Supplementary Information

for

A Quantification Scheme for Non-covalent Interactions in the Enantio-controlling Transition States in Asymmetric Catalysis

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1. An illustration of how to apply the proposed quantification scheme

(a) Model system: A simple n-pentylbenzene is considered here for quantifying the intramolecular C–H···π interaction. The definition of fragments is such that the terminal methyl group is placed in one layer and the remaining part of the molecule is in another layer. The partition scheme is shown in Fig. S1 as given below.

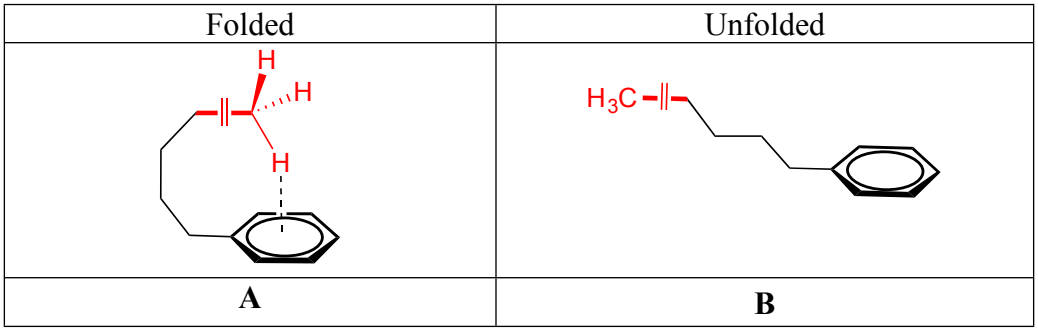


Fig. S1: The partition scheme used to estimate intramolecular non-covalent interaction between the terminal methyl group and the aryl ring in n-pentylbenzene

In a BSSE-CP calculation, the typical energy terms obtained are (a) the counterpoise corrected total electronic energy ($\Delta E_{int}(1,2)$), (b) BSSE energy ($\Delta E_{BSSE}(1) + \Delta E_{BSSE}(2)$), (c) the sum of the energies of the monomers ($E_1^{1,2} + E_2^{1,2}$) and (d) finally the complexation energy or the interaction energy between the sub-systems ($\Delta E_{int}^{CP}(1,2)$). 1 and 2 here refer to the interacting sub-systems obtained through partitioning of the super-system.

Step-1: Calculation of E_A

The partition involved yields interaction energy E_A which is defined as

E_A = (counterpoise corrected total electronic energy of the super-system) – (sum of energies of the sub-systems)

$= E_{1,2}^{1,2} - (E_1^{1,2} + E_2^{1,2})$

$= BD_{C\text{-}C} + NCI_{B\cdots M}$

Where $BD_{C\text{-}C}$ is the bond disassociation energy and $NCI_{B\cdots M}$ is the non-covalent interaction between the benzene and methyl fragment.

The respective values obtained from a BSSE-CP calculation are as follows,

Counterpoise corrected total electronic energy in hartree ($\Delta E_{int}(1,2)$)= -428.61753

BSSE energy in hartree ($\Delta E_{BSSE}(1) + \Delta E_{BSSE}(2)$) = 0.003978

Sum of monomers in hartree ($E_1^{1,2} + E_2^{1,2}$) = -428.43619

Complexation energy ($\Delta E_{int}^{CP}(1,2)$) = -113.79 kcal/mol

Hence $E_A = BD_{C\text{-}C} + NCI_{B\text{-}M}$ = -113.79 kcal/mol.

Step-2: Calculation of E_B

The partition involved yields interaction energy E_B which is defined as

E_B = counterpoise corrected total electronic energy - sum of monomers

$= E_{1,2}^{1,2} - (E_1^{1,2} + E_2^{1,2})$

$= BD_{C\text{-}C}$

Where $BD_{C\text{-}C}$ is the bond disassociation energy, which is the only interaction energy.

The respective values obtained from a BSSE-CP calculation are as follows:

Counterpoise corrected total electronic energy in hartree ($\Delta E_{int}(1,2)$) = -428.61732

BSSE energy in hartree ($\Delta E_{BSSE}(1) + \Delta E_{BSSE}(2)$) = 0.003227

Sum of monomers in hartree ($E_1^{1,2} + E_2^{1,2}$) = -428.43812

Complexation energy in hartree ($\Delta E_{int}^{CP}(1,2)$) = -112.45

Hence $E_B = BD_{C\text{-}C}$ = -112.45 kcal/mol

Therefore $NCI_{B\cdots M} = E_A - E_B$

= -1.34 kcal/mol

The NCI stabilization in the given system is about 1.34 kcal/mol.

(b) Calculation of E_A with scheme-1 partition for TS-1R involved in asymmetric sulfoxidation reaction

In scheme-1, four C–C bonds are cleaved (shown with red breaks). This leads to fragment-1 (consisting of all the substituted 3,3' aryl arms) and rest of the system as fragment-2 (consisting of the BINOL backbone and the activated substrates).

The **counterpoise corrected total electronic energy (**$E_{1,2}^{1,2}$) is equal to

[Total electronic energy of the optimized geometry] – [BSSE energy] (which is due to the fragmentation of the molecule into different layers, one such partition scheme, namely, scheme-1 is shown here).

Sum of monomers ($E_1^{1,2} + E_2^{1,2}$) is equal to:

[Electronic energy of fragment-1] (in the presence of the ghost atoms of fragment-2) + [Electronic energy of fragment-2] (in the presence of the ghost atoms of fragment-1).

The **complexation energy (corrected) (**$\Delta E_{int}^{CP}(1,2)$) as shown in Fig. S2 is the calculated value of $\mathbf{E_A}$.

$\mathbf{E_A}$ is then calculated as,

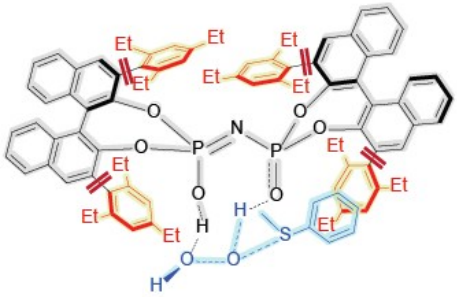
[Counterpoise corrected energy] – [Sum of monomers]

= -5415.569819 – (-5414.744456)

= -517.92 kcal/mol.

This complexation energy is the energy released when fragments 1 and 2 are together to get back the energy of the original super-system, which basically will consist of the 4 C–C bond energies and the 'not-so-obvious' interactions between the aryl arms of the catalyst with the BINOL backbone ($NCI_{A\ldots B}$) and also with the activated substrates ($NCI_{A\ldots C}$). The formulation of $\mathbf{E_A}$ as shown in the main text (Fig. 7) is therefore as a more generalized expression applicable to a wide range of intramolecular interactions. Along the similar lines, other desired quantities such as $\mathbf{E_B}$ and $\mathbf{E_C}$ can be calculated. The non-covalent interaction ($NCI_{A\ldots C}$) can then be computed as $NCI_{A\ldots C} = ½ [E_A + E_C – E_B]$.

It may be noted that some of the interactions are 'not-so-obvious' because when the fragment-1 is replaced with ghost atoms, the interactions due to fragment-1 on fragment-2 goes 'missing' and has to be taken into account in the formulation of the generalized expression.

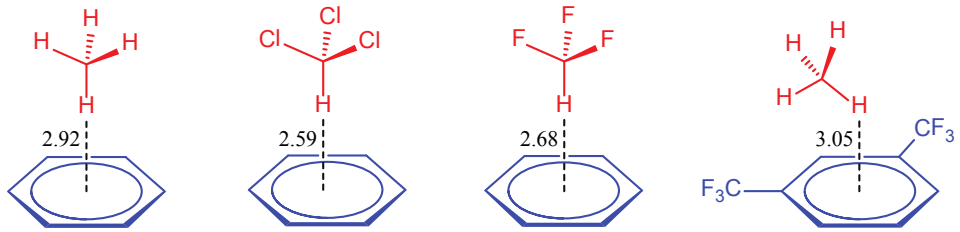


Scheme-1

```
Counterpoise corrected energy =   -5415.569819829777
                    BSSE energy =       0.043137746902
                sum of monomers =   -5414.744456956751
            complexation energy =    -544.99 kcal/mole (raw)
            complexation energy =    -517.92 kcal/mole (corrected)
```

Fig. S2. Scheme-1 partition for TS-1R involved in asymmetric sulfoxidation and an excerpt from the output file.

2. Studies on Model Systems



(-1.7, *-1.5*, **-1.5**) (-7.2, *-6.1*, **-5.6**) (-5.1, *-4.5*, **-4.1**) (-2.7, *-2.2*, **NA**)

Fig. S3 Comparison of intermolecular interaction energies (in kcal/mol) at the M06-2X/6-311+G** level of theory for a set of weakly interacting binary complexes with that obtained at the CBS limit. The values in parentheses are the interaction energies obtained using the super-system approach and respectively represent (a) uncorrected in normal font type, (b) BSSE-corrected in italics, and (c) at the CCSD(T)/CBS limit in bold font type.[1] The shortest contact (in armstrong) between the hydrogen of the interacting molecule and the benzene ring is also shown.

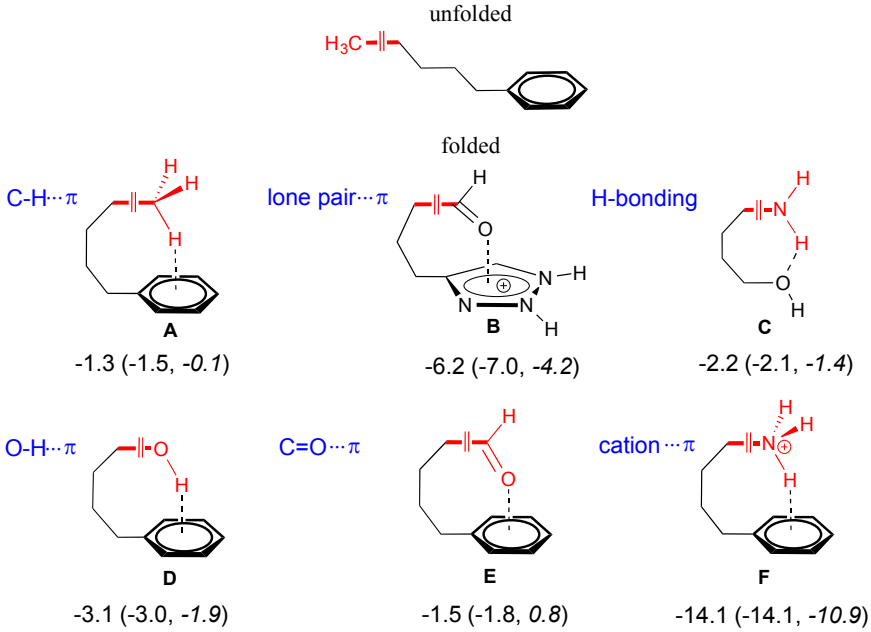
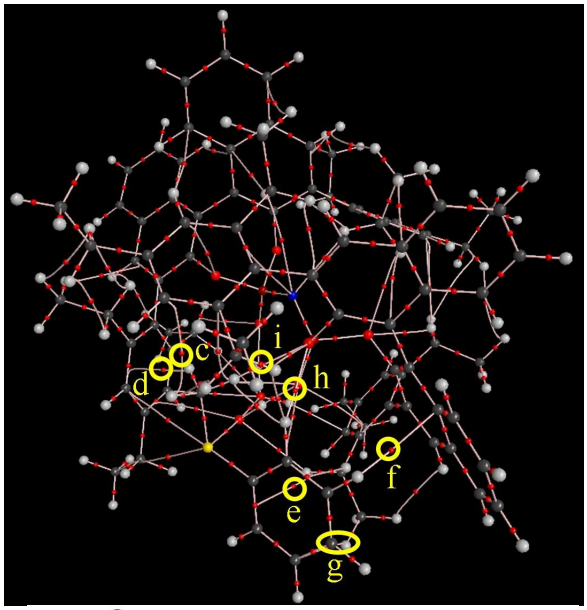


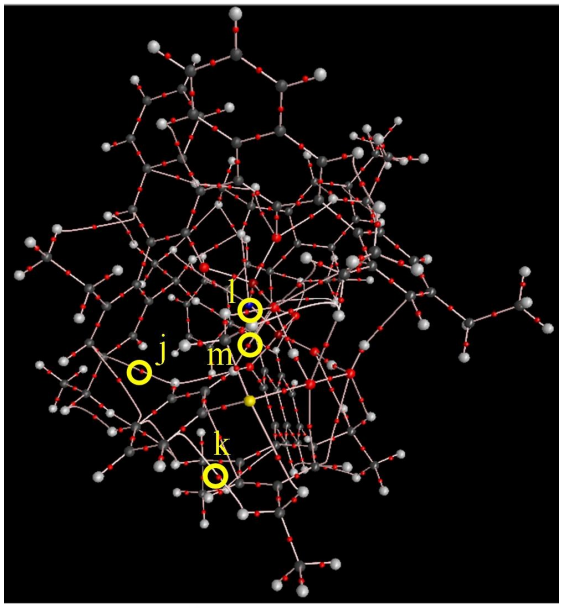
Fig. S4 The various substituted alkyl benzene models (**A** to **F**) with different types of non-covalent interactions and the corresponding partition scheme. The values outside and within parentheses are the strength of interactions (in kcal/mol) computed at the M06-2X level of theory respectively using 6-31G** and 6-311+G** basis sets. For comparison, the interaction

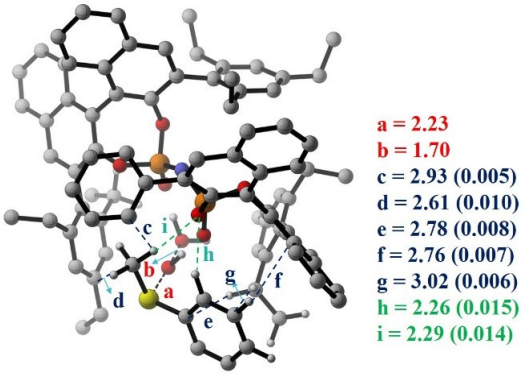
(1) (a) S. Tsuzuki, K. Honda, T. Uchimaru, M. Mikami and K.Tanabe. *J. Phys. Chem. A* 2002, **106**, 4423-4428; (b) A. L. Ringer, M. S. Figgs, M. O. Sinnokrot and C. D.Sherrill. *J. Phys. Chem. A* 2006, **110**, 10822-10828.

energies at the CCSD(T)/6-31G** is provided in italics font type within parentheses as the second entry.

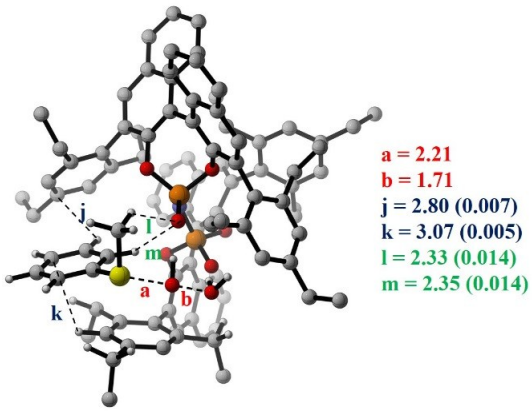
3. Evidence for the Presence of Weak Non-covalent Interactions in the Stereocontrolling Transition States







TS-1-*R*

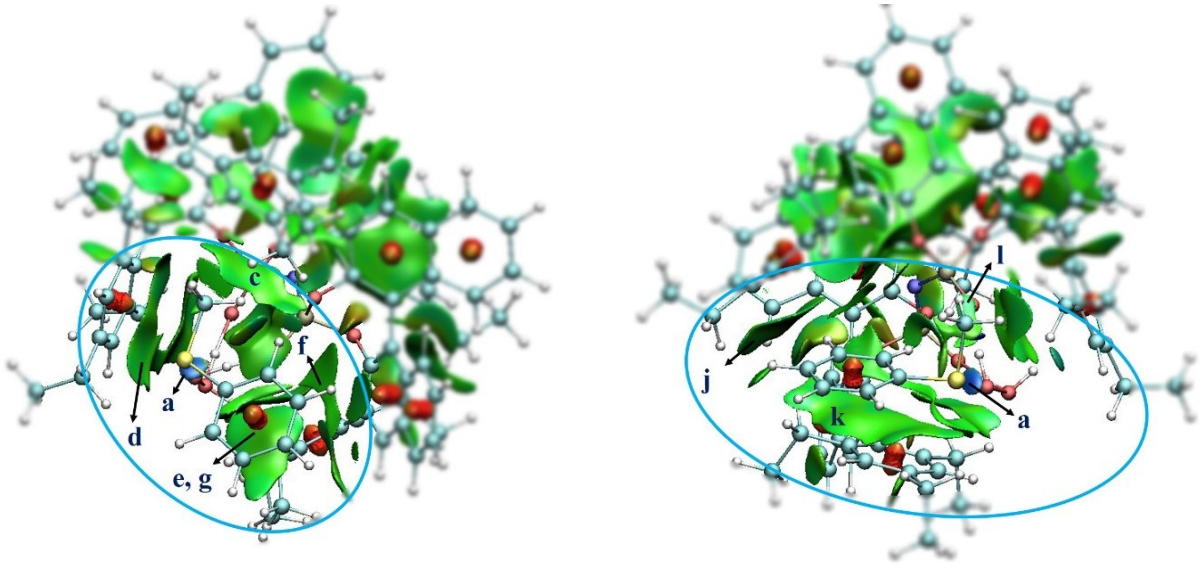


TS-1-*S*

Interaction		Interacting Substrate	Partners from Catalyst	**TS-1-*R*** ρ_{bcp}	**TS-1-*S*** ρ_{bcp}
C-H···π	**c**	Methyl	aryl arm	0.005	-
C-H···π	**d**	Methyl	aryl arm	0.010	-
C-H···π	**e**	Phenyl	aryl arm	0.008	-
C-H···π	**f**	Phenyl	aryl arm	0.007	-
C-H···π	**g**	Phenyl	ethyl of aryl arm	0.006	-

C-H···O	**h**	Phenyl	binol oxygen	0.015	-
C-H···O	**i**	Methyl	binol oxygen	0.014	-
C-H···π	**j**	Phenyl	aryl arm	-	0.007
C-H···π	**k**	Phenyl	aryl arm	-	0.005
C-H···O	**l**	Methyl phosphate oxygen		-	0.014
C-H···O	**m**	Phenyl phosphate oxygen		-	0.014

Fig. S5 The bond paths and corresponding bond critical points for various non-covalent interactions between the substrate and the catalyst as obtained using AIM analysis. The ρ_{bcp} is known to correlate with the strength of inter-atomic interactions.[2] A negative sign of the Laplacian $\nabla^2\rho$ suggests the presence of partial *covalent* type interactions while a positive sign indicates an *ionic* type interaction.[3] See Fig. 3(i) for the optimized geometries of the transition states.



TS-1-*R*		**TS-1-*S***	
Interaction	Interacting Partners from	Interaction	Interacting Partners from

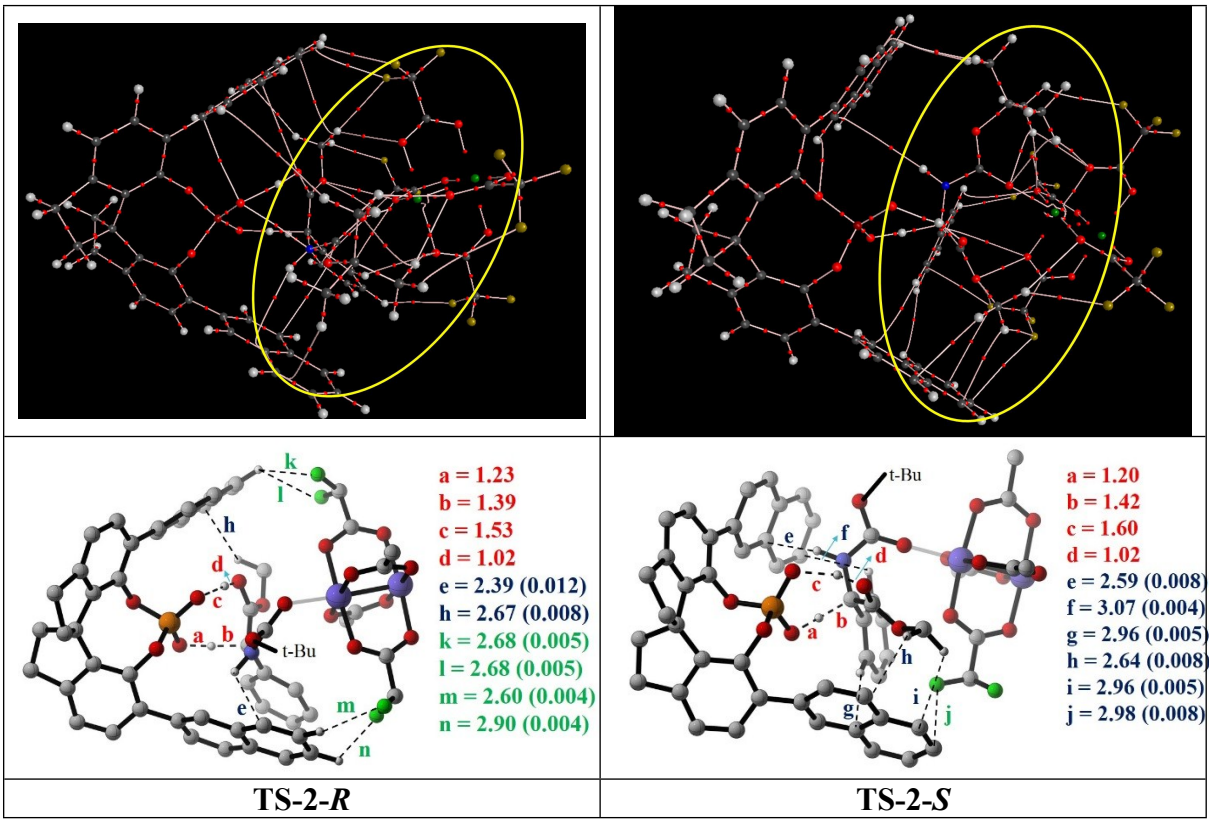
(2) (a) J. R. Premkumar and G. N. Sastry, *J. Chem. Phys. A* 2014, **118**, 11388-11398; (b) F. Zhou, R. Liu, J. Tang, P. Li, Y. Cui and H. Zhang, *J. Mol. Model.* 2016, **29**, 1.

(3) (a) S. J. Grabowski, *Chem. Rev.* 2011, **111**, 2597-2625.

	Substrate	Catalyst		Substrate	Catalyst
C–H···π **c**	Methyl	aryl arm	C–H···π **j**	Phenyl	aryl arm
C–H···π **d**	Methyl	aryl arm	C–H···π **k**	Phenyl	aryl arm
C–H···π **e**	Phenyl	aryl arm	C–H···O **l**	Methyl	phosphate oxygen
C–H···π **f**	Phenyl	aryl arm			
C–H···π **g**	Phenyl	ethyl of aryl arm			

Fig. S6 NCI plot[4] depicting the regions of non-covalent interactions (green surfaces) between the substrate and the catalyst arms at 3,3' positions of the BINOL backbone. The type of interactions is further marked using letters. The non-covalent interactions within catalyst backbone are shown only in a blurred background as these are noted as the same in the diastereomeric transition states.

Reaction 2: Asymmetric N-H Insertion



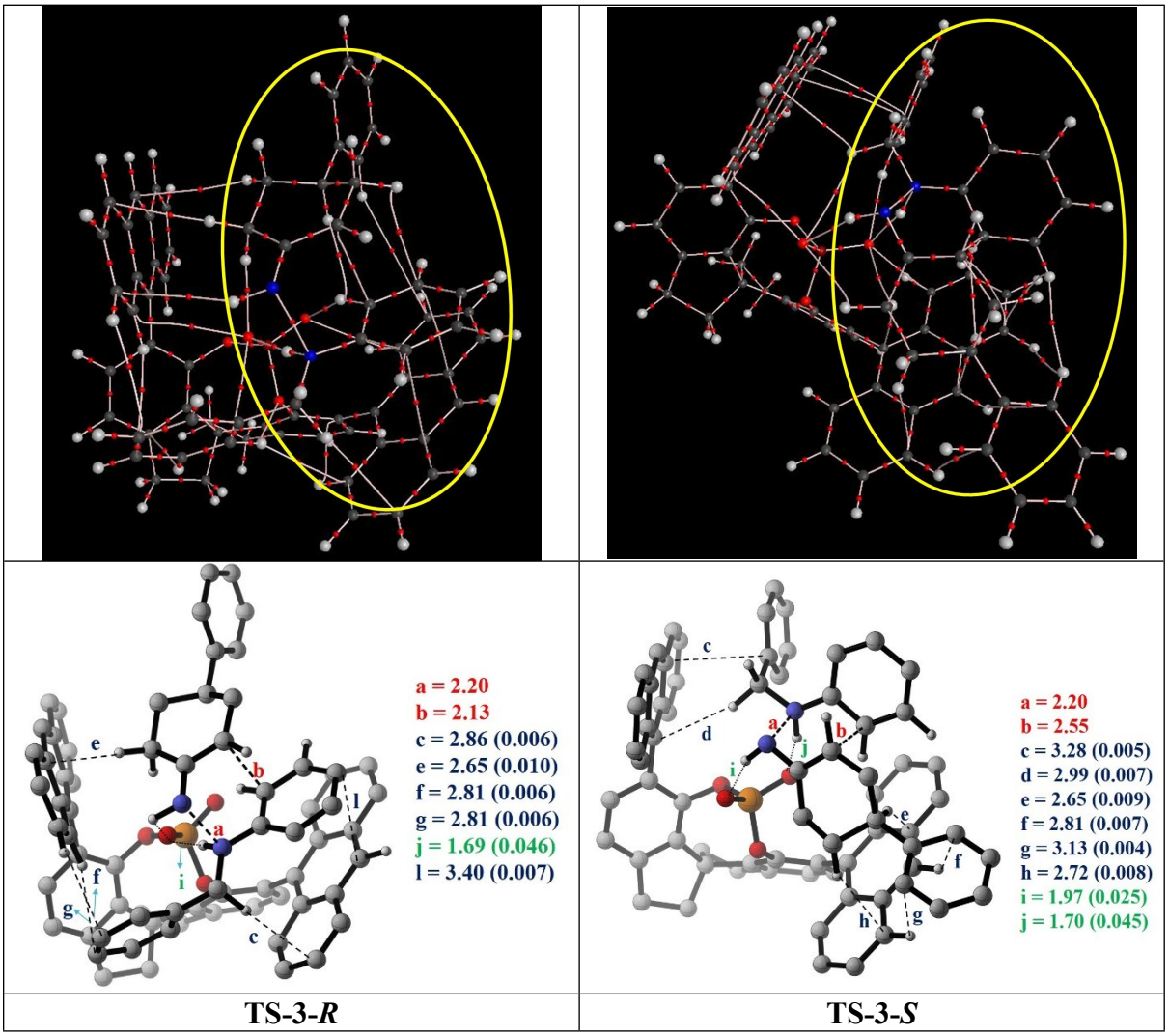
TS-2-*R* **TS-2-*S***

[4] (a) E. R. Johnson, S. Keinan, P. Mori-SanÀchez, J. Contreras- García, A. J. Cohen and W. Yang, *J. Am. Chem. Soc*. 2010, **132**, 6498-6506. (b) E. R. Johnson, S. Keinan, P. Mori-Sanchez, J. Contreras-Garcia, A. J. Cohen and W. T. Yang, *J. Am. Chem. Soc.* 2010, **132**, 6498-6506.

interaction	type	ρ_{BCP}	
		TS-2-*R*	**TS-2-*S***
e	N-H…π	0.012	0.008
f	C-H…π	*no bcp*	0.004
g	C-H…π	*no bcp*	0.005
h	C-H…π	0.008	0.008
i	C-H…π	*no bcp*	0.005
j	C-F…π	*no bcp*	0.008
k	C-F…H	0.005	*no bcp*
l	C-F…H	0.005	*no bcp*
m	C-F…H	0.004	*no bcp*
n	C-F…H	0.004	*no bcp*

Fig. S7 The bond paths and corresponding bond critical points for various non-covalent interactions between the substrate and the catalyst as obtained using AIM analysis of Reaction **2.**

Reaction 3: Asymmetric Fischer Indolization



TS-3-*R* | **TS-3-*S***

Interaction	Type	ρ_{BCP}	
		TS-3-*R*	**TS-3-*S***
c	π…π	0.006	0.005
d	C-H…π	*no bcp*	0.007
e	C-H…π	0.010	0.009
f	C-H…π	0.006	0.007
g	C-H…π	0.006	0.004
h	C-H…π	*no bcp*	0.008
i	N-H…O	*no bcp*	0.025
j	N-H…O	0.046	0.045
l	π…π	0.007	*no bcp*

Fig. S8 The bond paths and corresponding bond critical points for various non-covalent interactions between the substrate and the catalyst as obtained using AIM analysis of Reaction **3.**

4. Partition Scheme for Different Transition States

Reaction 1: Asymmetric Sulfoxidation

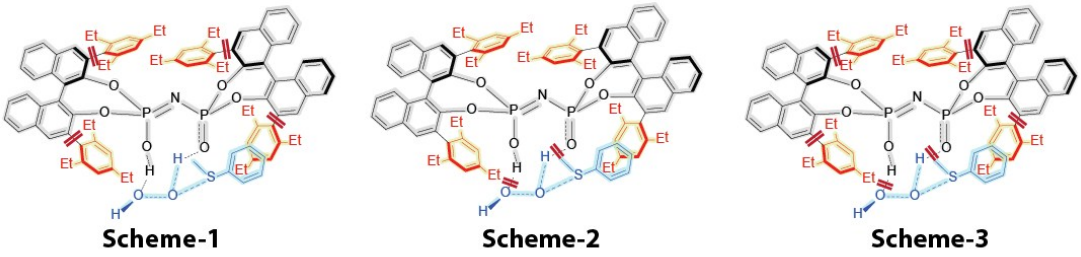


Fig. S9. The partition scheme for transition state (**TS-1**). Fragment **A** (in red) consists of aryl arms at the 3,3′-substituted backbone, fragment **B** (in black) consists of the BINOL phosphoric acid backbone, and fragment **C** (in blue) consists of the activated substrates.

In scheme-1 mode of partition (as described in the main manuscript)

BD_A = Sum of 4 C-C bond dissociation energies that connects **A** to the supersystem

$NCI_{A...C}$ = Non-covalent interactions between the 3,3′-substituted aryl arms and the substrates

$NCI_{A...B}$ = Non-covalent interactions between the 3,3′-substituted aryl arms and BINOL backbone

In scheme-2 mode of partition, we have

BD_C = Sum of H-bonding energies of the phosphoric acid and substrate that connects **C** to the super system

$NCI_{B...C}$ = Non-covalent interactions between BINOL backbone and activated substrates

Lastly, through scheme-3 partition, the terms that are used in schemes 1 and 2 will reappear such that suitable deduction of desirable quantities can be done.

As mentioned in Section 1.3, the energy calculation can be done for each scheme described above. Assuming the fragments to be in different layers 1 and 2 for a given partition scheme, the energy can be expressed as follows:

$$E_{(A/B/C)} = E_{1,2}^{1,2} - (E_1^{1,2} + E_2^{1,2})$$

where $E_{1,2}^{1,2}$ describes the counterpoise corrected total electronic energy of the transition state (which varies with respect to different type of fragmentation) and $E_1^{1,2} + E_2^{1,2}$ describes the sum of electronic energies of the fragments.

Table S4.1: BSSE Corrected Electronic Energies (in hartree) of Stereocontrolling Transition States

Fragmentation Schemes	Total electronic energy of transition state	Sum of electronic energies of fragments
	TS-1-*R*	
E_A	-5415.569820	-5414.744457
E_B	-5415.591494	-5415.403801
E_C	-5415.566447	-5414.590049
	TS-1-*S*	
E_A	-5415.560943	-5414.740292
E_B	-5415.584127	-5415.402488
E_C	-5415.560258	-5414.591530

Table S4.2: BSSE Corrected Non-Covalent Interaction Energies (in kcal/mol)

Transition State	E_A	E_B	E_C	$NCI_{A...C}$
TS-1-*R*	-517.9	-612.7	-117.8	-11.5
TS-1-*S*	-515.0	-608.0	-114.0	-10.5

Reaction 2: Asymmetric N-H insertion Reaction

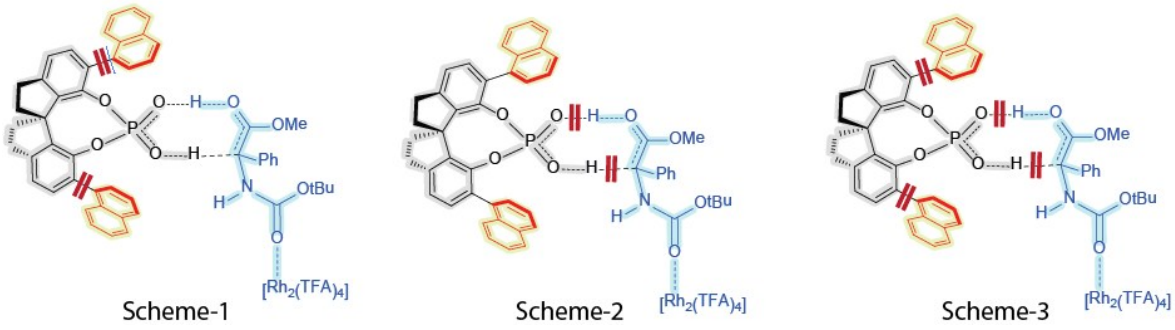


Fig. S10. The partition scheme for transition state **TS-2**. The fragments generated through the partition scheme are shown in different colors. Fragment A, shown in red color, consists of the aryl arms attached to the 3,3' positions of the SPINOL backbone. Fragment B (in black) contains the SPINOL phosphoric acid backbone, and C (in blue) consists of the activated substrates.

In scheme-1 mode of partition (as described in the main manuscript)

BD_A = Sum of two C-C bond dissociation energies that connects A to the SPINOL backbone.

$NCI_{A...C}$ = Non-covalent interactions between the 3,3'-aryl arms and the substrates.

$NCI_{A...B}$ = Non-covalent interactions between the 3,3'-aryl arms and the SPINOL backbone.

In scheme-2 mode of partition, we have

BD_C = Sum of hydrogen bonding energies of the phosphoric acid and the substrate that connects layer C to the rest of the super system.

$NCI_{B...C}$ = Non-covalent interactions between the SPINOL backbone and the activated substrates.

Lastly, through scheme-3 partition, the terms that are used in schemes 1 and 2 will reappear such that suitable deduction of desirable quantities can be done.

Table S4.3: BSSE Corrected Electronic Energies (in hartree) of Stereocontrolling Transition States

Partition Schemes	Total electronic energy of transition state	Sum of electronic energies of fragments
	TS-2-*R*	
E_A	-5290.541070	-5290.136172
E_B	-5290.542859	-5289.991559
E_C	-5290.541348	-5290.365217
	TS-2-*S*	
E_A	-5290.531160	-5290.129967
E_B	-5290.532920	-5290.067946
E_C	-5290.534921	-5290.446296

Table S4.4: BSSE Corrected Non-Covalent Interaction Energies (in kcal/mol)

Transition State	E_A	E_B	E_C	$NCI_{A...C}$
TS-2-*R*	-254.1	-346.0	-110.5	-9.3
TS-2-*S*	-251.8	-291.8	-55.6	-7.8

Reaction 3: Asymmetric Fischer Indolization

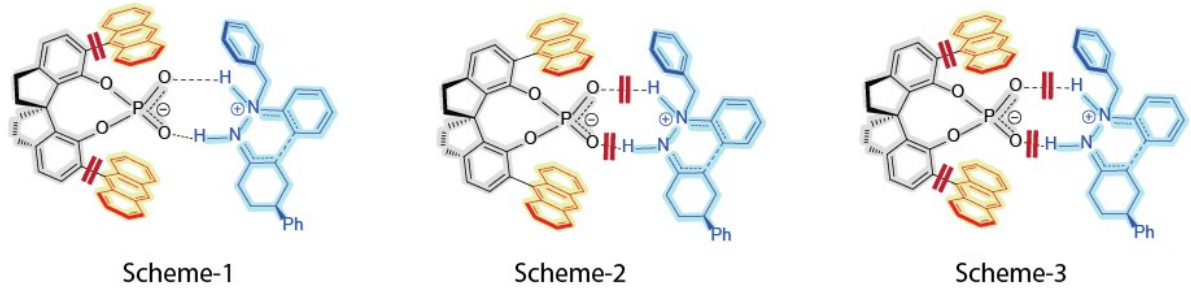


Fig. S11. The fragments generated through the partition scheme are shown in different colors. Fragment A, shown in red color, consists of the aryl arms attached to the 3,3' positions of the SPINOL backbone. Fragment B (in black) contains the BINOL phosphoric acid backbone, and C (in blue) consists of the substrates.

Table S4.5: BSSE Corrected Electronic Energies (in hartree) of Stereocontrolling Transition States

Partition Schemes	Total Electronic Energy of Transition State	Sum of electronic energies of fragments
	TS-3-*R*	
E_A	-3452.390477	-3451.973494
E_B	-3452.386066	-3451.842370
E_C	-3452.396539	-3452.218333
	TS-3-*S*	
E_A	-3452.398761	-3451.981785
E_B	-3452.395773	-3451.846256
E_C	-3452.406355	-3452.216718

Table S4.6: BSSE Corrected Non-Covalent Interaction Energies (in kcal/mol)

Transition State	E_A	E_B	E_C	$NCI_{A...C}$
TS-3-*R*	-261.7	-341.2	-111.8	-16.2
TS-3-*S*	-261.7	-344.8	-119.0	-17.9

5. Gibbs free energies between the diastereomeric transition states and enantiomeric excess (%ee)

Table S5.1a: The level of theory used for geometries and the respective ΔG(ΔG1) as obtained from literature in kcal/mol

	level of Theory used for	electronic energy (M06-2X/	reported energetic details	

	geometries[a]	6-31G**) (*e1*)	electronic energy (*e2*)	Gibbs free energy (*g1*)	ΔG1	ΔE1
TS-1-*R*	L1	-5415.612958	-5415.612958	-5414.023527	-3.9	-4.26
TS-1-*S*		-5415.606177	-5415.606177	-5414.017296		
TS-2-*R*	L2	-5290.567246	-5290.567246	-5289.688271	-6.1	-8.40
TS-2-*S*		-5290.55386	-5290.55386	-5289.678568		
TS-3-*R*	L3	-3452.413091	-3452.659263	-3451.712571	-2.8	-5.82
TS-3-*S*		-3452.422372	-3452.666029	-3451.717046		

Table S5.1b: The ratio of the difference in $NCI_{A...C}$ and the difference in Gibbs free energies between the diastereomeric transition states (ΔG and ΔNCI are in kcal/mol)

	Gibbs free energy correction factor *g2*=(*g1-e2*)	Gibbs free energy (M06-2X/ 6-31G**) (*e1*+*g2*)	ΔG2	ΔNCI	ΔNCI/ ΔE1	ΔNCI/ ΔG2
TS-1-*R*	1.589431	-5414.023527	-3.9	-1.0	0.24	0.25
TS-1-*S*	1.588881	-5414.017295				
TS-2-*R*	0.878975	-5289.688271	-6.1	-1.5	0.18	0.24
TS-2-*S*	0.875292	-5289.678568				
TS-3-*R*	0.946692	-3451.466399	-4.4	-1.7	0.29	0.38
TS-3-*S*	0.948983	-3451.473388				

[a] Geometries from literature at the level of theory indicated as L1= M06-2X/6-31G**: L2= M06/6-31G*; L3= ωB97X-D/6-31G*;

Table S5.2: Comparison of the computed enantiomeric excess (%ee) with that obtained from the experimental reports. Here, ΔG1 is as noted from the published literature at the respective levels of theory given in Table 5.1. ΔG2 is obtained at the M06-2X/6-31G** level of theory in the gas phase using the thermal and entropic correction factors obtained as indicated in Table 5.1

reaction	expt ee%	ref.[1]	ΔG1 (kcal/mol)	ee% (using ΔG1)	ref.[1]	ΔG2 (kcal/mol)	ee% (using ΔG2)
1	98	17a	3.9	99.7	16a	3.9	99.7
2	95	17d	6.1	>99	16b	6.1	>99
3	87	17e	2.8	98.2	16c	4.4	>99

[1]As cited in the main text

6. Comparison of Our Scheme with Other Quantification Methods

According to Wheeler's H-capping method, the energy difference between two competing transition state involved in the stereodetermining step ($\Delta\Delta E^{\ddagger}$) can be expressed in terms of

$$\Delta\Delta E^{\ddagger} = \Delta\Delta E_{sub} + \Delta\Delta E_{cat} + \Delta\Delta E_{int}$$

where, $\Delta\Delta E_{sub}$ is the difference in energy between the substrates in the transition state, $\Delta\Delta E_{cat}$ is the difference in energies between the catalyst in the respective TS geometries, and $\Delta\Delta E_{int}$ is the difference in interaction energies between the catalyst and substrate in the TS geometries. The $\Delta\Delta E_{int}$ has been calculated as the contributions arising through the interaction of the substrate with different fragments of the catalyst (considering as three different dimers).

Table S6.1: Interaction Energy ($\Delta\Delta E_{int}$) Computed at the ωB97X-D/6-31G* Level of Theory for Reaction **3**

Type of interaction	Interaction energy kcal/mol
H-bond	2.6
π···π	-2.4
C-H···π	5.0

In this study we have quantified the overall interactions by solving the equations described. The composition of different type of interactions can be quantified by substituting the overall interaction in the equation, as reported in the following section.

Fig. S12: The fragments generated through the partition scheme are shown in different colors. Fragment A, shown in red color, consists of the aryl arms attached to the 3,3' positions of the SPINOL backbone. Fragment B (in black) contains the BINOL phosphoric acid backbone, and C (in blue) consists of the substrates.

In scheme-1 mode of partition (as described in the main manuscript)

BD_A = Sum of two C-C bond dissociation energies that connects A to the SPINOL backbone.

$NCI_{A...C}$ = Non-covalent interactions between the 3,3'-aryl arms and the substrates.

$NCI_{A...B}$ = Non-covalent interactions between the 3,3'-aryl arms and the SPINOL backbone.

In scheme-2 mode of partition, we have

BD_C = Sum of hydrogen bonding energies of the phosphoric acid and the substrate that connects layer C to the rest of the super system.

$NCI_{B...C}$ = Non-covalent interactions between the SPINOL backbone and the activated substrates.

Lastly, through scheme-3 partition, the terms that are used in schemes 1 and 2 will reappear such that suitable deduction of desirable quantities can be done.

The equations are given below:

$$E_A = BD_A + NCI_{A...B} + NCI_{A...C}$$

$$E_B = BD_A + BD_C + NCI_{A...B} + NCI_{B...C}$$

$$E_C = BD_C + NCI_{A...C} + NCI_{B...C}$$

Table S6.2: BSSE Corrected Non-Covalent Interaction Energies Obtained at the M06-2X/6-31G** Level of Theory (in kcal/mol)

Transition State	E_A	E_B	E_C	$NCI_{A...C}$
TS-3-R	-261.7	-341.2	-111.8	-16.2
TS-3-S	-261.7	-344.8	-119.0	-17.9

Table S6.3: BSSE Corrected Non-Covalent Interaction Energies Obtained at the ωB97X-D/6-31G* Level of Theory (in kcal/mol)

Transition State	E_A	E_B	E_C	$NCI_{A...C}$
TS-3-R	-272.7	-347.46	-121.45	-23.3
TS-3-S	-273.3	-349.51	-127.29	-25.5

The comparison between the Wheeler's H-capping method is presented in **Table S6.4.**

Table S6.4: BSSE-Corrected Difference in the Non-Covalent Interaction Energies between the Diastereomeric Transition States Leading to *R* and *S* Enantiomeric Products Obtained at the ωB97X-D/6-31G* Level of Theory (in kcal/mol)

$\Delta\Delta E_{int}$ for $TS_{(R-S)}$	H-capping scheme (ωB97X-D/6-31G*)	Our scheme (ωB97X-D/6-31G*)	Our scheme (M06-2X/6-31G**)
H-bond	2.6	3.6	5.4
π···π	-2.4	2.2	1.7
C-H···π	5.0		

The $\Delta\Delta E_{int}$ for $TS_{(R-S)}$ is calculated with the following equation,

$$\Delta E_{NCI\ (H\text{-}bond)} = \Delta E_{NCI\ (B\ldots C)} = 1/2(\ E_B + E_C - E_A\ )$$

7. Comparison of non-covalent interaction computed using the M06-2X with the CCSD(T) level of theory in gas phase

Table S7.1: Comparison between CCSD(T) and M06-2X level of theories with 6-31G** basis set in kcal/mol

Model system	Type of interaction	CCSD(T)/6-31G**	M06-2X/6-31G**
A	C-H···π	-0.1	-1.3
B	Lone pair···π	-4.2	-6.2
C	H-bonding	-1.4	-2.2
D	O-H···π	-1.9	-3.1
E	C=O···π	0.8	-1.5
F	Cation···π	-10.9	-14.1

8. Quantification of Non-covalent interactions utilising F-sSAPT and H-capping methods

8.1 H-capping method

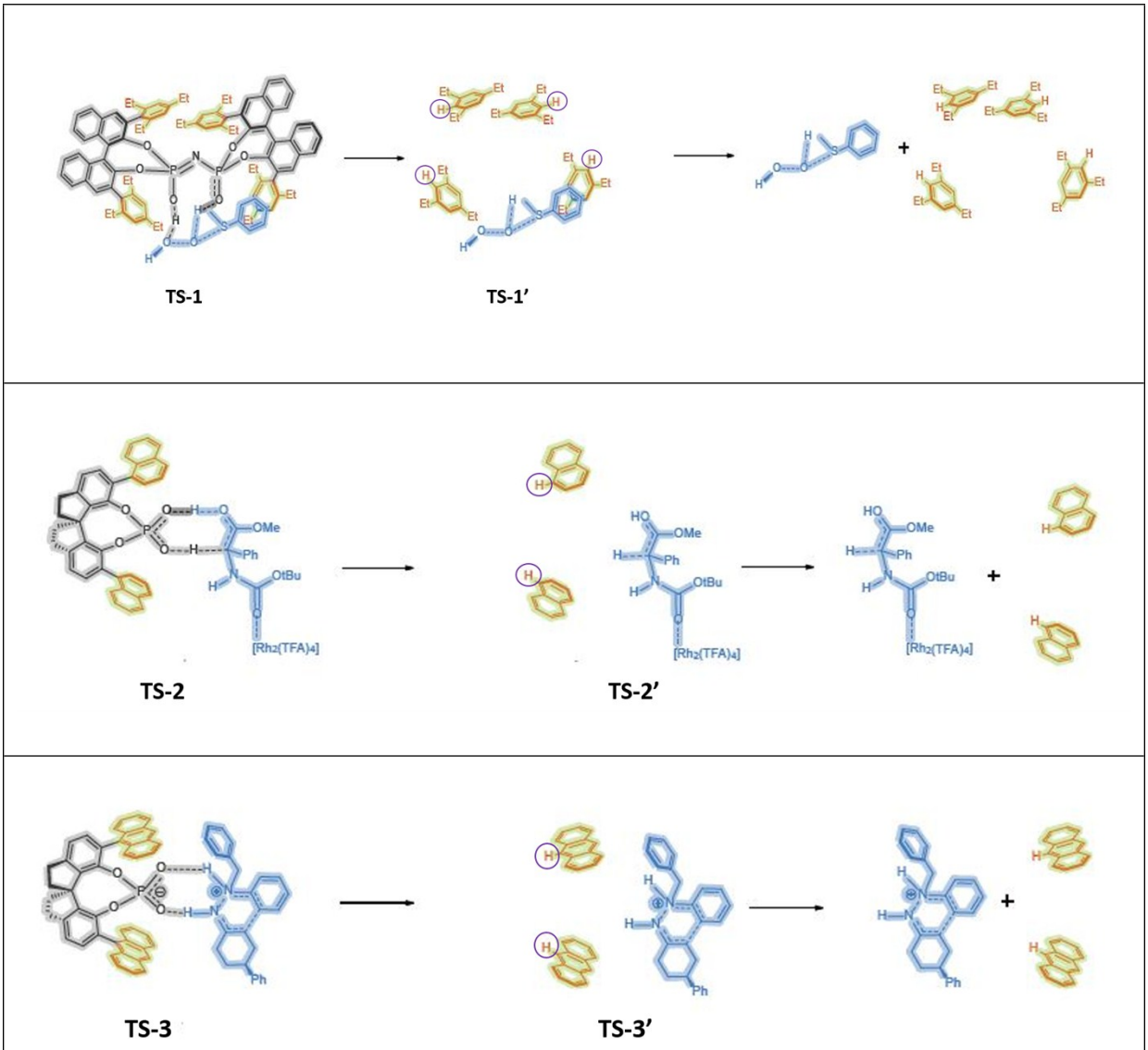


Fig. S13 Partitioning scheme for the stereocontrolling transition states for Reaction **1-3** employed in H-capped method in the determination of intramolecular non-covalent interactions. The full transition states are denoted as **TS-1, TS-2** and **TS-3** and the fragments obtained after the deletion of the backbone (black layer) is represented using **TS-1'**, **TS-2'** and **TS-3'**. The hydrogen that is capped to fill the open valency is shown encircled in the partitioned transition states. The interaction energy is calculated between the fragments in A (in red) and C (in blue) in this approach.

Table S8.1. Computed Strength of the Non-Covalent Interactions (kcal/mol) between the 3,3' Aryl Arms of the Catalyst (fragment-A, red) and the Substrate (fragment-C, blue) in the Stereocontrolling Transition States for Reactions **1** through **3** at the M06-2X/6-31G** using the H-Capping Methodology. In all Cases **TS-1-*R*** is Compared to **TS-1-*S***, as Reported in the Main Text

TS	NCI		ΔNCI $NCI_{(lower\ energy\ TS)}$-$NCI_{(higher\ energy\ TS)}$		ΔNCI/ΔE	
	H-Capped	Our Methodology	H-Capped	Our Methodology	H-Capped	Our Methodology
TS-1-*R*	-18.7	-11.5	-0.2	-1.0	0.1	0.24
TS-1-*S*	-18.5	-10.5	0.0	0.0		
TS-2-*R*	-4.3	-9.3	-5.6	-1.5	0.7	0.18
TS-2-*S*	1.3	-7.8	0.0	0.0		
TS-3-*S*	-19.6	-17.9	-1.9	-1.7	0.3	0.29
TS-3-*R*	-17.7	-16.2	0.0	0.0		

8.2 F-sSAPT method

Exchange-scaled variant of the symmetry adapted perturbation theory, namely, SAPT0 (F-sSAPT)[5] as the reactions considered take place between strongly interacting molecules[6] (here, "0" refers to the use of the simplest truncation of SAPT whereas "F" stands for the functional group).

(5) (a) T. M. Parker, L. A. Burns, R. M. Parrish, A. G. Ryno and C. D. Sherrill, *J. Chem. Phys.,* 2014, **140**, 094106. (b) R. M. Parrish, T. M. Parker and C. D. Sherrill, *J. Chem. Theory Comput.,* 2014, **10**, 4417–4431.

(6) B. W. Bakra and C. D. Sherrill, *Phys. Chem. Chem. Phys.,* 2016, **18**, 10297-10308.

Fig. S14 Partitioning scheme of the stereocontrolling transition states employed in F-sSAPT analysis used in the determination of intramolecular non-covalent interactions between the 3,3' aryl arms of the catalyst (in red) and the substrate (in blue). As F-SAPT analysis requires two interacting monomers, the transition states are partitioned in to catalyst and substrate. Further, the catalyst is broken down into the backbone (colored black) and the 3,3' aryl arms (in red). The substrate (in blue) is considered as a single fragment.

Table S8.2: F-sSAPT Analysis[a] of Non-Covalent Interaction Energies (in kcal/mol). The highlighted rows represent $NCI_{A\cdots C}$ where A is the 3,3' aryl arms of the catalyst (shown in in red color in Fig. S14) and C is the substrate (in blue). The columns labeled 'Frag1' contain all possible interacting fragments of the catalyst and 'Frag2' that of the substrate. The 'Elst', 'Exch', and 'Disp' columns respectively represent the computed electrostatics, exchange-repulsion, and dispersion. 'IndAB' or 'IndBA' refers to the induction of monomer A or B in the presence of the electrostatic potential of monomer B or A, respectively

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
TS-1-*S*							
B	C	-87.18	108.35	-15.63	-111.16	-21.59	-127.20
A	C	-17.57	44.49	-4.41	2.65	-26.74	-1.58
B	All	-87.18	108.35	-15.63	-111.16	-21.59	-127.20
A	All	-17.57	44.49	-4.41	2.65	-26.74	-1.58
All	C	-104.75	152.84	-20.04	-108.51	-48.33	-128.79
All	All	-104.75	152.84	-20.04	-108.51	-48.33	-128.79
TS-1-*R*							
B	C	-91.93	121.82	-18.28	-114.06	-27.02	-129.47
A	C	-15.30	36.68	-4.88	3.63	-22.66	-2.54

B	All	-91.93	121.82	-18.28	-114.06	-27.02	-129.47
A	All	-15.30	36.68	-4.88	3.63	-22.66	-2.54
All	C	-107.23	158.49	-23.17	-110.43	-49.69	-132.02
All	All	-107.23	158.49	-23.17	-110.43	-49.69	-132.02
TS-2-*S*							
A	C	-14.10	24.71	-3.02	-0.12	-19.67	-12.19
B	C	-63.10	92.45	-13.17	-49.27	-17.93	-51.03
A	All	-14.10	24.71	-3.02	-0.12	-19.67	-12.19
B	All	-63.10	92.45	-13.17	-49.27	-17.93	-51.03
All	C	-77.20	117.16	-16.19	-49.39	-37.60	-63.22
All	All	-77.20	117.16	-16.19	-49.39	-37.60	-63.22
TS-2-*R*							
A	C	-19.74	30.65	-6.30	0.23	-24.03	-19.19
B	C	-70.20	106.30	-17.59	-58.73	-23.48	-63.70
A	All	-19.74	30.65	-6.30	0.23	-24.03	-19.19
B	All	-70.20	106.30	-17.59	-58.73	-23.48	-63.70
All	C	-89.94	136.95	-23.88	-58.50	-47.51	-82.89
All	All	-89.94	136.95	-23.88	-58.50	-47.51	-82.89
TS-3-*R*							
B	C	-96.67	41.71	-8.01	-18.05	-17.16	-98.19
A	C	-14.38	25.18	-3.99	-0.17	-24.55	-17.91
B	All	-96.67	41.71	-8.01	-18.05	-17.16	-98.19
A	All	-14.38	25.18	-3.99	-0.17	-24.55	-17.91
All	C	-111.05	66.89	-12.00	-18.22	-41.72	-116.10
All	All	-111.05	66.89	-12.00	-18.22	-41.72	-116.10
TS-3-*S*							
B	C	-101.70	37.30	-8.87	-17.64	-12.43	-103.34
A	C	-13.56	25.37	-4.91	-0.47	-26.47	-20.04
B	All	-101.70	37.30	-8.87	-17.64	-12.43	-103.34
A	All	-13.56	25.37	-4.91	-0.47	-26.47	-20.04
All	C	-115.27	62.67	-13.78	-18.11	-38.90	-123.38
All	All	-115.27	62.67	-13.78	-18.11	-38.90	-123.38

[a] Auxiliary basis set cc-pVDZ-JKfit for 6-31G**, as defined in PSI4 is used for self-consistent field (SCF) procedure and for two-body contributions from SAPT0 cc-pVDZ-RI basis set is employed. For the heavy atoms, def2-QZVPP-JKfit for self-consistent field (SCF) procedure and def2-QZVPP-RI for the two-body contributions from SAPT0 are used.

Table S8.3. Computed Strength of the Non-Covalent Interactions (kcal/mol) between the 3,3' Aryl arms of the Catalyst (fragment-A, red) and the Substrate (fragment-C, blue) in the Stereocontrolling Transition States for Reactions **1** through **3** at the M06-2X/6-31G** Obtained using the F-SAPT Analysis. In all Cases **TS-1-*R*** is Compared to **TS-1-*S*** as Reported in the Main Text

TS	NCI		ΔNCI $NCI_{(lower\ energy\ TS)}$-$NCI_{(higher\ energy\ TS)}$		ΔNCI/ΔE	
	F-SAPT	our method	F-SAPT	our method	F-SAPT	our method
TS-1-*R*	-2.5	-11.5	-0.9	-1.0	0.2	0.2
TS-1-*S*	-1.6	-10.5	0.0	0.0		
TS-2-*R*	-19.2	-9.3	-7.0	-1.5	0.8	0.2
TS-2-*S*	-12.2	-7.8	0.0	0.0		
TS-3-*S*	-20.0	-17.9	-2.1	-1.7	0.4	0.3
TS-3-*R*	-17.9	-16.2	0.0	0.0		

9. Optimized Cartesian Coordinates of the Transition State Geometries Employed in Single Point Energy Calculations (M06-2X/6-31G**)

TS-1-*S*

6	3.025791	-2.875080	-2.850737	6	6.397064	-0.845350	2.238326
6	3.427576	-1.544983	-2.634367	8	2.430295	0.012428	-0.461292
6	3.042806	-0.537921	-3.537222	5	1.234832	-0.847154	0.227539
6	2.292234	-0.882552	-4.661408	8	1.780621	-0.987884	1.756348
6	1.915116	-2.198859	-4.920592	6	2.425090	0.068879	2.372782
6	2.298890	-3.181894	-4.006652	6	3.693116	0.433702	1.957835
6	4.249995	-1.224766	-1.429131	6	4.317261	1.562520	2.583582
6	3.702233	-0.513050	-0.327930	6	3.701990	2.152337	3.720230
6	4.368497	-0.311378	0.861202	6	2.440812	1.670640	4.151183
6	5.678112	-0.878162	1.012787	6	1.768326	0.680273	3.476133
6	6.276033	-1.529679	-0.102148	6	5.508735	2.151846	2.079131
6	5.540961	-1.677276	-1.306128	6	6.068725	3.241896	2.695138
6	7.583122	-2.070442	0.023099	6	5.481600	3.794955	3.857385
6	8.262505	-1.997380	1.210097	6	4.323120	3.259927	4.356126
6	7.652956	-1.388768	2.331743	6	0.387045	0.303253	3.912494

6	-0.692429	1.139833	3.577439	6	-3.562851	-4.655581	-0.693274
6	-1.954854	0.855948	4.098878	6	-4.128185	-3.987789	0.390570
6	-2.165417	-0.207658	4.975131	6	-4.487525	-2.642109	0.311699
6	-1.082683	-1.029461	5.280956	6	-3.626346	-1.957352	-3.370804
6	0.183352	-0.813467	4.736172	6	-4.812225	-2.280623	-4.285384
6	-0.521782	2.367812	2.716835	6	-3.165672	-6.108192	-0.604511
6	-0.522332	3.652696	3.551332	6	-4.240526	-7.031198	-1.188214
6	-3.533845	-0.452608	5.567422	6	-5.094683	-1.958953	1.516216
6	-3.965501	0.665822	6.520901	6	-6.625672	-1.926240	1.459960
6	1.308889	-1.760261	5.081906	6	2.174791	3.173118	0.174471
6	2.067763	-1.328640	6.340826	6	2.370091	4.308799	1.181865
6	3.454776	0.900277	-3.341595	6	3.849912	4.718245	-4.311389
6	4.878091	1.163125	-3.842147	6	3.797215	6.190783	-4.730355
6	1.129995	-2.562036	-6.156866	6	-1.090580	4.149576	-3.638717
6	2.047643	-3.014168	-7.297650	6	-1.822608	5.461811	-3.335467
6	3.297347	-3.992716	-1.867161	8	-1.202384	-0.887012	-1.987012
6	4.419591	-4.933198	-2.313386	8	1.206825	-2.234525	-0.340187
7	-0.040545	0.083979	0.222727	8	-0.468807	-3.105689	-2.702834
5	-1.189500	0.103970	-0.867408	8	-0.180300	-4.107793	-1.343641
8	-2.549699	0.065669	0.018492	6	0.137205	-5.382542	0.438230
6	-3.724800	0.481253	-0.586785	6	1.752903	-4.962494	1.164361
6	-3.943235	1.833687	-0.717133	6	-0.923313	-4.600406	1.644541
6	-5.155607	2.274993	-1.346034	6	-1.449687	-5.381989	2.672136
6	-6.120289	1.300896	-1.727348	6	-2.240796	-4.782454	3.649640
6	-5.839860	-0.077046	-1.539588	6	-2.480722	-3.411726	3.604682
6	-4.653041	-0.510278	-1.004206	6	-1.956941	-2.636404	2.571203
6	-5.424008	3.639655	-1.642308	6	-1.195339	-3.234614	1.576268
6	-6.603268	4.011083	-2.237176	1	6.003327	-2.195071	-2.142881
6	-7.579055	3.044889	-2.573805	1	8.027103	-2.555229	-0.842123
6	-7.335207	1.719199	-2.330254	1	9.258973	-2.417567	1.298515
6	-2.883064	2.794152	-0.311790	1	8.182603	-1.356777	3.278383
6	-1.614892	2.670274	-0.846587	1	5.938480	-0.390746	3.108944
6	-0.641525	3.704405	-0.769267	1	1.970692	2.128094	5.018250
6	-0.930415	4.782009	0.035016	1	3.843129	3.691435	5.230195
6	-2.142682	4.874929	0.767157	1	5.941902	4.650949	4.339656
6	-3.140155	3.878854	0.586523	1	6.969726	3.686488	2.285104
6	-2.393050	5.954606	1.654323	1	5.964563	1.740564	1.184977
6	-3.565254	6.025615	2.360696	1	1.994467	-4.215715	-4.176308
6	-4.544778	5.015974	2.206262	1	1.984798	-0.095570	-5.347340
6	-4.342713	3.973891	1.337283	1	0.420229	-3.361120	-5.914492
8	-1.302591	1.557226	-1.599661	1	0.537899	-1.698904	-6.477659
6	0.538973	3.764454	-1.692280	1	2.747749	-2.217742	-7.565064
6	1.855103	3.646936	-1.223021	1	1.470563	-3.278662	-8.187445
6	2.914053	3.958778	-2.082356	1	2.634996	-3.886690	-6.997531
6	2.704838	4.339420	-3.402056	1	3.374779	1.178934	-2.287451
6	1.390162	4.358136	-3.873649	1	2.750418	1.548594	-3.873760
6	0.303584	4.077504	-3.048913	1	5.600161	0.533613	-3.313411
6	-4.305764	-1.958924	-0.901081	1	5.155148	2.208634	-3.679791
6	-3.769797	-2.621040	-2.019262	1	4.961701	0.947650	-4.911663
6	-3.396955	-3.958241	-1.887600	1	-2.790630	1.494903	3.813233

1	-1.229945	-1.885226	5.938525
1	-1.333512	2.398498	1.981163
1	0.406733	2.298637	2.149402
1	-1.487516	3.799575	4.046976
1	-0.331716	4.525180	2.921198
1	0.252705	3.615472	4.323760
1	-4.270389	-0.547740	4.758693
1	-3.531217	-1.407105	6.106480
1	-4.957924	0.471428	6.936191
1	-3.995692	1.627990	6.002225
1	-3.256418	0.756840	7.348119
1	2.000478	-1.837573	4.237024
1	0.885904	-2.760049	5.231218
1	1.386978	-1.257778	7.194242
1	2.527689	-0.346942	6.195613
1	2.857955	-2.042228	6.589909
1	-6.578158	-0.810671	-1.854693
1	-8.063266	0.960666	-2.604756
1	-8.509500	3.355268	-3.038000
1	-6.786181	5.057796	-2.458043
1	-4.680337	4.392026	-1.404921
1	-0.231213	5.613365	0.072084
1	-1.625934	6.715139	1.774514
1	-3.742266	6.848268	3.045695
1	-5.463644	5.066954	2.781423
1	-5.095867	3.201375	1.221914
1	-2.934295	-4.458964	-2.736998
1	-4.240542	-4.509298	1.341365
1	-3.521807	-0.875504	-3.260400
1	-2.698885	-2.311422	-3.833252
1	-4.923781	-3.362019	-4.410053
1	-4.679591	-1.832519	-5.274059
1	-5.746167	-1.898011	-3.862927
1	-2.221983	-6.253360	-1.144465
1	-2.981336	-6.374262	0.442612
1	-5.184969	-6.906403	-0.650772
1	-3.942307	-8.081274	-1.122783
1	-4.423537	-6.791530	-2.239669
1	-4.780664	-2.497450	2.416194
1	-4.702562	-0.938293	1.607381
1	-7.024452	-2.940831	1.370597
1	-6.972913	-1.350526	0.597940
1	-7.042607	-1.471374	2.363145
1	3.932044	3.879198	-1.701471
1	1.201200	4.605738	-4.917397
1	3.095952	2.579138	0.129413
1	1.391337	2.483367	0.503889
1	2.624576	3.914543	2.169272
1	1.462055	4.908505	1.283941
1	3.179978	4.972363	0.861802
1	-1.000193	4.038457	-4.724481
1	-1.691973	3.301651	-3.297748
1	-2.791296	5.485805	-3.842524
1	-1.234690	6.318729	-3.677475
1	-1.999317	5.581461	-2.263168
1	4.798338	4.520116	-3.800779
1	3.836135	4.081961	-5.205362
1	2.871007	6.412461	-5.267763
1	3.833729	6.839805	-3.851252
1	4.636952	6.445556	-5.382303
1	2.365848	-4.563035	-1.760101
1	3.517422	-3.574805	-0.881523
1	5.376244	-4.406991	-2.369510
1	4.534367	-5.764163	-1.611249
1	4.210953	-5.351518	-3.302454
1	-0.812815	-2.192497	-2.314641
1	0.438803	-2.934761	-3.023483
1	0.356121	-3.372997	-0.891008
1	-0.836142	-2.649518	0.740146
1	-1.241295	-6.447475	2.702468
1	-2.144034	-1.566374	2.525875
1	-2.659415	-5.386061	4.448711
1	-3.083869	-2.941155	4.375633
1	2.518368	-5.443576	0.553055
1	1.891833	-3.879769	1.159036
1	1.789383	-5.358679	2.180591

TS-1-*R*

6	3.478394	2.618455	-2.013403
6	3.004849	3.873637	-1.629825
6	3.910096	4.897308	-1.331225
6	5.278168	4.659978	-1.406500
6	5.754505	3.405540	-1.782860
6	4.851140	2.393628	-2.094430
16	1.286680	4.284691	-1.396281
6	0.365460	2.960036	-2.218584
8	0.790350	3.805811	0.722937
8	0.340714	3.299062	2.288828
8	-1.182143	1.409821	1.907476
15	-1.417672	0.296014	0.937645
8	-2.259987	-0.829405	1.751976
6	-2.880722	-1.838427	1.042800
6	-4.010428	-1.546336	0.301501
6	-4.605062	-2.596582	-0.471795
6	-4.119856	-3.924234	-0.319395
6	-3.023858	-4.171242	0.547419
6	-2.375776	-3.157567	1.212306
6	-5.654500	-2.361403	-1.401612
6	-6.217467	-3.398261	-2.102480
6	-5.771013	-4.726683	-1.907005

6	-4.742743	-4.979132	-1.037574	6	3.128432	-1.964937	-1.723046
6	-4.593153	-0.179027	0.366925	6	1.982084	-1.305321	-2.120426
6	-3.789614	0.919434	0.144989	6	1.106781	-1.787626	-3.129864
6	-4.246902	2.260321	0.256134	6	1.390563	-3.012594	-3.681156
6	-5.575014	2.453764	0.544344	6	2.490369	-3.793135	-3.241589
6	-6.452227	1.371279	0.807704	6	3.365648	-3.277808	-2.244128
6	-5.955709	0.038497	0.764761	6	2.719483	-5.093533	-3.763299
6	-7.804230	1.604092	1.172420	6	3.757510	-5.861323	-3.305237
6	-8.628316	0.565474	1.515769	6	4.614550	-5.359592	-2.297621
6	-8.123689	-0.755436	1.524767	6	4.426489	-4.102386	-1.781964
6	-6.826352	-1.013372	1.162186	6	-0.074025	-0.978934	-3.559728
8	-2.473506	0.709314	-0.229799	6	-1.370676	-1.395707	-3.220429
6	-3.307035	3.417851	0.151734	6	-2.461325	-0.636275	-3.651010
6	-2.834525	4.023009	1.332243	6	-2.299693	0.501669	-4.433991
6	-1.991436	5.126113	1.229334	6	-1.001096	0.906498	-4.748837
6	-1.604428	5.651064	-0.002730	6	0.115456	0.193907	-4.315112
6	-2.081698	5.034700	-1.155877	6	-1.631847	-2.651962	-2.426656
6	-2.915592	3.913974	-1.098840	6	-2.434136	-3.691283	-3.214299
6	-1.280518	-3.459534	2.188965	6	1.490741	0.643031	-4.755711
6	0.016525	-3.785542	1.759763	6	1.933810	-0.067405	-6.039640
6	0.960148	-4.179737	2.711507	6	-3.497752	1.214070	-5.011637
6	0.664840	-4.234502	4.069423	6	-3.916797	0.599035	-6.351566
6	-0.615872	-3.862320	4.476391	8	1.697956	-0.063267	-1.594924
6	-1.593100	-3.473839	3.562747	6	3.721046	0.582015	2.537106
6	0.443027	-3.720945	0.310987	6	3.188577	-0.231735	3.554879
6	0.257780	-5.039502	-0.446045	6	2.548097	0.362958	4.641562
6	1.685571	-4.713890	5.073217	6	2.426698	1.745716	4.756248
6	1.459761	-6.179804	5.457579	6	2.987624	2.535243	3.752744
6	-2.974019	-3.132543	4.078639	6	3.619370	1.982489	2.632776
6	-3.916485	-4.341117	4.060545	6	3.346170	-1.733693	3.537049
6	-3.215961	3.532907	2.711440	6	4.747215	-2.162574	3.985858
6	-4.318619	4.388782	3.342076	6	1.749507	2.380222	5.945716
6	-0.672762	6.836771	-0.061784	6	2.760615	2.797565	7.018656
6	-1.315171	8.115439	0.483101	6	4.142457	2.942303	1.586307
6	-3.403054	3.285066	-2.382552	6	5.418256	3.652656	2.049036
6	-4.749436	3.866554	-2.825152	1	6.310424	0.703317	1.718689
7	-0.222453	-0.397583	0.165116	1	8.190507	0.532833	0.194511
15	1.248029	0.122669	-0.032758	1	9.130630	-0.122262	-1.998035
8	1.657333	1.518156	0.318347	1	7.698072	-1.315580	-3.651148
8	2.226558	-0.957088	0.682409	1	5.378718	-1.884236	-3.109060
6	3.571483	-0.771748	0.400003	1	0.737654	-3.408769	-4.455965
6	4.061943	-1.287537	-0.779947	1	2.044019	-5.470813	-4.526073
6	5.430988	-1.025549	-1.117877	1	3.919629	-6.856532	-3.705916
6	6.241181	-0.312304	-0.189905	1	5.424786	-5.978470	-1.925966
6	5.679655	0.148803	1.028413	1	5.083414	-3.727221	-1.004084
6	4.353175	-0.033752	1.331622	1	2.916971	3.621689	3.828970
6	5.993413	-1.373682	-2.376330	1	2.122398	-0.275954	5.412903
6	7.292012	-1.049851	-2.680448	1	1.180277	3.256228	5.614373
6	8.104272	-0.367531	-1.745241	1	1.027710	1.675821	6.371326
6	7.586318	-0.008657	-0.528347	1	3.323551	1.929484	7.373114

1	2.261162	3.257824	7.875154
1	3.478575	3.516330	6.613390
1	3.132191	-2.131784	2.541452
1	2.594576	-2.169792	4.202544
1	5.511109	-1.753771	3.317761
1	4.842929	-3.252447	3.983018
1	4.955618	-1.802299	4.997388
1	-3.464926	-0.955632	-3.369576
1	-0.853695	1.795672	-5.362386
1	-2.165227	-2.378755	-1.510237
1	-0.688338	-3.097782	-2.114876
1	-3.462001	-3.357967	-3.392440
1	-2.485227	-4.634342	-2.663245
1	-1.967341	-3.885616	-4.185766
1	-4.334389	1.158646	-4.305675
1	-3.269962	2.276885	-5.152829
1	-4.787506	1.112013	-6.769104
1	-4.166270	-0.458324	-6.225397
1	-3.099165	0.663299	-7.075307
1	2.229176	0.461240	-3.968571
1	1.477073	1.726210	-4.924187
1	1.218130	0.117134	-6.845820
1	1.988812	-1.148195	-5.879755
1	2.917666	0.281845	-6.364099
1	-5.958223	3.468995	0.614681
1	-8.165713	2.628661	1.187318
1	-9.659118	0.753364	1.797834
1	-8.767335	-1.574264	1.829614
1	-6.452685	-2.030197	1.191895
1	-2.697885	-5.196811	0.702845
1	-4.370814	-5.990497	-0.895572
1	-6.235346	-5.538649	-2.456916
1	-7.013787	-3.198806	-2.812306
1	-6.006136	-1.345712	-1.550146
1	-1.589631	5.561074	2.143488
1	-1.778218	5.416799	-2.130830
1	-3.527061	2.486470	2.673666
1	-2.320968	3.563051	3.342730
1	-4.018091	5.439965	3.387450
1	-4.543623	4.051943	4.357634
1	-5.240405	4.332734	2.755336
1	0.228806	6.594417	0.514658
1	-0.349724	6.994695	-1.096471
1	-2.203173	8.378696	-0.098262
1	-0.617272	8.956126	0.443451
1	-1.627366	7.982980	1.522925
1	-2.653245	3.454232	-3.165498
1	-3.478121	2.197808	-2.263963
1	-4.674156	4.950753	-2.950414
1	-5.518180	3.667978	-2.072826
1	-5.079786	3.433455	-3.773697
1	1.964070	-4.435527	2.373892
1	-0.863767	-3.873962	5.537241
1	1.502732	-3.441451	0.284057
1	-0.095175	-2.910565	-0.187454
1	0.692019	-4.973279	-1.449126
1	-0.801931	-5.290398	-0.553295
1	0.749574	-5.863428	0.080519
1	-2.877780	-2.766851	5.106289
1	-3.410107	-2.312013	3.501865
1	-4.894607	-4.080988	4.474544
1	-3.499537	-5.161114	4.652724
1	-4.064603	-4.704911	3.039896
1	2.691647	-4.594388	4.655016
1	1.640612	-4.088754	5.972942
1	0.467176	-6.313660	5.897117
1	1.519805	-6.820025	4.573041
1	2.204363	-6.520807	6.181971
1	3.362622	3.688149	1.387071
1	4.317096	2.429533	0.638021
1	6.236701	2.940183	2.192487
1	5.737860	4.390439	1.309153
1	5.259874	4.165550	3.002782
1	-0.335407	2.524651	2.081765
1	1.155113	2.859560	2.605954
1	1.128323	2.867418	0.498689
1	3.540009	5.875706	-1.037373
1	2.798594	1.804590	-2.225717
1	5.972709	5.460600	-1.170839
1	5.213144	1.413467	-2.392931
1	6.821583	3.215066	-1.836298
1	0.870819	1.999641	-2.140495
1	-0.590411	2.898800	-1.692868
1	0.197776	3.213506	-3.266848

TS-2-*S*

6	-5.316807	1.955719	0.477038
6	-6.390058	1.409668	1.162416
6	-6.836669	2.010647	2.342038
6	-6.249366	3.180367	2.800780
6	-5.195159	3.732976	2.081561
6	-4.693286	3.132369	0.920665
6	-7.919815	1.177951	2.969764
6	-7.746956	-0.167603	2.255460
6	-7.240481	0.203952	0.837142
6	-6.708850	-1.011945	0.108913
6	-7.742227	-1.618865	-0.611635
6	-8.981377	-0.768823	-0.564630
6	-8.435314	0.577250	-0.075844

6	-7.533937	-2.817821	-1.276354
6	-6.275424	-3.405475	-1.226553
6	-5.206045	-2.802089	-0.554954
6	-5.443950	-1.583182	0.097553
8	-4.383549	-0.900242	0.685179
15	-3.638984	0.199842	-0.248333
8	-3.247988	-0.415652	-1.593834
8	-4.809582	1.257739	-0.615740
8	-2.559419	0.807884	0.594715
7	-0.787824	-1.347013	-0.260329
6	-0.321160	-0.831036	0.895594
8	-0.982650	-1.316033	1.927612
6	-0.791920	-0.846867	3.308431
6	-0.676100	-0.802304	-1.588770
6	-0.331741	0.583295	-1.726806
8	0.315385	0.917112	-2.808074
6	0.629231	2.301214	-3.013194
8	0.562082	0.034677	0.975333
8	-0.700177	1.548344	-0.962472
1	-4.721929	4.649584	2.429389
1	-6.593066	3.651014	3.720098
1	-8.339416	-3.289065	-1.836556
1	-6.096377	-4.353851	-1.730162
1	-9.482768	-0.701479	-1.537361
1	-9.718590	-1.181411	0.140780
1	-8.049560	1.152959	-0.928585
1	-9.177881	1.198181	0.439660
1	-8.914111	1.608168	2.775785
1	-7.818546	1.102687	4.058844
1	-6.964336	-0.753496	2.757309
1	-8.657199	-0.778891	2.229303
1	-2.040351	-0.594939	-1.772437
1	-1.549042	-2.009108	-0.128671
1	-0.283701	2.893823	-3.125129
1	1.208475	2.682521	-2.165596
1	1.221107	2.321747	-3.928442
1	-1.367510	1.289434	-0.229020
6	-0.103651	-1.752588	-2.592660
6	-0.602391	-1.774174	-3.896478
6	0.921339	-2.634246	-2.245028
6	-0.059874	-2.628993	-4.848731
1	-1.423354	-1.107223	-4.160321
6	1.462495	-3.492788	-3.195789
1	1.289080	-2.653920	-1.219232
6	0.978921	-3.489116	-4.501631
1	-0.454676	-2.630427	-5.862346
1	2.262494	-4.172354	-2.906197
1	1.404469	-4.160381	-5.244340
6	-3.876249	-3.446435	-0.581530
6	-3.139560	-3.654624	0.567778
6	-3.354440	-3.901008	-1.822247
6	-1.881721	-4.305725	0.529109
1	-3.516175	-3.299842	1.526961
6	-2.146363	-4.544299	-1.888181
1	-3.918578	-3.695078	-2.730089
6	-1.375591	-4.764752	-0.721488
1	-1.742789	-4.863998	-2.848268
6	-3.509670	3.712528	0.250774
6	-2.385033	4.078422	1.040628
6	-3.462870	3.918217	-1.110836
6	-1.270732	4.634225	0.471873
1	-2.413375	3.877103	2.110022
6	-2.332372	4.506676	-1.726140
1	-4.312325	3.640062	-1.733327
6	-1.216466	4.879780	-0.921766
1	-0.402930	4.888352	1.079907
6	-2.073168	-1.328948	3.966912
1	-2.167042	-2.419401	3.899153
1	-2.082077	-1.047939	5.025768
1	-2.935893	-0.873477	3.464245
6	-0.709023	0.668992	3.404532
1	0.258784	1.053992	3.078525
1	-1.501266	1.131620	2.805293
1	-0.859696	0.947123	4.454875
6	0.437888	-1.531237	3.873046
1	1.340137	-1.229614	3.330082
1	0.565529	-1.248041	4.925020
1	0.334813	-2.621612	3.817203
6	-2.280916	4.757076	-3.120510
1	-3.138581	4.477792	-3.731234
6	-0.091983	5.478558	-1.536949
1	0.756570	5.752564	-0.913127
6	-1.178715	5.346912	-3.689878
6	-0.070208	5.708595	-2.890619
1	-1.155551	5.538151	-4.760427
1	0.800160	6.171801	-3.350609
6	-1.081472	-4.462603	1.688932
1	-1.469866	-4.098995	2.639389
6	-0.099424	-5.376671	-0.765613
1	0.276969	-5.724727	-1.726481
6	0.164276	-5.029824	1.609846
6	0.657178	-5.499997	0.371132
1	0.778385	-5.127954	2.502525
1	1.644089	-5.952285	0.324730
8	2.608923	2.181395	0.164794
6	3.704728	2.793399	0.078140
8	4.874913	2.347781	0.138532
45	5.112225	0.293856	0.279935
8	5.137957	-1.780930	0.395407
6	4.052050	-2.373945	0.590128

8	2.897685	-1.898100	0.758512
45	2.692975	0.138982	0.490202
8	2.932569	0.454685	2.516603
6	4.106988	0.478692	2.967202
8	5.195500	0.417201	2.350243
8	2.641913	-0.123971	-1.560405
6	3.713294	0.008380	-2.200365
8	4.880161	0.169577	-1.764399
6	4.095734	-3.911314	0.581720
6	3.550566	4.303793	-0.177746
6	3.598035	0.058891	-3.735486
6	4.169683	0.595253	4.499196
9	5.413771	0.600035	4.944821
9	3.521649	-0.434575	5.040945
9	3.569325	1.718457	4.882504
9	2.692920	4.834873	0.690026
9	4.702346	4.941493	-0.085077
9	3.060643	4.481547	-1.408238
9	4.582558	-0.624192	-4.301721
9	3.708239	1.343064	-4.100710
9	2.442754	-0.400898	-4.174746
9	3.439750	-4.400798	1.629208
9	5.333524	-4.371509	0.599381
9	3.494736	-4.343513	-0.530974

TS-2-*R*

7	-0.873037	-1.470271	0.214694
6	0.256818	-1.916488	-0.387622
8	0.191652	-3.202798	-0.694989
6	1.354505	-3.920938	-1.242581
6	-0.990260	-0.075570	0.560891
6	-0.805595	0.714988	-0.624022
8	-0.160143	1.835622	-0.575230
6	0.172524	2.499297	-1.801060
8	1.194344	-1.156625	-0.653781
8	-1.311455	0.376664	-1.765929
1	-2.356403	0.231721	0.771738
1	-1.641984	-2.122920	0.336937
1	0.803859	1.843477	-2.408078
1	0.721506	3.393499	-1.496214
1	-0.733351	2.771388	-2.347822
1	-2.056266	-0.308065	-1.653578
6	-0.312443	0.357751	1.817699
6	-0.549902	1.637451	2.329742
6	0.535755	-0.497271	2.524505
6	0.097713	2.073715	3.477719
1	-1.228382	2.311347	1.802726
6	1.168676	-0.066711	3.684969
1	0.708729	-1.510652	2.164316
6	0.969084	1.226755	4.158478
1	-0.075757	3.088786	3.832956
1	1.831902	-0.747926	4.214217
1	1.478045	1.565243	5.058452
6	0.803581	-5.307596	-1.521465
1	0.459468	-5.782670	-0.596618
1	1.592341	-5.931310	-1.956665
1	-0.034095	-5.258690	-2.226276
6	1.810298	-3.295227	-2.552078
1	2.168569	-2.272713	-2.436764
1	0.983416	-3.304562	-3.272077
1	2.629956	-3.897130	-2.962954
6	2.423344	-3.994356	-0.165092
1	2.707328	-3.008043	0.206061
1	3.326822	-4.469370	-0.565747
1	2.058813	-4.588841	0.681498
8	3.002923	0.732903	-2.171156
6	3.978528	1.405282	-2.597339
8	5.074763	1.652804	-2.043454
45	5.373460	0.923315	-0.128554
8	5.522211	0.125935	1.769182
6	4.610616	-0.653565	2.141563
8	3.583957	-1.030533	1.523563
45	3.217431	-0.178291	-0.324077
8	4.220445	-1.745445	-1.227531
6	5.474736	-1.698603	-1.281164
8	6.249116	-0.782871	-0.917393
8	2.388387	1.493969	0.551101
6	3.134945	2.481334	0.744379
8	4.383689	2.571565	0.617484
6	4.767021	-1.180895	3.578378
6	3.755155	2.001280	-3.998072
6	2.445888	3.796237	1.155486
6	6.107734	-2.986424	-1.836535
9	5.976002	-3.949204	-0.921213
9	5.471227	-3.372025	-2.938193
9	7.389763	-2.831187	-2.112040
9	3.485415	1.027603	-4.860613
9	4.808059	2.673987	-4.423013
9	2.707275	2.827466	-3.954949
9	2.793483	4.746388	0.282662
9	1.131033	3.689620	1.143411
9	2.845342	4.165612	2.366557
9	3.981880	-2.226365	3.801305
9	6.022871	-1.532703	3.813762
9	4.429938	-0.208606	4.424682
6	-6.070975	-2.018139	-0.243085
6	-7.218254	-1.591093	-0.886313
6	-7.849516	-2.431201	-1.804759
6	-7.396905	-3.731653	-1.977461

6	-6.294279	-4.171179	-1.251135
6	-5.577433	-3.325208	-0.392525
6	-8.956855	-1.688859	-2.503117
6	-8.670345	-0.226321	-2.123087
6	-8.011719	-0.314455	-0.724162
6	-7.402691	0.993673	-0.254467
6	-8.332926	1.704360	0.512851
6	-9.586852	0.898261	0.695964
6	-9.104996	-0.514188	0.361959
6	-8.025480	2.950429	1.037159
6	-6.767211	3.490459	0.801821
6	-5.799871	2.798713	0.064755
6	-6.142251	1.542066	-0.454588
8	-5.179851	0.814690	-1.140851
15	-4.267916	-0.216126	-0.286083
8	-3.517115	0.514661	0.833027
8	-5.368976	-1.091778	0.511369
8	-3.439645	-1.002221	-1.251411
1	-5.960847	-5.199938	-1.368192
1	-7.889527	-4.403867	-2.677571
1	-8.754494	3.493192	1.636009
1	-6.509480	4.472354	1.194011
1	-10.004663	0.985734	1.705772
1	-10.372932	1.228172	-0.000395
1	-8.630601	-0.959380	1.247437
1	-9.900278	-1.193618	0.032980
1	-9.945320	-2.010824	-2.142994
1	-8.952394	-1.855536	-3.586842
1	-7.942598	0.205839	-2.823735
1	-9.561968	0.412504	-2.128489
6	-4.471843	3.415182	-0.144121
6	-3.774539	3.939513	0.923048
6	-3.936181	3.562203	-1.451111
6	-2.570646	4.659511	0.741948
1	-4.154416	3.797272	1.935057
6	-2.783864	4.274995	-1.659735
1	-4.476012	3.133899	-2.292496
6	-2.075437	4.857240	-0.579339
1	-2.411918	4.429782	-2.673037
6	-4.338053	-3.780067	0.275065
6	-3.538798	-4.787199	-0.334004
6	-3.906640	-3.259439	1.482813
6	-2.383244	-5.235655	0.248401
1	-3.838782	-5.191430	-1.297857
6	-2.686249	-3.656437	2.075701
1	-4.490041	-2.501288	1.996588
6	-1.906163	-4.675043	1.457556
1	-1.794351	-6.011077	-0.239035
6	-2.193582	-3.026516	3.247520
1	-2.786668	-2.233870	3.701923
6	-0.672476	-5.043881	2.045295
1	-0.089538	-5.840926	1.583237
6	-0.979771	-3.384295	3.775865
6	-0.213348	-4.408179	3.172080
1	-0.596218	-2.871166	4.654791
1	0.743977	-4.690327	3.605312
6	-1.861334	5.226188	1.831028
1	-2.238028	5.058801	2.839971
6	-0.909291	5.639107	-0.765528
1	-0.545788	5.800393	-1.780847
6	-0.736939	5.982788	1.618870
6	-0.259219	6.198022	0.306063
1	-0.204185	6.417105	2.461984
1	0.632176	6.800876	0.149844

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15	0.591972	-0.189209	-0.689624
8	1.122225	-1.501411	-1.537542
8	2.010814	0.632719	-0.427415
6	3.383497	-2.060737	-1.018438
6	2.025032	-2.336154	-0.919215
6	1.576819	-3.458435	-0.205892
6	2.527675	-4.248712	0.451349
6	3.882132	-3.931951	0.433999
6	4.301449	-2.833920	-0.303323
6	5.694286	-2.269186	-0.449760
1	6.295301	-2.878714	-1.139476
1	6.232718	-2.237662	0.505164
6	5.421626	-0.869372	-1.027609
1	5.221531	-0.159682	-0.205495
1	6.255281	-0.470948	-1.626758
6	4.117922	-1.036017	-1.863085
6	4.453685	-1.588110	-3.278238
1	3.534528	-2.014850	-3.715116
1	5.219982	-2.378512	-3.248184
6	4.885708	-0.346711	-4.083465
1	4.675695	-0.442414	-5.155240
1	5.964000	-0.159227	-3.980696
6	4.083526	0.758269	-3.435858
6	3.845504	2.050157	-3.885795
1	4.274128	2.403940	-4.821040
6	3.052720	2.895673	-3.113937
1	2.877877	3.919653	-3.436947
6	2.436789	2.453271	-1.937138
6	2.661070	1.131931	-1.529711
6	3.538008	0.315355	-2.229726
1	4.594652	-4.538485	0.989158
1	2.182350	-5.119123	1.004757
8	-0.325051	0.557529	-1.590330

8	0.194046	-0.608131	0.697803
6	0.144328	-3.872069	-0.154642
6	-0.508139	-3.980564	1.091201
6	-0.520414	-4.272477	-1.334230
6	0.072250	-3.497900	2.310543
6	-1.813245	-4.573799	1.163617
6	-1.857998	-4.789320	-1.254830
6	0.091427	-4.212679	-2.629195
6	-0.561150	-3.664133	3.507653
1	1.017843	-2.967930	2.267525
6	-2.433428	-4.752716	2.442463
6	-2.463134	-4.951033	-0.009172
6	-2.538665	-5.165414	-2.456653
1	1.114981	-3.862886	-2.715138
6	-0.587238	-4.585674	-3.751493
6	-1.823731	-4.322555	3.582445
1	-0.100911	-3.282028	4.415022
1	-3.410898	-5.230469	2.478375
1	-3.461239	-5.384021	0.047993
6	-1.928312	-5.060365	-3.669615
1	-3.556442	-5.542848	-2.374408
1	-0.101437	-4.522466	-4.722274
1	-2.303049	-4.459573	4.549093
1	-2.453966	-5.346258	-4.577689
6	1.601263	3.399506	-1.144049
6	0.446858	3.968462	-1.720518
6	2.011004	3.796875	0.146686
6	-0.091396	3.512130	-2.968586
6	-0.243925	5.023329	-1.037859
6	1.269505	4.806298	0.848165
6	3.160585	3.244598	0.802770
6	-1.200414	4.090824	-3.511111
1	0.375894	2.665011	-3.459205
6	-1.387428	5.624158	-1.654366
6	0.184366	5.420300	0.226788
6	1.664827	5.175448	2.174119
1	3.765558	2.510886	0.279078
6	3.505837	3.619660	2.068149
6	-1.851056	5.177028	-2.854863
1	-1.602756	3.714906	-4.448913
1	-1.888444	6.435564	-1.129260
1	-0.358971	6.203562	0.752844
6	2.742612	4.596260	2.774139
1	1.076962	5.931039	2.692253
1	4.375220	3.172980	2.544992
1	-2.726482	5.633533	-3.311306
1	3.032592	4.880281	3.783205
6	-2.602891	3.327785	0.533704
6	-1.347768	3.462837	3.034722
6	-2.845159	4.396267	1.370776
6	-2.213117	4.454967	2.627470
6	-1.092913	2.365129	2.180199
1	-0.059813	0.638085	1.814363
1	-1.525277	1.477627	0.255865
1	-3.059146	3.276893	-0.451439
1	-3.502915	5.202528	1.056281
1	-2.402041	5.300283	3.285354
1	-0.857127	3.529189	4.000526
1	-1.194335	-0.830620	3.328070
1	-3.613936	1.718083	2.982326
6	0.598683	1.388082	3.695787
1	1.197659	2.326980	3.565819
1	0.011142	1.469259	4.639106
6	-4.672519	0.960296	1.171983
1	-4.861903	1.993806	0.850938
1	-5.612746	0.617084	1.645146
6	-4.328281	0.046031	-0.015238
1	-3.413949	0.443545	-0.493924
6	-3.995671	-1.351999	0.524359
1	-4.866767	-1.744991	1.079666
1	-3.801385	-2.047998	-0.308377
6	-2.765116	-1.305082	1.433024
1	-2.698106	-2.223070	2.023527
1	-1.845754	-1.254805	0.839082
6	-2.748480	-0.135839	2.387757
6	-3.616348	0.938191	2.222435
7	-1.832907	-0.006209	3.352870
7	-0.340775	1.295948	2.573656
6	-1.770583	2.277769	0.948370
6	1.515188	0.190688	3.738115
6	1.431061	-0.742664	4.770945
6	2.468253	0.008445	2.732358
6	2.285526	-1.844792	4.799656
1	0.688819	-0.609855	5.556561
6	3.309039	-1.097381	2.749361
1	2.530634	0.721510	1.916049
6	3.220256	-2.027778	3.784106
1	2.211952	-2.566262	5.610466
1	4.025498	-1.241336	1.944955
1	3.875409	-2.895983	3.792548
6	-5.425185	0.053095	-1.056375
6	-5.191162	0.610592	-2.315736
6	-6.691005	-0.479072	-0.789199
6	-6.192111	0.637817	-3.284391
1	-4.208595	1.024306	-2.539498
6	-7.693610	-0.455648	-1.754285
1	-6.896283	-0.921264	0.184287
6	-7.447792	0.104162	-3.006835
1	-5.988535	1.076040	-4.259002
1	-8.670434	-0.878451	-1.529233

1	-8.230233	0.121902	-3.761923

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15	0.902246	0.841411	0.294853
8	0.263658	2.362114	0.368718
8	2.452463	1.130361	-0.197893
6	1.424900	3.879284	-1.062015
6	0.295427	3.116926	-0.784071
6	-0.794103	3.111509	-1.667246
6	-0.688938	3.844288	-2.855549
6	0.465805	4.548113	-3.181719
6	1.518902	4.559860	-2.278244
6	2.871324	5.217505	-2.412990
1	2.798774	6.297991	-2.223043
1	3.300745	5.092477	-3.413994
6	3.688304	4.508720	-1.319157
1	4.098749	3.564736	-1.717568
1	4.525662	5.111793	-0.934704
6	2.649423	4.166181	-0.210510
6	2.439026	5.386979	0.730046
1	1.487602	5.251863	1.272464
1	2.388045	6.338051	0.176831
6	3.619009	5.317419	1.720445
1	3.379176	5.752102	2.697915
1	4.496578	5.855334	1.334478
6	3.892672	3.832850	1.800947
6	4.654854	3.126252	2.721287
1	5.176034	3.639945	3.526459
6	4.750352	1.741279	2.596124
1	5.365773	1.173831	3.291109
6	4.042037	1.043721	1.612221
6	3.247979	1.780206	0.722023
6	3.230829	3.165657	0.768281
1	0.538211	5.075960	-4.130226
1	-1.531554	3.836151	-3.543728
8	0.879092	0.325366	1.693938
8	0.283309	0.083684	-0.844938
6	-2.082824	2.405984	-1.395511
6	-2.469525	1.311202	-2.196288
6	-2.974422	2.923383	-0.433156
6	-1.581029	0.697307	-3.138549
6	-3.792832	0.770012	-2.071266
6	-4.294130	2.369515	-0.315028
6	-2.629711	4.013001	0.432454
6	-1.979151	-0.365009	-3.895450
1	-0.565939	1.071071	-3.213556
6	-4.178000	-0.335997	-2.895119
6	-4.680856	1.325406	-1.151446
6	-5.197740	2.902497	0.659564
1	-1.644246	4.461203	0.348413
6	-3.514047	4.488192	1.355556
6	-3.300104	-0.888174	-3.779372
1	-1.280571	-0.827267	-4.588819
1	-5.189389	-0.726838	-2.791915
1	-5.687977	0.920799	-1.066526
6	-4.818070	3.923834	1.477463
1	-6.186980	2.455532	0.742046
1	-3.225361	5.308906	2.008123
1	-3.597474	-1.735660	-4.392935
1	-5.506544	4.317142	2.221870
6	4.173571	-0.438252	1.500275
6	3.682589	-1.281143	2.517779
6	4.841943	-0.989986	0.386061
6	2.944624	-0.782795	3.641158
6	3.886584	-2.699790	2.425355
6	5.029192	-2.409677	0.300567
6	5.363777	-0.183892	-0.678605
6	2.459392	-1.626147	4.596146
1	2.744672	0.281130	3.701521
6	3.366397	-3.550477	3.452974
6	4.558940	-3.228928	1.325515
6	5.689869	-2.962528	-0.841380
1	5.257783	0.895198	-0.622550
6	5.987132	-0.748372	-1.751773
6	2.674678	-3.032743	4.505836
1	1.890957	-1.226036	5.432393
1	3.531818	-4.622980	3.365868
1	4.703333	-4.306380	1.253311
6	6.147326	-2.161111	-1.842089
1	5.800994	-4.042994	-0.899303
1	6.368162	-0.114979	-2.549621
1	2.277598	-3.688011	5.277792
1	6.633057	-2.593205	-2.713543
6	-3.297112	-3.517936	-1.371119
6	-0.876152	-4.759889	-0.689569
6	-3.181687	-4.888144	-1.443607
6	-1.962120	-5.504031	-1.089009
6	-0.973980	-3.346606	-0.638575
1	-0.030958	-1.546257	-0.456449
1	-2.279658	-1.652387	-0.954131
1	-4.221682	-3.018407	-1.648076
1	-4.016819	-5.496558	-1.781004
1	-1.872125	-6.586332	-1.147243
1	0.061005	-5.248454	-0.445335
1	0.082968	-1.449418	2.003522
1	-2.426742	-3.871344	1.643564
6	1.411507	-2.995468	-0.004160
1	1.419479	-3.860276	0.695736
1	1.923792	-2.147748	0.510017

6	-4.224707	-2.557855	1.554900
1	-4.733334	-3.254344	0.873523
1	-4.600094	-2.805580	2.567368
6	-4.549133	-1.091100	1.231287
1	-4.245406	-0.919997	0.182805
6	-3.682724	-0.186929	2.112866
1	-3.848792	-0.434721	3.177684
1	-3.954284	0.869905	1.980516
6	-2.205671	-0.376264	1.772637
1	-1.563578	0.194989	2.449429
1	-2.001911	0.015835	0.763432
6	-1.800827	-1.834978	1.807360
6	-2.761146	-2.829670	1.575528
7	-0.552383	-2.260655	1.903581
7	0.031699	-2.551333	-0.201285
6	-2.220873	-2.738146	-0.909423
6	2.109168	-3.315990	-1.307101
6	2.620841	-4.589505	-1.550674
6	2.260373	-2.322550	-2.278626
6	3.270746	-4.875294	-2.749882
1	2.518020	-5.363519	-0.791162
6	2.905963	-2.607227	-3.476570
1	1.872697	-1.324144	-2.085399
6	3.411161	-3.884567	-3.716764
1	3.667798	-5.872638	-2.926485
1	3.022821	-1.825667	-4.223977
1	3.917345	-4.103697	-4.654282
6	-6.038807	-0.832316	1.304425
6	-6.854224	-1.265176	0.252149
6	-6.641112	-0.178538	2.380856
6	-8.227990	-1.048866	0.268251
1	-6.395677	-1.767167	-0.599909
6	-8.018154	0.041270	2.402612
1	-6.033563	0.177800	3.208828
6	-8.816316	-0.391302	1.347781
1	-8.840273	-1.387150	-0.564887
1	-8.466827	0.556327	3.249282
1	-9.889366	-0.215258	1.363912