Supporting Information for

Unusual Non-bifunctional Mechanism for Co-PNP Complex Catalyzed Transfer Hydrogenation Governed by the Electronic Configuration of Metal Center

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1. Complete Citation for Ref. 55

(19) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; B. Mennucci; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; J. A. Montgomery, J.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; J. J. Heyd, E. B.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2009.

2. The Potential Energy Surface of Fe-PNP catalyst

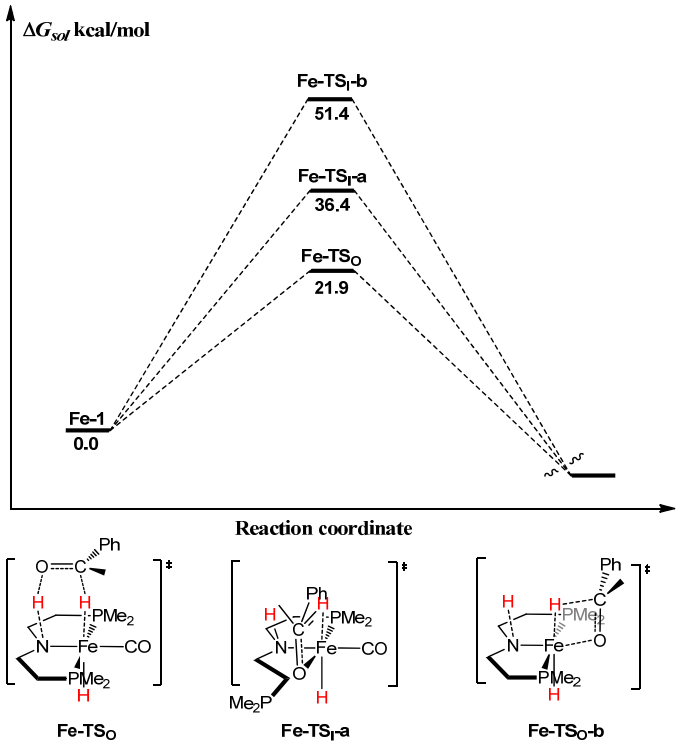

Figure S1. The hydride transfer mechanism of Fe-PNP catalyst through inner sphere and outer sphere

The hydride transfer mechanisms of Fe-PNP catalyst are depicted in Figure S1. As shown in the figure, the hydrogenation process via a bifunctional transition state **Fe-TS$_O$** has the lowest activation free energy 21.9 kcal/mol. However, the non-bifunctional mechanisms via the inner sphere are difficult to occur due to the high energy barrier. The inner sphere hydride transfer through the dissociation of phosphors ligand **Fe-TS$_I$-a** will lead to an activation energy of 36.4 kcal/mol. Moreover, the hydride transfer with the dissociation of carbonyl compound **Fe-TS$_I$-b** is even higher energy barrier (51.4 kcal/mol). This is because the back-donation effect of CO will stabilize the complex. Thus, it cost an extra energetic penalty to dissociate this compound. Finally, the Fe-PNP hydrogenation catalyst will follow a typical bifunctional pathway.

3. The molecular orbital explanation of β-hydride elimination process.

For β-hydride elimination process, it is required that the complex has an open coordination site, which means there's empty orbital on the metal center. We have illuminated the change of molecular orbital during the *β*-hydride elimination process. For the complex **I-4$_{vacant}$**, because the vacant site of X axis, the dx^2-y^2 will mix with $4p_x$ to form a polarized molecular orbital. This empty orbital can interact with the electron pair of C-H bond to form the agostic complex **I-4$_{Agostic}$** and lead to the *β*-hydride elimination process. We can consider the polarized dx^2-y^2 mixed with $4p_x$ as the empty orbital to accept the electron pair of hydride.

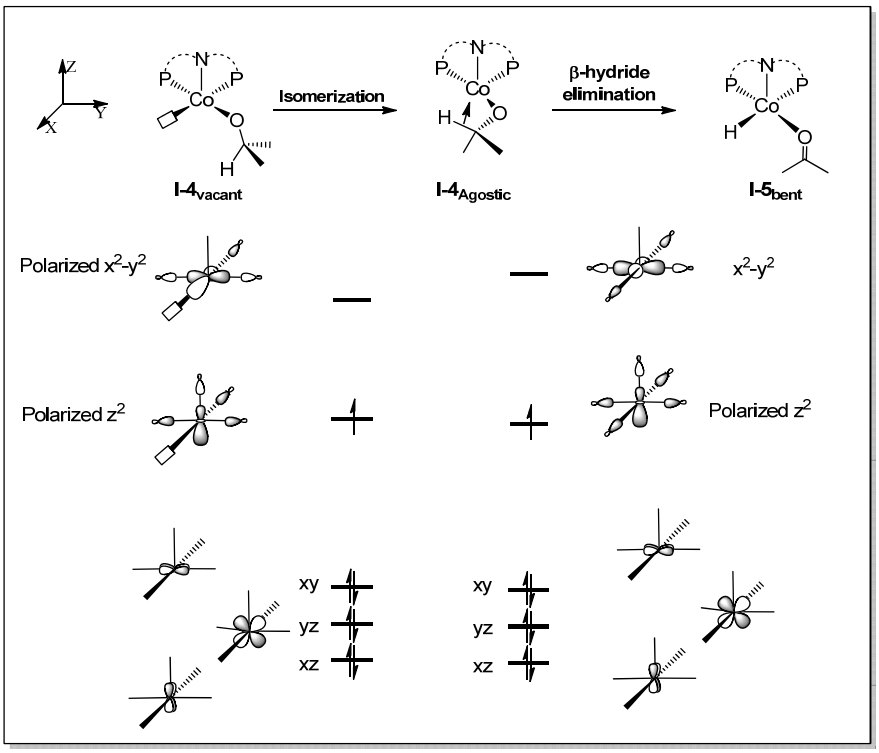

Figure S2. The molecular orbital explanation of β-hydride elimination process

4. The bifunctional mechanism via the tetrahedral geometry at quartet spin status and the "butterfly" type complex.

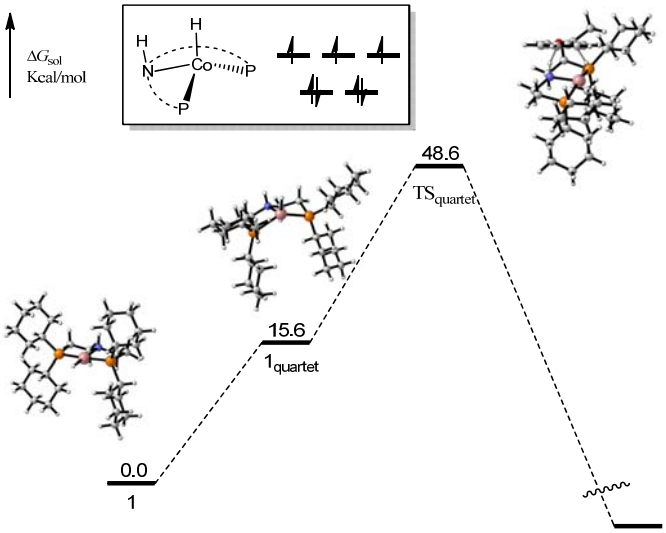

Figure S3. The bifunctional mechanism via the complex at quartet spin state.

The geometry of the complex changes along the change of spin state. By reading the geometry and wavefunctions information in chk file of quartet, we set the spin state at doublet. However, the geometry changes from tetrahedron to square plane. Thus, the quartet complex at tetrahedral geometry is 15.6 kcal/mol higher than doublet complex. By reading the geometry and wavefunctions information in chk file of doublet, we set the spin state at quartet. Somehow, the geometry changes into a "butterfly" type geometry. In this geometry, the quartet is 21.9 kcal/mol higher than the doublet square planar complex. The spin contamination of the tetrahedral geometry is 0.28%. The spin contamination of butterfly type is 0.42%. The spin contamination for the **O-TS1$_{\mathbf{quartet}}$** is 0.68%. These data are all very small, indicating no spin contamination in our studied system.

With respect to the quartet situation, the bifunctional transfer mode will occur with a total energy barrier of 48.6 kcal/mol. Another bifunctional transfer model via a "butterfly" type complex bearing a bent PNP ligand is also verified to be inaccessible ($\Delta G^{\neq}$ = 48.4 kcal/mol). The full model situation is unable to be located by computational method due to the high steric repulsion. Therefore, we rule these two mechanisms.

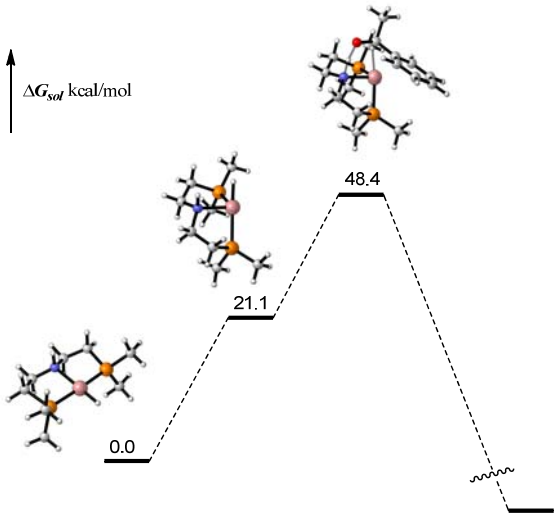

Figure S4. The bifunctional mechanism via the "butterfly" type complex.

5. The MO comparison of different coordination status of Co^{II} center

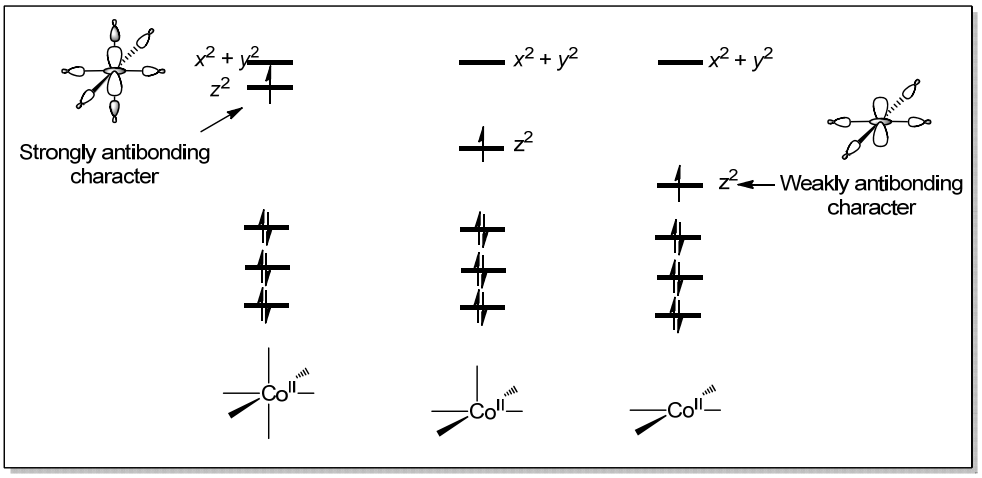

Figure S5. The MO comparison of different coordination status of Co^{II} center.

In organometallic chemistry, a classical principle, known as "18-Electron rule", is generally used to predict stable metal complexes. In the terms of the molecular orbital theory, which means the bonding orbital and nonbonding orbital need to be fully occupied to gain the maximum stabilization energy. Many d^7 and d^8 complex choose the square-planar geometry because there's no extra ligand on the direction of Z axis. In this situation, the ligand MO linearly combined of the ligand orbitals on the XY planar will have small interaction (small overlap) with the d_z^2 orbital will lead to a weakly antibonding orbital.

From this perspective, the most stable geometry for d^7 Co^{II} center should be the square-planar geometry. On the other hand, the maximum numbers of the coordination ligands is 5, which leads to a 17e complex. It does not violate the "18-Electron rule" and can be located by computational method. Thus, the five-coordinated complex is already saturated for a d^7 complex. The six-coordinated geometry will lead to singly occupied d_z^2 orbital with strongly antibonding character. In other words, it violates the "18-Electron rule" as the six-coordinated d^7 complex is an unstable "19e complex".

6. The bifunctional transfer mechanism of Co^{III} six-coordinated catalyst

For the Co^{II} d^7 center, six-coordinated geometry will lead to an unreasonable 19e complex (please see next reply). On the other hand, Co^{III} offers a chance for six coordinated geometry by forming an 18e complex. However, it is found that Co^{II}, rather than Co^{III}, is the active catalyst for the transfer hydrogenation of C=O and C=N bonds (*Chem Commun*. 2013, 49, 10151). Therefore, six-coordinated Co^{II} or Co^{III} did not be further considered according to the analysis above and experimental observation. Even though we use six-coordinated Co^{III} to calculate the energy barrier for the metal-ligand cooperation mechanism, the results suggest it is much higher than Co^{II} inner-sphere mechanism ($\Delta G^{\neq}$ = 43.3 kcal/mol). Therefore, calculation also suggests that Co^{III} metal-ligand cooperation mechanism is less possible. It can also explain the low efficiency of Co^{III} catalyst found in *Chem Commun* paper.

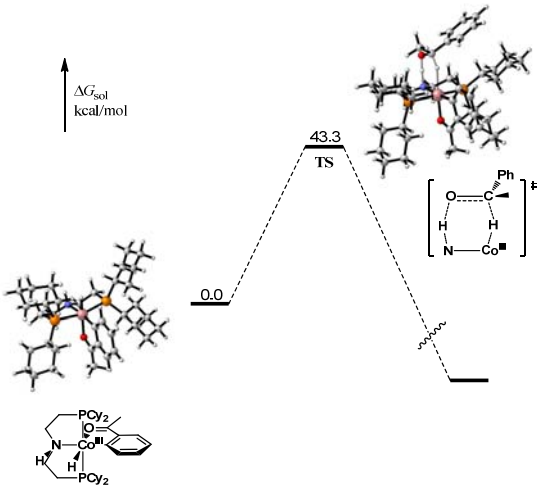

Figure S6. The energy barrier of Co^{III} complex based on bifunctional transfer mechanism

7. The absolute energies of all optimized structures.

Table S1. The absolute energies of all optimized structures

Species	$Zero_c$ (BSI)	H_c (BSI)	G_c (BSI)	E_0 (BSI)	H (BSI)	G (BSI)	SP+SOL (BSII)	SP (BSII)	Sol G Kcal/mol	Final Free energy
AcPh	0.138211	0.14694	0.105593	-384.762	-384.753	-384.795	-385.015214	-385.001707	-8.48	-384.903
THF	0.11676	0.121268	0.090086	-232.334	-232.33	-232.361	-232.520446	-232.513622	-4.28	-232.424
IPA	0.108279	0.114647	0.080911	-194.257	-194.251	-194.284	-194.431547	-194.424272	-4.56	-194.344
Acetone	0.083763	0.090125	0.055931	-193.077	-193.07	-193.105	-193.227579	-193.218205	-5.88	-193.165
PE	0.161367	0.170706	0.127881	-385.937	-385.928	-385.971	-386.215707	-386.203198	-7.85	-386.081
Inner sphere										
1	0.294776	0.313386	0.249722	-1200.22261	-1200.204	-1200.267664	-1200.739519	-1200.659715	-50.08	-1200.482945
***cis*-I-1**	0.434544	0.461753	0.377677	-1585.014238	-1584.987028	-1585.071105	-1585.759704	-1585.68726	-45.46	-1585.375175
***trans*--I-1**	0.434948	0.462862	0.376374	-1585.010835	-1584.982921	-1585.069409	-1585.757263	-1585.683686	-46.17	-1585.374037
***cis*-I-TS1**	0.434451	0.461389	0.379071	-1584.975983	-1584.949045	-1585.031362	-1585.724681	-1585.648634	-47.72	-1585.338758
***trans*-I-TS1**	0.434337	0.46134	0.378213	-1584.971685	-1584.944682	-1585.027809	-1585.720273	-1585.643795	-47.99	-1585.335208
I-2	0.43915	0.466557	0.381513	-1585.001233	-1584.973825	-1585.058869	-1585.762056	-1585.677787	-52.88	-1585.373691
$I\text{-}1_{bent}$	0.435058	0.462839	0.377718	-1584.996519	-1584.968738	-1585.053859	-1585.74	-1585.67	-43.68	-1585.354813
$I\text{-}TS1_{bent}$	0.434349	0.461213	0.378861	-1584.988326	-1584.961462	-1585.043813	-1585.73	-1585.66	-46.5	-1585.34904
$I\text{-}2_{Agostic}$	0.437338	0.464559	0.38	-1584.992383	-1584.965162	-1585.04931	-1585.75	-1585.67	-49.96	-1585.359666
I-TS3	0.433301	0.460636	0.375635	-1584.959683	-1584.932349	-1585.017349	-1585.72	-1585.63	-53.68	-1585.334652
$I\text{-}TS3_{shuttle}$	0.541752	0.575062	0.477962	-1779.262228	-1779.228918	-1779.326019	-1780.17	-1780.09	-46.11	-1779.680643
$I\text{-}3_a$	0.272915	0.291347	0.227477	-1199.004332	-1198.9859	-1199.04977	-1199.5	-1199.42	-51.44	-1199.265154
$I\text{-}3_b$	0.384856	0.409567	0.331149	-1393.310162	-1393.285452	-1393.36387	-1393.959554	-1393.8885	-44.6	-1393.621553
I-TS4	0.380056	0.404357	0.327602	-1393.277906	-1393.253605	-1393.33036	-1393.932196	-1393.851454	-50.67	-1393.597742
$I\text{-}TS4_{shuttle}$	0.487509	0.518133	0.426034	-1587.57	-1587.54	-1587.635817	-1588.245952	-1588.174241	-45	-1587.819918

Species	$Zero_c$ (BSI)	H_c (BSI)	G_c (BSI)	E_0 (BSI)	H (BSI)	G (BSI)	SP+SOL (BSII)	SP (BSII)	Sol G Kcal/mol	Final Free energy
***cis*-I-TS2**	0.65475	0.693979	0.5843	-1973.55066	-1973.511431	-1973.621109	-1974.620483	-1974.545103	-47.3	-1974.029331
***cis*-I-TS2$_{shuttle}$**	0.547588	0.579945	0.486855	-1779.1562	-1779.1238	-1779.2169	-1780.1787	-1780.1006	-49.02	-1779.685
***trans*-TS2**	0.655113	0.69436	0.585425	-1973.5423	-1973.5031	-1973.612	-1974.6147	-1974.5374	-48.54	-1974.0224
***trans*-TS2$_{shuttle}$**	0.548084	0.580417	0.487805	-1779.1492	-1779.1169	-1779.2095	-1780.1695	-1780.0907	-49.44	-1779.6748
I-TS5	0.54649	0.579438	0.484101	-1779.2657	-1779.2327	-1779.3281	-1780.1739	-1780.0993	-46.82	-1779.683
I-TS5$_{shuttle}$	0.653646	0.693509	0.580097	-1973.5496	-1973.5097	-1973.6231	-1974.6156	-1974.5415	-46.48	-1974.0286
I-4$_{vacant}$	0.385812	0.4103	0.333128	-1393.3031	-1393.2786	-1393.4	-1393.9549	-1393.8801	-46.98	-1393.6149
***cis*-I-TS6**	0.381113	0.405174	0.32927	-1393.29	-1393.2659	-1393.3418	-1393.9393	-1393.8644	-46.97	-1393.6032
***trans*-I-TS6**	0.38125	0.405209	0.329294	-1393.2857	-1393.2617	-1393.3376	-1393.9354	-1393.8598	-47.44	-1393.5993
***cis*-I-5**	0.380421	0.405869	0.325153	-1393.3268	-1393.3013	-1393.382	-1393.9724	-1393.9016	-44.39	-1393.6404
***trans*-I-5**	0.380501	0.405886	0.325524	-1393.3236	-1393.2983	-1393.3786	-1393.9697	-1393.898	-45	-1393.6373
I-4	0.386171	0.410433	0.333832	-1393.32	-1393.2958	-1393.3724	-1393.9771	-1393.8982	-49.51	-1393.6364
I-4$_{Agostic}$	0.384725	0.408754	0.333724	-1393.3099	-1393.2859	-1393.361	-1393.9616	-1393.8867	-47	-1393.621038
I-TS6$_{bent}$	0.380729	0.404672	0.329903	-1393.3029	-1393.279	-1393.3537	-1393.948	-1393.8773	-44.35	-1393.611259
I-5$_{bent}$	0.38105	0.406126	0.327286	-1393.3104	-1393.2853	-1393.3642	-1393.9531	-1393.8855	-42.41	-1393.618944
Cy-I-2	0.941872	0.986449	0.861629	-2365.48	-2365.43	-2365.56	-2367.400329	-2367.309241	-57.16	-2366.451326
Cy-I-4	0.888339	0.929909	0.81333	-2173.83	-2173.79	-2173.91	-2175.611072	-2175.525191	-53.89	-2174.716137
Cy-I-TS1	0.936252	0.980602	0.858156	-2365.44	-2365.39	-2365.5	-2367.359537	-2367.278577	-50.8	-2366.415669
Cy-I-TS2	1.160365	1.216846	1.068718	-2753.89	-2753.84	-2754.0	-2756.234626	-2756.15223	-51.7	-2755.062218
Cy-I-TS3	0.882137	0.92361	0.808502	-2173.8	-2173.75	-2173.9	-2175.574963	-2175.496654	-49.14	-2174.685885
Outer-sphere										
1	0.294776	0.313386	0.249722	-1200.2226	-1200.204	-1200.2677	-1200.7395	-1200.6597	-50.08	-1200.482945
O-2$_{AcPh}$	0.434553	0.46247	0.376537	-1585.0093	-1584.9814	-1585.0673	-1585.7528	-1585.6817	-44.64	-1585.369432

Species	$Zero_c$ (BSI)	H_c (BSI)	G_c (BSI)	E_0 (BSI)	H (BSI)	G (BSI)	SP+SOL (BSII)	SP (BSII)	Sol G Kcal/mol	Final Free energy
O-TS1$_{AcPh}$	0.572462	0.608921	0.503567	-1969.7454	-1969.7089	-1969.8143	-1970.731	-1970.6535	-48.68	-1970.220616
O-3$_{AcPh}$	0.41399	0.441489	0.355452	-1583.8275	-1583.8	-1583.8861	-1584.5483	-1584.4785	-43.83	-1584.186021
O-TS2$_{AcPh}$	0.519071	0.55253	0.454546	-1778.0586	-1778.0251	-1778.1231	-1778.9451	-1778.8692	-47.62	-1778.483732
O-2$_{THF}$	0.413631	0.438641	0.359933	-1432.5752	-1432.5502	-1432.6289	-1433.2598	-1433.1891	-44.34	-1432.892996
O-TS1$_{THF}$	0.551871	0.585223	0.487614	-1817.3136	-1817.2803	-1817.3779	-1818.2409	-1818.1632	-48.76	-1817.7464
O-3$_{THF}$	0.392969	0.41751	0.338237	-1431.3932	-1431.3686	-1431.4479	-1432.0556	-1431.9856	-43.92	-1431.710473
O-TS2$_{THF}$	0.498518	0.528843	0.438396	-1625.6266	-1625.5963	-1625.6867	-1626.4549	-1626.3789	-47.64	-1626.009603
O-2$_{IPA}$	0.405276	0.430581	0.35189	-1394.4914	-1394.4661	-1394.5448	-1395.1623	-1395.0912	-44.63	-1394.80359
O-TS1$_{IPA}$	0.54278	0.576683	0.478485	-1779.2307	-1779.1968	-1779.295	-1780.144	-1780.0654	-49.32	-1779.658685
O-3$_{IPA}$	0.384856	0.409567	0.331149	-1393.3102	-1393.2855	-1393.3639	-1393.9596	-1393.8885	-44.6	-1393.621553
O-TS2$_{IPA}$	0.489471	0.520342	0.429517	-1587.5434	-1587.5125	-1587.6033	-1588.3583	-1588.2808	-48.6	-1587.921917
O-TS1$_{shuttle}$	0.540888	0.574532	0.476125	-1779.224	-1779.1904	-1779.2888	-1780.1237	-1780.0541	-43.69	-1779.640698
O-3	0.272915	0.291347	0.227477	-1199.0043	-1198.9859	-1199.0498	-1199.4995	-1199.4175	-51.44	-1199.265154
O-TS2$_{shuttle}$	0.538287	0.57192	0.473109	-1779.2219	-1779.1883	-1779.2871	-1780.1228	-1780.0498	-45.82	-1779.64287
Cy-2	0.795356	0.831365	0.725881	-1980.8	-1980.76	-1980.87	-1982.39	-1982.3	-54.79	-1981.589865
Cy-O-2	0.915344	0.95767	0.839257	-2213.06	-2213.02	-2213.14	-2214.89	-2214.81	-49.35	-2213.963749
Cy-O-3	0.895262	0.936863	0.819469	-2211.89	-2211.85	-2211.96	-2213.69	-2213.61	-49.47	-2212.787575
Cy-O-TS1	1.055527	1.106081	0.969745	-2597.7	-2597.65	-2597.79	-2599.86	-2599.78	-54.51	-2598.799328
Cy-O-TS2	1.000527	1.04861	0.916685	-2406.06	-2406.01	-2406.14	-2408.08	-2408	-52.95	-2407.072665
Quartet										
2$_{quartet}$	0.292566	0.312027	0.245279	-1200.1969	-1200.1775	-1200.2442	-1200.7188	-1200.6326	-54.09	-1200.466683
TS1$_{quartet}$	0.431746	0.459363	0.373659	-1584.9443	-1584.9167	-1585.0024	-1585.7071	-1585.6164	-56.91	-1585.326611
Fe-PNP										

Species	$Zero_c$ (BSI)	H_c (BSI)	G_c (BSI)	E_0 (BSI)	H (BSI)	G (BSI)	SP+SOL (BSII)	SP (BSII)	Sol G Kcal/mol	Final Free energy
CO	0.007397	0.008341	-0.014102	-113.29952	-113.29857	-113.32102	-113.34453	-113.34883	2.7	-113.3517805
Fe-1	0.310542	0.330885	0.264424	-1292.6699	-1292.6496	-1292.716	-1293.1898	-1293.1659	-14.96	-1292.918483
Fe-TSo	0.450112	0.47885	0.393533	-1677.4292	-1677.4004	-1677.4858	-1678.1868	-1678.1637	-14.47	-1677.78643
Fe-TSI-a	0.440887	0.467416	0.38757	-1564.0597	-1564.0332	-1564.113	-1564.771	-1564.7452	-16.18	-1564.37654
Fe-TSI-b	0.448436	0.478491	0.386998	-1677.394	-1677.3639	-1677.4554	-1678.1574	-1678.1237	-21.11	-1677.763519

- The **Zero c, H c and G c** designate the thermal correction to Energy, Enthalpy and Gibbs Free Energy.
- The **E, H and G** designate the thermal correction to Energy, Enthalpy and Gibbs Free Energy.
- **SP** designate the single point energy.

8. The comparison of energy barrier using different functionals.

Table S2. The comparison of energy barrier using different functionals (Simple model)

Functionals	$\mathbf{I\text{-}TS2_{shuttle}}$	$\mathbf{O\text{-}TS1_{THF}}$
B3LYP	27.6	39.4
M06L	13.7	25.0
M06	10.2	26.2
TPSS	36.4	39.5
BMK	17.3	28.6
TPSSH	34.4	41.3

In order to compare the performance using different functionals, we have tested several functionals of different percentage HF exchange. In former B3LYP/BSII calculation results, the rate-determining step of inner sphere mechanism is $\mathbf{I\text{-}TS2_{shuttle}}$ and the rate-determining step of outer sphere mechanism is $\mathbf{O\text{-}TS1_{THF}}$. Therefore, we chose these two simple-model TSs to evaluate the performance of different functionals. Although the energy barrier does change with different functional, the mechanistic preference is still the same, which all suggest the outer sphere bifunctional mechanism is not favored. We noted that the M06l significantly lower the energy barrier with nearly ~10 kcal/mol. Therefore, we assume M06L will provide more accurate results.

Table S3. The comparison of energy barrier using different functionals (Full model)

Functionals	$\mathbf{I\text{-}TS2_{shuttle}}$	$\mathbf{O\text{-}TS1_{THF}}$
B3LYP	36.7	47.8
M06L	32.2	44.1
M06	30.6	44.2
TPSS	63.0	60.8

We then used full model of $\mathbf{I\text{-}TS2_{shuttle}}$ and $\mathbf{O\text{-}TS1_{THF}}$ to further confirmed the mechanistic preference. For wB97XD, BMK and TPSSH, we found it so hard to converge at full model at BSII level (with nearly 1500 basis functions) that we are not able to get the data. For TPSS, the mechanistic preference is inversed. M06 and M06L give more reasonable results. Compared with M06L, M06 is very slow to converge. However, few inconsistencies with B3LYP emerge when using M06L. **I-TS2** becomes more favored than $\mathbf{I\text{-}TS2_{shuttle}}$ when using M06l functional both in simplified model and full model. On the other hand, the rate-determining step slightly shifts to **I-TS3**, but the energy difference between **I-TS3** and **I-TS2** is very tiny (0.5 kcal/mol).

Above all, the mechanistic preference is consistent with the experimental observation (Inner sphere: 26.9 kcal/mol *vs.* Outer sphere: 44.1 kcal/mol). The original B3LYP/BSII data are used for the main discussion. The M06-L/BSII data based on the single point energy is shown along with the B3LYP data in the main context as a comparison.

9. The overall mechanistic comparison based on the full model at M06-L/BSII level calculation

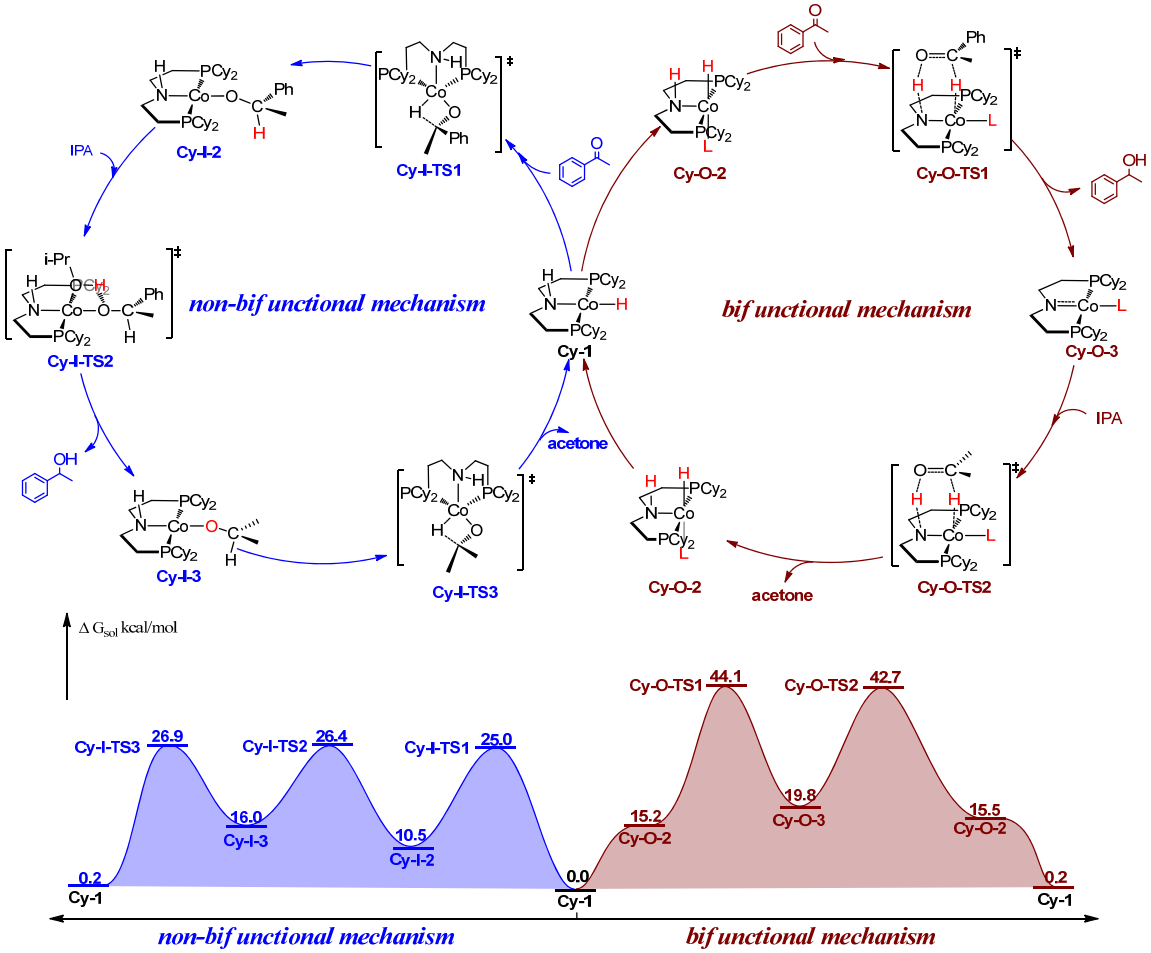

Figure S7. The overall comparison of non-bifunctional mechanism and bifunctional mechanism for Co-PNP catalyzed transfer hydrogenation based on the full model catalyst. The relative free energies are given in kcal/mol.

10. The comparison of different functionals include dispersion effects

Table S4. The relative activation energy of two rate-determining transition states optimized by different functionals. The results in the table are calculated at M06-L/BSII level. The relative free energies are given in kcal/mol.

Functionals	$\mathbf{I\text{-}TS2_{shuttle}}$	$\mathbf{O\text{-}TS1_{THF}}$
M06-L/BSII/SMD//B3LYP/BSI	13.7	25.0
M06-L/BSII/SMD//B3LYP-D3/BSI	15.8	26.4
M06-L/BSII/SMD//M06L/BSI	14.3	26.2

At M06-L/BSII level, we checked the relative energy of the rate-determining transition states optimized by different functionals with dispersion effects (B3LYP-D3 and M06-L). The difference in the energy results is quite small. The predicted mechanism is still the same when changing different functional to optimize the structure. But the difference in optimized geometries between B3LYP, B3LYP-D3 and M06-L do exist.

Therefore, the original B3LYP/BSII data are used for the main discussion. The M06-L/BSII data based on the single point energy is shown along with the B3LYP data in the main context as a comparison.

11. The explanation of the difference of relative energy of Cis-I-TS2 between B3LYP and M06L (S16).

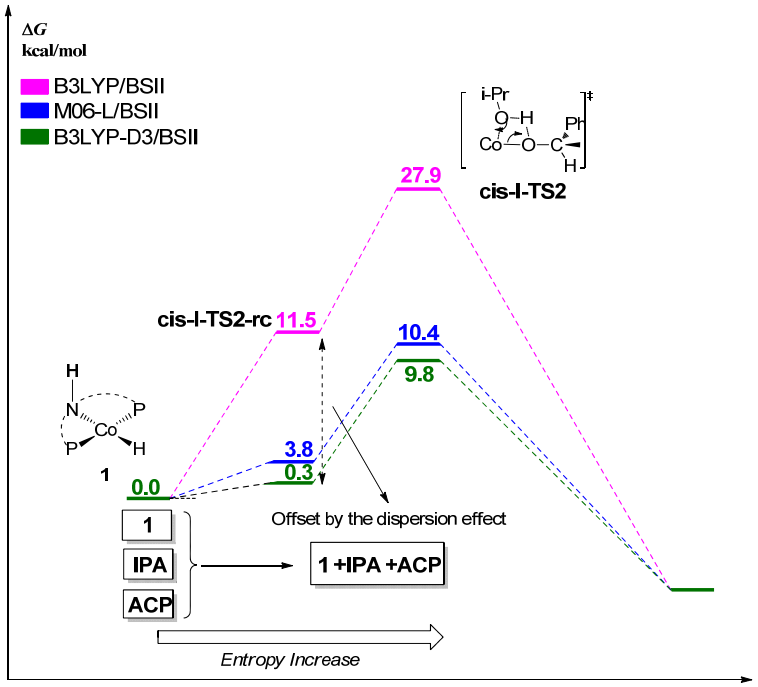

Figure S8. The explanation of the difference of relative energy of Cis-I-TS2 between B3LYP and M06L. The relative free energies are given in kcal/mol.

We have also noted that the relative energy barrier deviation between M06L/BSII and B3LYP/BSII becomes very large when the number of the reaction components changed. For **Cis-I-TS2**, the components changes from 3 to 1. This is an entropy increase process. Although we performed MHP method to reduce the overestimation of entropy, the entropy change of B3LYP/BSII data is still very high (ΔG = 11.5 kcal/mol). However, the M06L functional which include the dispersion effect, will offset the entropy increase. The relative energy of **Cis-I-TS2-rc** dropped to 3.8 kcal/mol for M06-L functional. The dispersion force will also stabilize the transition states to give a lower energy barrier ($\Delta G^{\ddagger}$ = 10.4 kcal/mol). In other places which don't include too much entropy change, the difference between M06L/BSII and B3LYP/BSII is not so great.

We justify this data by perform the B3LYP-D3 calculation. The activation free energy of B3LYP-D3/BSII of **Cis-I-TS2** is even lower ($\Delta G^{\ddagger}$ = 9.8 kcal/mol). This indicates the entropy increase is indeed offset by the dispersion effect.

11. The Cartesian coordinates (xyz) for all optimized structures are presented

1

27	0.000271	-0.585406	-0.081715
15	2.242751	-0.461389	-0.001355
15	-2.242891	-0.461789	-0.001807
7	-0.000123	1.487400	-0.375900
6	3.006277	-0.734231	1.652010
1	2.903962	-1.788515	1.921308
6	3.349996	-1.355283	-1.163930
1	4.387462	-1.025574	-1.056603
6	2.481747	1.358303	-0.360714
1	3.394089	1.759260	0.092423
1	2.585731	1.472367	-1.446932
6	1.250269	2.126420	0.135904
1	1.198177	2.102361	1.229534
1	1.299602	3.180398	-0.165375
6	-1.250398	2.126113	0.136483
1	-1.299918	3.180211	-0.164354
1	-1.198027	2.101622	1.230090
6	-2.481903	1.358091	-0.360159
1	-2.586181	1.472689	-1.446297
1	-3.394176	1.758728	0.093409
6	-3.353239	-1.354387	-1.162406
1	-3.294624	-2.425592	-0.953266
6	-3.003320	-0.734238	1.653104
1	-4.063663	-0.464788	1.649809
1	0.001051	-2.060745	0.115229
1	-0.000387	1.602395	-1.392890
1	-4.390149	-1.023768	-1.052546
1	-3.028829	-1.190854	-2.193173
1	3.290814	-2.426322	-0.954087
1	3.023434	-1.192023	-2.194063
1	2.490293	-0.140342	2.411195
1	4.066749	-0.465337	1.646415
1	-2.900950	-1.788533	1.922319
1	-2.485381	-0.140545	2.411124

O-1$_{AcPh}$

27	-1.318320	0.028634	-0.534549
15	-1.431072	2.289397	-0.431840
15	-1.665657	-2.204818	-0.326717
7	-1.868052	0.105063	1.618793
6	0.103883	3.293857	-0.661838
1	0.401789	3.273285	-1.714209
6	-2.704082	3.265261	-1.333774
1	-2.475141	3.256348	-2.402974
6	-1.852611	2.538707	1.376895
1	-1.440838	3.481384	1.751299
1	-2.944350	2.615434	1.450856
6	-1.359486	1.351523	2.218028
1	-0.265674	1.300134	2.208388
1	-1.677565	1.470386	3.264269
6	-1.492115	-1.159284	2.275552
1	-1.817113	-1.195454	3.325767
1	-0.398869	-1.224241	2.265581
6	-2.110856	-2.325043	1.488853
1	-3.204354	-2.282106	1.564278
1	-1.800103	-3.287909	1.906979
6	-3.039333	-3.074112	-1.189766
1	-2.811593	-3.139728	-2.257265
6	-0.257335	-3.392177	-0.495959
1	0.070095	-3.432023	-1.538722
1	-2.730760	0.089735	-1.000446
1	-2.885518	0.158463	1.581103
6	3.191887	0.001885	1.143511
6	4.461382	0.043011	1.706609
6	5.592372	-0.034815	0.886185
6	5.449523	-0.155386	-0.498306
6	4.179161	-0.198781	-1.066261
6	3.033482	-0.119510	-0.251370
6	1.675128	-0.150169	-0.826055
1	2.308305	0.060582	1.768989
1	4.575788	0.135529	2.781990
1	6.584151	-0.001821	1.326723
1	6.327344	-0.215356	-1.133408
1	4.085371	-0.290267	-2.142886
1	-3.681826	2.798228	-1.195558
1	-2.738953	4.302373	-0.987206
1	-0.050156	4.335721	-0.365275
1	0.915589	2.867850	-0.066751
1	-3.959120	-2.495776	-1.077338
1	-3.188421	-4.084180	-0.796676
1	0.584529	-3.060083	0.117060

1	-0.547884	-4.399908	-0.183706
8	0.683153	-0.043639	-0.078058
6	1.481243	-0.297414	-2.315729
1	1.886741	0.573174	-2.843051
1	2.005001	-1.178427	-2.698877
1	0.416789	-0.384785	-2.544297

O-1$_{THF}$

27	-0.061482	-0.422165	-0.613070
15	-2.329936	-0.470328	-0.523024
15	2.153090	-0.919412	-0.500073
7	-0.183555	-1.553014	1.302182
6	-3.261182	1.104082	-0.253563
1	-3.225265	1.709124	-1.163920
6	-3.364893	-1.351911	-1.763696
1	-3.339453	-0.804008	-2.709593
6	-2.614399	-1.429927	1.062435
1	-3.554040	-1.134711	1.540285
1	-2.716558	-2.486512	0.785777
6	-1.432501	-1.266636	2.031313
1	-1.377704	-0.238805	2.406478
1	-1.563839	-1.924046	2.903094
6	1.082067	-1.486665	2.055123
1	1.076514	-2.146896	2.934879
1	1.205992	-0.461700	2.421442
6	2.233768	-1.874171	1.114295
1	2.157887	-2.939130	0.862774
1	3.202412	-1.733215	1.604241
6	2.963673	-2.041643	-1.713646
1	3.054522	-1.529089	-2.675251
6	3.417781	0.413617	-0.280648
1	3.508000	0.989325	-1.206380
1	-0.182203	-1.671643	-1.407889
1	-0.261958	-2.490026	0.906966
1	-2.949550	-2.346816	-1.939581
1	-4.404115	-1.440230	-1.433435
1	-4.308950	0.912563	-0.003218
1	-2.798881	1.677185	0.553727
1	2.338656	-2.925151	-1.861664
1	3.959620	-2.346629	-1.379054
1	3.113283	1.095765	0.517023
1	4.398676	-0.004892	-0.035258
6	0.268241	2.247500	1.315614
8	0.101021	1.608330	0.023495
6	0.276109	2.579045	-1.050106
6	0.852068	3.824559	-0.379334
6	0.244096	3.748506	1.030337
1	-0.540269	1.912517	1.971026
1	1.226116	1.929035	1.745314
1	0.933899	2.134791	-1.802382
1	-0.703865	2.768834	-1.502478
1	1.944365	3.766188	-0.331486
1	0.585788	4.739784	-0.912698
1	0.806786	4.318479	1.773163
1	-0.785429	4.120784	1.025464

O-1$_{IPA}$

27	0.125721	-0.306997	-0.575583
15	-2.027814	-1.072037	-0.426924
15	2.400200	-0.237449	-0.531018
7	0.331908	-1.191566	1.457596
6	-3.583058	-0.071340	-0.543252
1	-3.690729	0.327413	-1.555626
6	-2.475081	-2.544043	-1.442050
1	-2.554771	-2.245554	-2.490996
6	-2.054855	-1.715025	1.339418
1	-3.035214	-1.551267	1.797225
1	-1.902419	-2.800304	1.299467
6	-0.945007	-1.068817	2.183332
1	-1.140622	-0.001165	2.332643
1	-0.905005	-1.536976	3.177757
6	1.538925	-0.655745	2.112611
1	1.718346	-1.115444	3.095352
1	1.382021	0.416336	2.272895
6	2.742348	-0.899245	1.187961
1	2.924164	-1.977100	1.095846
1	3.653268	-0.458135	1.604866
6	3.422162	-1.282160	-1.647912
1	3.353136	-0.893659	-2.667645
6	3.312411	1.376991	-0.544914
1	3.205425	1.862371	-1.519834
1	0.330827	-1.603118	-1.260637
1	0.491398	-2.179691	1.261714
1	-1.683150	-3.292010	-1.366442
1	-3.426956	-2.979421	-1.123435
1	-4.455126	-0.693523	-0.320168

1	-3.565364	0.767297	0.156322
1	3.029122	-2.301247	-1.649199
1	4.472239	-1.292219	-1.341396
1	2.919444	2.044283	0.228746
1	4.379116	1.226937	-0.353162
6	-1.114212	2.661297	0.202336
1	-1.876861	2.054564	0.696016
6	-0.682173	3.794608	1.125056
1	0.107249	4.398768	0.662081
1	-1.525485	4.460376	1.330791
1	-0.311262	3.406717	2.077607
6	-1.613394	3.136379	-1.155824
1	-0.849923	3.737693	-1.663720
1	-1.869997	2.289363	-1.797727
1	-2.501622	3.764523	-1.039535
8	0.002234	1.728055	0.032907
1	0.718877	2.214537	-0.396949

O-TS1$_{AcPh}$

27	0.021718	0.793800	0.355465
15	0.588573	-0.681088	1.991214
15	-0.459526	2.676312	-0.846971
7	1.621897	1.884607	1.047647
6	-0.543121	-0.591187	3.449149
1	-1.531733	-0.962407	3.166230
6	0.856170	-2.482977	1.766640
1	-0.093491	-2.959460	1.506984
6	2.186034	0.032170	2.589778
1	2.396229	-0.236853	3.629932
1	2.984536	-0.380691	1.965190
6	2.102747	1.549935	2.414134
1	1.406576	1.986884	3.139688
1	3.084575	2.009959	2.588272
6	1.557032	3.356516	0.838021
1	2.545504	3.800611	1.013175
1	0.869307	3.784893	1.576547
6	1.091936	3.646849	-0.590478
1	1.842599	3.261200	-1.288255
1	0.954121	4.719093	-0.761757
6	-0.883952	2.761333	-2.634775
1	-1.862997	2.300903	-2.795060
6	-1.792652	3.691385	-0.067226
1	-2.746135	3.162911	-0.151143
1	1.041031	0.099863	-0.838873
1	2.334892	1.537602	0.354348
6	-4.496055	-0.415008	0.679781
6	-5.841576	-0.670424	0.913821
6	-6.524319	-1.600860	0.122186
6	-5.858033	-2.274508	-0.904652
6	-4.510145	-2.021162	-1.143522
6	-3.812543	-1.087908	-0.353002
6	-2.384088	-0.802988	-0.583291
1	-3.955757	0.303294	1.286463
1	-6.362593	-0.148736	1.710358
1	-7.575618	-1.800127	0.306336
1	-6.389106	-2.995516	-1.517543
1	-4.005814	-2.550981	-1.944336
1	1.566907	-2.655347	0.956908
1	1.232536	-2.934669	2.689355
1	-0.165534	-1.188995	4.284544
1	-0.652205	0.446794	3.775454
1	-0.145234	2.219095	-3.225942
1	-0.927383	3.800880	-2.973198
1	-1.581681	3.840493	0.995103
1	-1.884632	4.668600	-0.551378
8	-1.806433	0.026937	0.149417
6	-1.625179	-1.497129	-1.681564
1	-1.646828	-2.582706	-1.538029
1	-2.084825	-1.293271	-2.654647
1	-0.592784	-1.144718	-1.676592
6	4.129611	-1.352872	-0.285727
6	4.635875	-2.602734	0.075939
6	4.048541	-3.767527	-0.422008
6	2.955016	-3.672310	-1.288657
6	2.448641	-2.422426	-1.646117
6	3.023246	-1.245034	-1.141658
6	2.567071	0.144272	-1.549547
1	4.601513	-0.437505	0.056186
1	5.500835	-2.666949	0.730070
1	4.446609	-4.740791	-0.151114
1	2.503095	-4.573692	-1.692891
1	1.601081	-2.369154	-2.322374
8	3.144664	1.142579	-1.020453
6	2.109229	0.286092	-3.000660
1	1.317393	-0.407949	-3.288991
1	1.781510	1.311041	-3.177352
1	2.975364	0.098074	-3.647493

O-TS1$_{THF}$

27	0.817239	-0.070662	0.423011
15	-0.632572	0.717756	2.016812
15	2.502876	-1.204556	-0.684177
7	0.274335	-1.907440	1.093665
6	0.161471	1.363731	3.558203
1	0.648352	2.321057	3.352554
6	-1.975958	1.928859	1.701955
1	-1.536315	2.899747	1.456506
6	-1.439685	-0.859861	2.542028
1	-1.846498	-0.804561	3.556763
1	-2.268869	-1.046869	1.852527
6	-0.388764	-1.964389	2.425560
1	0.380854	-1.852124	3.198171
1	-0.849336	-2.950899	2.565411
6	1.282222	-2.995469	0.950267
1	0.797845	-3.966994	1.110546
1	2.042462	-2.874702	1.731017
6	1.900976	-2.935792	-0.446904
1	1.115138	-3.124538	-1.185709
1	2.695815	-3.678395	-0.568022
6	2.934671	-1.016105	-2.464065
1	3.418844	-0.047921	-2.621190
6	4.168202	-1.191776	0.125424
1	4.636791	-0.211266	0.002232
1	-0.314754	-0.215619	-0.835881
1	-0.457230	-2.112726	0.361435
1	-2.585956	1.598879	0.859565
1	-2.606491	2.044617	2.588726
1	-0.579855	1.514740	4.349310
1	0.922767	0.664535	3.914527
1	2.033475	-1.055974	-3.077022
1	3.623694	-1.804198	-2.782352
1	4.071269	-1.389924	1.196111
1	4.826205	-1.946988	-0.316128
6	-3.671734	-1.037116	-0.469804
6	-4.865438	-0.370005	-0.186850
6	-5.095513	0.905367	-0.706319
6	-4.125717	1.506624	-1.515410
6	-2.932887	0.839698	-1.794802
6	-2.685857	-0.438116	-1.268032
6	-1.443119	-1.242529	-1.594981
1	-3.495843	-2.045654	-0.110153
1	-5.623749	-0.853833	0.422184
1	-6.027007	1.422345	-0.496328
1	-4.304616	2.492472	-1.935095
1	-2.192407	1.319872	-2.427285
8	-1.284340	-2.364599	-1.026073
6	-0.914404	-1.092334	-3.019826
1	-0.724371	-0.059095	-3.316046
1	-0.004054	-1.682152	-3.132749
1	-1.665547	-1.507612	-3.703537
6	1.029667	2.401432	-1.361041
8	1.427188	1.792475	-0.095794
6	2.553047	2.505836	0.491690
6	3.032493	3.461615	-0.599464
6	1.738040	3.753141	-1.377051
1	1.357910	1.743958	-2.172599
1	-0.059625	2.456273	-1.369511
1	2.192228	3.039996	1.377968
1	3.300046	1.770605	0.801530
1	3.497640	4.358606	-0.184516
1	3.766348	2.969495	-1.246644
1	1.139286	4.508666	-0.857781
1	1.922111	4.108276	-2.393577

O-TS1$_{IPA}$

27	0.942356	0.151872	0.466326
15	-0.656511	0.343657	2.090638
15	2.839750	-0.413397	-0.712861
7	0.838812	-1.850292	0.880292
6	0.061420	0.940593	3.684927
1	0.353525	1.989155	3.582098
6	-2.247816	1.252324	1.971535
1	-2.051321	2.324274	1.879959
6	-1.078988	-1.429158	2.390315
1	-1.485070	-1.598210	3.392748
1	-1.847203	-1.705672	1.661198
6	0.193336	-2.245593	2.161842
1	0.910611	-2.082488	2.974610
1	-0.037387	-3.318689	2.143522
6	2.071657	-2.647136	0.633973
1	1.828265	-3.717239	0.643182
1	2.776852	-2.463728	1.453026
6	2.670855	-2.253082	-0.716075

1	1.962136	-2.519957	-1.507263
1	3.623623	-2.759755	-0.899429
6	3.273494	0.080832	-2.431827
1	3.494914	1.150862	-2.466897
6	4.417769	-0.092716	0.201497
1	4.620306	0.982088	0.238058
1	-0.115357	-0.032974	-0.855588
1	0.181327	-2.103411	0.094173
1	-2.802012	0.921067	1.091763
1	-2.851316	1.085370	2.868992
1	-0.659962	0.853343	4.503348
1	0.955034	0.363136	3.937154
1	2.438365	-0.121162	-3.103768
1	4.154402	-0.468751	-2.777017
1	4.341323	-0.457401	1.229310
1	5.264654	-0.584758	-0.286824
6	-3.177702	-1.670540	-0.703283
6	-4.495160	-1.354619	-0.363804
6	-5.018430	-0.099267	-0.679203
6	-4.216330	0.836722	-1.340807
6	-2.899713	0.520347	-1.675868
6	-2.360253	-0.735193	-1.354408
6	-0.963198	-1.166402	-1.761176
1	-2.769308	-2.656009	-0.504150
1	-5.118779	-2.095244	0.128786
1	-6.045650	0.145106	-0.425961
1	-4.621691	1.810058	-1.602252
1	-2.290649	1.257376	-2.190962
8	-0.541139	-2.294193	-1.360693
6	-0.509587	-0.697640	-3.142572
1	-0.596622	0.379290	-3.297036
1	0.519997	-1.013749	-3.314634
1	-1.139004	-1.198380	-3.888926
6	0.330903	3.071989	-0.434059
1	-0.623395	2.540916	-0.442690
6	0.196536	4.419694	0.262397
1	-0.183217	4.303517	1.281208
1	1.160513	4.939540	0.310786
1	-0.496398	5.061178	-0.290282
6	0.881853	3.162542	-1.849193
1	1.863057	3.654325	-1.860464
1	0.972585	2.166041	-2.287109
1	0.214244	3.758579	-2.478550
8	1.185752	2.197055	0.384201
1	2.093935	2.524874	0.333043

O-TS1$_{shuttle}$

27	0.549582	-0.875520	0.366797
15	1.683290	-2.047136	-1.208176
15	-0.127220	-0.146141	2.394406
7	2.252102	-0.060598	0.786227
6	2.134120	-3.719793	-0.565698
1	1.242740	-4.351965	-0.528144
6	1.287137	-2.389169	-2.976348
1	0.375943	-2.989906	-3.043387
6	3.264221	-1.089546	-1.225144
1	4.111491	-1.674689	-1.597456
1	3.112934	-0.241421	-1.902353
6	3.494820	-0.589808	0.204262
1	3.895466	-1.412937	0.821137
1	4.278322	0.185186	0.199193
6	2.522175	0.428463	2.147880
1	3.315032	1.193595	2.130003
1	2.908843	-0.384586	2.786862
6	1.257980	1.016542	2.782951
1	1.005710	1.975301	2.315453
1	1.380328	1.188975	3.857330
6	-1.672462	0.736614	2.854794
1	-2.533334	0.083104	2.693411
6	-0.004013	-1.484918	3.659569
1	0.959511	-1.992647	3.568339
1	1.129627	-1.454511	-3.519098
1	2.104422	-2.938686	-3.453016
1	2.881792	-4.199908	-1.204461
1	2.535070	-3.633033	0.447332
1	-1.786650	1.617272	2.220441
1	-1.646587	1.042892	3.904835
1	-0.101525	-1.083324	4.672798
1	-0.795776	-2.220477	3.493285
8	1.190270	1.969488	-0.828425
6	1.747104	3.309710	-0.750822
6	0.876559	4.218181	-1.609422
6	3.203806	3.286740	-1.201658
1	1.695416	3.643625	0.295956
1	0.899732	3.895050	-2.655268
1	-0.162683	4.215850	-1.266156
1	1.242447	5.247573	-1.562363

1	3.802149	2.613245	-0.579434
1	3.277831	2.956857	-2.242899
1	3.642234	4.286485	-1.126307
1	1.676185	1.313400	-0.224786
1	-0.083207	0.470052	-2.479405
6	-1.148967	0.247498	-2.451523
6	-1.724336	0.548428	-1.093752
1	-1.327236	-0.779818	-2.760159
1	-1.662658	0.910694	-3.161545
1	-0.906251	-0.975148	-0.246210
8	-1.248955	1.564009	-0.440067
1	-0.242223	1.787232	-0.660993
6	-3.111767	0.164460	-0.778487
6	-3.678535	-1.016768	-1.292867
6	-3.908657	1.027817	-0.003838
6	-5.007379	-1.328993	-1.030611
1	-3.072801	-1.707501	-1.869313
6	-5.242523	0.716172	0.245569
1	-3.483656	1.951713	0.369814
6	-5.793131	-0.462600	-0.262966
1	-5.433429	-2.247030	-1.422286
1	-5.854619	1.395669	0.830093
1	-6.832523	-0.705950	-0.065194

O-2$_{AcPh}$

27	-1.053224	-0.000014	0.008009
15	-1.246878	2.272731	0.143356
15	-1.246820	-2.272750	0.142992
7	-2.882286	-0.000037	-0.249646
6	-1.277824	2.963371	1.852852
1	-0.289834	2.859740	2.309610
6	-0.175492	3.450376	-0.783671
1	0.845581	3.412945	-0.393778
6	-2.951458	2.453742	-0.519276
1	-3.441718	3.376289	-0.192767
1	-2.872851	2.470184	-1.611563
6	-3.705662	1.199942	-0.069148
1	-4.027302	1.317276	0.981491
1	-4.630697	1.103770	-0.656449
6	-3.705732	-1.199905	-0.068724
1	-4.630909	-1.103724	-0.655793
1	-4.027074	-1.317055	0.982026
6	-2.951713	-2.453806	-0.518894
1	-2.873561	-2.470524	-1.611207
1	-3.441806	-3.376291	-0.191966
6	-0.175623	-3.449043	-0.785995
1	0.845605	-3.411975	-0.396475
6	-1.276464	-2.965108	1.851795
1	-0.288327	-2.861384	2.308206
6	3.446112	-0.000973	1.156551
6	4.738484	-0.001156	1.665809
6	5.833185	-0.000251	0.793750
6	5.632472	0.000831	-0.589225
6	4.339788	0.000970	-1.104896
6	3.230244	0.000069	-0.236958
6	1.853158	0.000219	-0.753951
1	2.589624	-0.001637	1.821547
1	4.898592	-0.001998	2.739242
1	6.842818	-0.000390	1.193075
1	6.483036	0.001552	-1.262974
1	4.199486	0.001810	-2.180407
1	-0.156714	3.178619	-1.842254
1	-0.547517	4.474866	-0.688374
1	-1.557323	4.021308	1.849058
1	-1.995063	2.406623	2.461080
1	-0.157328	-3.175824	-1.844207
1	-0.547434	-4.473728	-0.691946
1	-1.993752	-2.409401	2.460928
1	-1.555377	-4.023194	1.847023
8	0.898541	-0.000147	0.051792
6	1.580785	0.000870	-2.236039
1	2.024373	0.881912	-2.711457
1	2.026316	-0.878456	-2.712764
1	0.503787	-0.000105	-2.411056

O-2$_{THF}$

27	-0.210131	0.184447	-0.008079
15	1.441906	1.792835	0.090744
15	-2.110816	-1.088211	0.131079
7	-1.344790	1.580820	-0.436546
6	1.856178	2.423354	1.775737
1	2.423632	1.672555	2.332780
6	3.080430	1.670789	-0.744746
1	3.692087	0.899479	-0.268298
6	0.527572	3.158890	-0.733041
1	0.919196	4.147188	-0.472329

1	0.632682	3.016021	-1.813694
6	-0.936083	2.984150	-0.324595
1	-1.086466	3.371935	0.699272
1	-1.570400	3.602849	-0.975906
6	-2.800687	1.476812	-0.289866
1	-3.287183	2.217284	-0.941281
1	-3.125372	1.720932	0.738070
6	-3.289248	0.075950	-0.665657
1	-3.207796	-0.069975	-1.747894
1	-4.328251	-0.097721	-0.368583
6	-2.303400	-2.718679	-0.703945
1	-1.631310	-3.452316	-0.250624
6	-2.760214	-1.387044	1.831886
1	-2.089081	-2.057524	2.375764
1	2.939228	1.404148	-1.795486
1	3.618218	2.622240	-0.691840
1	2.451105	3.339968	1.719155
1	0.934349	2.631211	2.325081
1	-2.053127	-2.624075	-1.763829
1	-3.331128	-3.083234	-0.614666
1	-2.813065	-0.440898	2.376598
1	-3.757178	-1.836857	1.800560
6	1.803917	-1.910374	1.127740
8	1.033630	-1.439300	-0.020430
6	1.587484	-1.966380	-1.261887
6	2.439516	-3.152509	-0.824091
6	2.985740	-2.678870	0.533359
1	2.098824	-1.043101	1.725252
1	1.147874	-2.549232	1.728191
1	0.748835	-2.224694	-1.911625
1	2.184546	-1.181358	-1.739801
1	1.819065	-4.046228	-0.702525
1	3.227949	-3.381082	-1.544640
1	3.303736	-3.500967	1.178209
1	3.843486	-2.013874	0.388799

O-2$_{IPA}$

27	0.066520	-0.092538	0.087057
15	-2.078612	-0.936617	0.232468
15	2.352355	0.195398	0.276875
7	0.488300	-1.717643	-0.691401
6	-2.414056	-1.684549	1.884956
1	-2.537715	-0.893931	2.630282
6	-3.678394	-0.123914	-0.195048
1	-3.885984	0.697265	0.496520
6	-1.891670	-2.343640	-0.933323
1	-2.625590	-3.137631	-0.762818
1	-2.038781	-1.945565	-1.943060
6	-0.454962	-2.838030	-0.767257
1	-0.386636	-3.483372	0.127062
1	-0.190534	-3.480107	-1.620054
6	1.858380	-2.236946	-0.751724
1	1.948972	-2.928223	-1.602222
1	2.108387	-2.831455	0.145623
6	2.869423	-1.101637	-0.915952
1	2.790559	-0.670673	-1.919513
1	3.900228	-1.434035	-0.757372
6	3.266462	1.733981	-0.174798
1	3.068188	2.529053	0.551073
6	3.085468	-0.290430	1.897926
1	2.811525	0.435546	2.668412
1	-3.641315	0.271639	-1.213543
1	-4.498561	-0.845487	-0.130666
1	-3.320332	-2.297388	1.866311
1	-1.567258	-2.306841	2.184553
1	2.953801	2.076210	-1.164751
1	4.345272	1.551721	-0.188904
1	2.694143	-1.266438	2.195638
1	4.176480	-0.345723	1.836888
6	-1.231277	2.708331	-0.345662
1	-2.105573	2.090261	-0.554463
6	-1.633955	3.934418	0.461139
1	-2.136870	3.649058	1.388743
1	-0.760324	4.548733	0.710853
1	-2.316046	4.559370	-0.122505
6	-0.496871	3.028715	-1.640236
1	0.399236	3.630325	-1.447010
1	-0.202315	2.112675	-2.160790
1	-1.143350	3.608152	-2.305923
8	-0.399648	1.834564	0.504134
1	0.366010	2.352853	0.787546

O-3

27	-0.474728	-0.673698	0.000000
15	-0.506952	0.057594	2.241576
15	-0.506952	0.057594	-2.241576

7	1.438113	-0.357308	0.000000
6	-0.750724	1.848750	2.601436
1	-1.809264	2.099854	2.495108
6	-1.349692	-0.801479	3.634653
1	-0.971299	-0.447734	4.598320
6	1.309474	-0.257885	2.478357
1	1.705562	0.254043	3.361411
1	1.426915	-1.336128	2.635395
6	2.061970	0.171856	1.211565
1	2.126265	1.272102	1.164281
1	3.102045	-0.185935	1.254206
6	2.061970	0.171856	-1.211565
1	3.102045	-0.185935	-1.254206
1	2.126265	1.272102	-1.164281
6	1.309474	-0.257885	-2.478357
1	1.426915	-1.336128	-2.635395
1	1.705562	0.254043	-3.361411
6	-1.349692	-0.801479	-3.634653
1	-2.424964	-0.609994	-3.585357
6	-0.750724	1.848750	-2.601436
1	-0.429264	2.090523	-3.619050
1	-0.971299	-0.447734	-4.598320
1	-1.188744	-1.880005	-3.560809
1	-2.424964	-0.609994	3.585357
1	-1.188744	-1.880005	3.560809
1	-0.183704	2.457406	1.892745
1	-0.429264	2.090523	3.619050
1	-1.809264	2.099854	-2.495108
1	-0.183704	2.457406	-1.892745

O-TS2$_{AcPh}$

27	0.653056	0.042331	-0.282322
15	0.796798	2.310243	-0.440451
15	0.748882	-2.198712	-0.672876
7	2.549443	0.065059	-1.101848
6	-0.190592	2.971985	-1.854150
1	-1.255387	2.845921	-1.640736
6	0.473986	3.529462	0.898545
1	-0.589270	3.513111	1.153795
6	2.562893	2.529991	-0.956014
1	2.722306	3.463695	-1.504838
1	3.178149	2.562611	-0.051185
6	2.947600	1.313045	-1.800730
1	2.445014	1.341394	-2.774635
1	4.028816	1.309609	-1.992320
6	2.950257	-1.146051	-1.867194
1	4.035853	-1.141980	-2.030073
1	2.470546	-1.112874	-2.852490
6	2.537890	-2.396964	-1.088115
1	3.095752	-2.420695	-0.145887
1	2.742763	-3.311700	-1.653154
6	0.298201	-3.537876	0.503884
1	-0.781050	-3.518332	0.679738
6	-0.159629	-2.682981	-2.206984
1	-1.234347	-2.565100	-2.043913
1	1.320045	-0.094004	1.279362
1	3.083866	0.012464	-0.195925
6	-3.996810	0.045212	-0.958044
6	-5.337124	0.043483	-1.324058
6	-6.330459	-0.004934	-0.339378
6	-5.980103	-0.051672	1.012344
6	-4.638451	-0.051951	1.383778
6	-3.630217	-0.003435	0.402081
6	-2.201522	-0.006931	0.768482
1	-3.217647	0.081876	-1.711366
1	-5.613596	0.079177	-2.373049
1	-7.377494	-0.006515	-0.626774
1	-6.751829	-0.088504	1.774299
1	-4.380470	-0.089039	2.436502
1	1.047850	3.268815	1.788940
1	0.739626	4.540585	0.575967
1	0.015147	4.032966	-2.026100
1	0.038744	2.413174	-2.765516
1	0.807591	-3.392954	1.457091
1	0.566531	-4.516495	0.094747
1	0.129300	-2.032597	-3.036775
1	0.045287	-3.722301	-2.482059
8	-1.344061	0.057933	-0.137030
6	-1.775687	-0.088383	2.210038
1	-2.157695	0.771984	2.770579
1	-2.186898	-0.985624	2.684458
1	-0.686018	-0.107988	2.261473
6	2.684347	1.109729	2.850754
6	2.746601	-0.245816	2.147360
8	3.648627	-0.439981	1.281953
6	2.330655	-1.416482	3.034929
1	1.345136	-1.280244	3.487915

1	2.360491	-2.350384	2.471950
1	3.065902	-1.501804	3.846243
1	2.907501	1.918916	2.153346
1	1.722618	1.289604	3.338820
1	3.465523	1.121725	3.622553

O-TS2$_{THF}$

27	0.039531	-0.049164	-0.321157
15	-0.156471	-2.334501	-0.515921
15	-0.003246	2.225734	-0.740388
7	-1.892534	-0.013645	-0.929966
6	0.602384	-3.100951	-2.018614
1	1.692639	-3.074101	-1.936393
6	0.280975	-3.527210	0.814177
1	1.366469	-3.538208	0.946557
6	-1.979860	-2.482369	-0.799975
1	-2.249725	-3.403516	-1.325921
1	-2.477827	-2.491954	0.174779
6	-2.408908	-1.244192	-1.588837
1	-2.018281	-1.279427	-2.612533
1	-3.503031	-1.193870	-1.658420
6	-2.344795	1.209393	-1.652122
1	-3.440973	1.222148	-1.697695
1	-1.972887	1.166159	-2.682606
6	-1.828553	2.449455	-0.921656
1	-2.267817	2.471209	0.081013
1	-2.091679	3.369904	-1.452070
6	0.598184	3.515040	0.426630
1	1.690590	3.483169	0.472343
6	0.686325	2.801917	-2.358813
1	1.777316	2.730094	-2.348159
1	-0.479201	0.075050	1.289017
1	-2.340055	0.050899	0.023673
1	-0.178976	-3.220833	1.754789
1	-0.050240	-4.538232	0.558761
1	0.288512	-4.143195	-2.133985
1	0.314552	-2.542496	-2.913410
1	0.204634	3.329194	1.426699
1	0.292503	4.512445	0.096735
1	0.314274	2.175953	-3.174012
1	0.408333	3.842231	-2.555550
6	-1.728372	-1.075648	3.018109
6	-1.840792	0.273839	2.313395
8	-2.807478	0.472733	1.524562
6	-1.314406	1.448385	3.131739
1	-0.296825	1.289242	3.497523
1	-1.368500	2.372334	2.554039
1	-1.970437	1.570920	4.004071
1	-2.018676	-1.888158	2.349727
1	-0.728568	-1.259098	3.419811
1	-2.437767	-1.074870	3.856671
6	3.116650	-0.059071	-0.773005
8	2.006127	-0.138375	0.159946
6	2.477699	-0.022824	1.539447
6	3.973976	0.272224	1.424020
6	4.348992	-0.360833	0.073373
1	2.932699	-0.777144	-1.576072
1	3.152211	0.950557	-1.200546
1	1.897736	0.761789	2.026962
1	2.270259	-0.975180	2.036520
1	4.153717	1.352135	1.401412
1	4.538121	-0.143609	2.261817
1	5.260478	0.057431	-0.359722
1	4.486396	-1.442314	0.176544

O-TS2$_{IPA}$

27	0.040951	0.040260	-0.420000
15	2.095770	-0.963882	-0.474313
15	-2.145823	0.615201	-0.823934
7	-0.669922	-1.893553	-0.471845
6	2.857816	-0.870979	-2.153779
1	3.127208	0.165817	-2.372007
6	3.515720	-0.638300	0.648524
1	3.904492	0.366613	0.462130
6	1.641909	-2.744552	-0.260241
1	2.393855	-3.418300	-0.683214
1	1.571463	-2.950981	0.812544
6	0.276424	-2.948317	-0.919730
1	0.360738	-2.899961	-2.011757
1	-0.123455	-3.939375	-0.668709
6	-2.021407	-2.091778	-1.062279
1	-2.398719	-3.087920	-0.797790
1	-1.937249	-2.052774	-2.154735
6	-2.967230	-1.012656	-0.534288
1	-3.070583	-1.137722	0.548732
1	-3.954068	-1.072411	-1.003583

6	-3.143624	1.880611	0.063688
1	-2.761143	2.880353	-0.158547
6	-2.491480	1.007090	-2.600208
1	-2.060874	1.978098	-2.863657
1	-0.108960	0.109830	1.273408
1	-0.803108	-1.991333	0.571256
1	3.192802	-0.699275	1.688959
1	4.319844	-1.359620	0.474632
1	3.755872	-1.492779	-2.220913
1	2.140972	-1.200607	-2.910749
1	-3.082979	1.720159	1.140766
1	-4.190684	1.829505	-0.249593
1	-2.043811	0.251031	-3.250647
1	-3.568053	1.047058	-2.793741
6	0.723760	-0.959069	3.241938
6	-0.641716	-0.742881	2.589378
8	-1.255921	-1.747618	2.122028
6	-1.462781	0.363519	3.247233
1	-0.924176	1.312404	3.310315
1	-2.409254	0.501086	2.722500
1	-1.702347	0.041196	4.269236
6	1.434744	2.756156	0.261571
1	1.828235	2.026778	0.973126
6	2.559240	3.595873	-0.329554
1	3.313642	2.966735	-0.810010
1	2.176746	4.304811	-1.073155
1	3.048612	4.176997	0.457799
6	0.336119	3.575358	0.922384
1	-0.112401	4.281206	0.211457
1	-0.442342	2.921883	1.322549
1	0.748935	4.164369	1.746748
8	0.868603	1.905182	-0.797085
1	0.386134	2.471277	-1.414906
1	1.291576	-0.030995	3.349385
1	0.552033	-1.372094	4.244729
1	1.309208	-1.693954	2.686689

O-TS2$_{shuttle}$

27	1.720760	0.021339	0.403192
15	2.056242	-2.218043	0.453091
15	2.040624	2.213061	-0.095074
7	1.365096	-0.222550	-1.508932
6	3.864416	-2.577010	0.348489
1	4.342585	-2.337958	1.302277
6	1.448970	-3.495380	1.633614
1	1.850182	-3.296898	2.631091
6	1.371958	-2.679816	-1.201078
1	1.770470	-3.628359	-1.575487
1	0.288463	-2.788191	-1.078129
6	1.681707	-1.513528	-2.145279
1	2.743905	-1.550492	-2.440369
1	1.107538	-1.633983	-3.077596
6	1.680787	0.872112	-2.443643
1	1.109211	0.756104	-3.378343
1	2.743461	0.835851	-2.737082
6	1.372302	2.237264	-1.820526
1	0.289658	2.388062	-1.738834
1	1.779461	3.059644	-2.417949
6	1.357061	3.713127	0.723608
1	1.814191	3.835678	1.709310
6	3.836526	2.605763	-0.268880
1	4.308376	2.606483	0.717525
1	0.358293	-3.477013	1.687185
1	1.768885	-4.492685	1.317538
1	4.045244	-3.630940	0.116035
1	4.320942	-1.958196	-0.428254
1	0.277370	3.605911	0.845928
1	1.568766	4.606276	0.128134
1	4.327835	1.845640	-0.881840
1	3.985189	3.585918	-0.732168
8	-1.185281	-0.240711	-0.697161
6	-2.287471	0.081508	-1.597920
6	-2.253925	-0.869307	-2.792991
1	-2.149139	1.110813	-1.955772
1	-1.308308	-0.782346	-3.338542
1	-2.379429	-1.906740	-2.470438
1	-3.066503	-0.627704	-3.483595
1	-0.235539	-0.223670	-1.145973
1	-0.957332	-1.411080	1.686226
6	-0.821237	-0.838254	2.602582
6	-0.426701	0.584315	2.314737
1	-0.106648	-1.327305	3.263329
1	-1.791296	-0.791967	3.118177
1	1.423416	0.233526	1.935788
8	-0.882605	1.167712	1.267902
1	-1.112767	0.503234	0.398109
6	-0.075818	1.467829	3.476520

1	0.373121	2.401739	3.142830
1	-1.015470	1.706244	3.994758
1	0.585113	0.961590	4.180263
6	-3.578633	0.015499	-0.808195
6	-4.433310	1.121874	-0.759443
6	-3.945216	-1.156868	-0.130550
6	-5.637211	1.060392	-0.053820
1	-4.160307	2.036671	-1.280077
6	-5.143120	-1.217883	0.579958
1	-3.291764	-2.024361	-0.162566
6	-5.993168	-0.108897	0.618249
1	-6.293096	1.925305	-0.028664
1	-5.419103	-2.132038	1.097452
1	-6.928546	-0.158782	1.167301

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27	-0.101373	-0.068165	-0.115015
15	-2.347996	0.253366	-0.082715
15	2.110973	-0.757211	-0.040285
7	-0.556520	-2.082284	-0.251151
6	-2.948228	0.922284	1.515842
1	-2.445076	1.878864	1.676631
6	-3.190492	1.258141	-1.365857
1	-2.796943	2.276347	-1.310032
6	-2.981569	-1.490166	-0.234493
1	-3.932208	-1.652457	0.282639
1	-3.152671	-1.699050	-1.297680
6	-1.899537	-2.420468	0.325550
1	-1.814751	-2.303288	1.410186
1	-2.139731	-3.471730	0.124065
6	0.517537	-2.991034	0.259276
1	0.279166	-4.033468	0.014370
1	0.518802	-2.902035	1.350010
6	1.873851	-2.584071	-0.318515
1	1.898180	-2.766635	-1.400037
1	2.676987	-3.179978	0.126602
6	3.458071	-0.277852	-1.199666
1	3.699202	0.778306	-1.058297
6	2.882832	-0.646122	1.629390
1	3.057224	0.402989	1.879962
1	-0.620968	-2.241131	-1.262247
6	1.259258	3.014609	-1.311061
6	1.138844	2.536018	0.138873
1	2.072377	2.005338	0.404693
1	-2.973075	0.860482	-2.360423
1	-4.273219	1.280714	-1.212515
1	-4.032594	1.064954	1.514904
1	-2.669633	0.252168	2.333192
1	3.129593	-0.418470	-2.232602
1	4.357631	-0.874963	-1.022992
1	2.206034	-1.061083	2.380641
1	3.834818	-1.184486	1.663348
8	0.024224	1.678402	0.290636
6	0.971218	3.702645	1.116285
1	0.062843	4.266013	0.878752
1	0.886738	3.333365	2.142520
1	1.824168	4.387174	1.062768
1	2.115214	3.685381	-1.441741
1	1.381850	2.164326	-1.991800
1	0.353562	3.555348	-1.605302

***cis*-I-TS1**

27	-0.641546	0.021415	0.170266
15	0.650809	1.928295	0.635103
15	-2.731644	-1.101440	0.416268
7	-1.596840	1.187917	-1.215167
6	-0.063625	2.997892	1.963171
1	0.167868	2.560293	2.938205
6	2.460464	2.127875	0.881416
1	2.749503	1.667141	1.828844
6	0.264339	2.837099	-0.939763
1	0.494504	3.906069	-0.873460
1	0.898193	2.408717	-1.724591
6	-1.214730	2.632866	-1.267826
1	-1.838276	3.155379	-0.535565
1	-1.459609	3.047374	-2.253389
6	-3.078005	1.023423	-1.324999
1	-3.426741	1.415606	-2.288572
1	-3.528329	1.642659	-0.542401
6	-3.489440	-0.436259	-1.148971
1	-3.103379	-1.044924	-1.974944
1	-4.581097	-0.525932	-1.152539
6	-3.145953	-2.896666	0.356115
1	-2.776736	-3.395665	1.255819
6	-3.839310	-0.475358	1.757706
1	-3.501731	-0.875454	2.717871

1	0.289565	-1.023191	0.924006
1	-1.168906	0.718053	-2.018131
6	2.916133	-0.762844	-1.341276
6	4.283678	-0.477580	-1.337300
6	5.036444	-0.669108	-0.176564
6	4.417916	-1.151285	0.981030
6	3.055071	-1.445306	0.974881
6	2.292374	-1.249289	-0.185170
6	0.829609	-1.650703	-0.267841
1	2.321064	-0.635292	-2.239371
1	4.762810	-0.117896	-2.243210
1	6.100386	-0.452679	-0.174547
1	4.999586	-1.304548	1.885084
1	2.584458	-1.820815	1.880140
1	3.007602	1.627332	0.080789
1	2.725704	3.189188	0.904955
1	0.353555	4.009003	1.924792
1	-1.151245	3.057091	1.872938
1	-2.677391	-3.357742	-0.516313
1	-4.229111	-3.039275	0.294450
1	-3.790285	0.615353	1.816547
1	-4.878691	-0.777730	1.596576
8	0.130816	-1.161457	-1.259631
6	0.569870	-3.108938	0.118739
1	1.043892	-3.735173	-0.644779
1	1.006348	-3.368494	1.085190
1	-0.496929	-3.324130	0.130990

***trans*-I-TS1**

27	-0.679922	0.107078	0.241604
15	-2.837800	-0.933441	0.456891
15	0.711191	1.967417	0.648462
7	-1.637710	1.384829	-1.011402
6	-3.238649	-2.690726	0.060825
1	-2.884139	-3.345610	0.860802
6	-3.893978	-0.605351	1.936552
1	-3.533848	-1.205321	2.776888
6	-3.682176	0.019454	-0.920618
1	-4.357617	-0.625273	-1.490607
1	-4.299812	0.807117	-0.471092
6	-2.625210	0.636120	-1.840789
1	-2.068476	-0.135429	-2.378273
1	-3.088059	1.308086	-2.574719
6	-0.612557	2.125271	-1.803121
1	-1.098112	2.746322	-2.566586
1	-0.002809	1.370185	-2.304725
6	0.239089	2.983009	-0.858536
1	-0.316672	3.870338	-0.533410
1	1.133763	3.340154	-1.376339
6	0.166590	3.008255	2.076125
1	0.458766	2.521347	3.010587
6	2.543662	2.065453	0.754236
1	2.885090	1.521175	1.637397
1	0.205853	-0.972494	0.992678
1	-2.165139	2.076901	-0.472943
6	2.853682	-0.897709	-1.317060
6	4.235881	-0.695390	-1.320716
6	4.976498	-0.893870	-0.153544
6	4.331151	-1.302024	1.017778
6	2.953006	-1.514779	1.019120
6	2.202322	-1.308453	-0.146777
6	0.720239	-1.631702	-0.225679
1	2.268033	-0.764141	-2.220620
1	4.735056	-0.394488	-2.237215
1	6.051388	-0.740815	-0.156965
1	4.903438	-1.461745	1.926725
1	2.460807	-1.833830	1.934568
1	-3.825267	0.448233	2.220867
1	-4.941974	-0.857029	1.748248
1	-4.320113	-2.820845	-0.043859
1	-2.748487	-2.981144	-0.871318
1	-0.921863	3.114587	2.076770
1	0.621048	4.003132	2.041198
1	2.994743	1.596846	-0.121939
1	2.865553	3.108771	0.825796
8	0.042149	-1.101510	-1.205745
6	0.395122	-3.074427	0.167173
1	0.827087	-3.349987	1.131228
1	-0.679176	-3.242701	0.186231
1	0.836719	-3.723593	-0.597016

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27	-0.831243	0.091363	0.036163
15	-0.715704	2.359413	0.054196
15	-1.303264	-2.184212	-0.072061
7	-2.681928	0.352217	-0.855136

6	-0.712818	3.062140	1.747109
1	0.146428	2.639315	2.273015
6	0.605724	3.250889	-0.854225
1	1.573769	2.912194	-0.477154
6	-2.332231	2.821598	-0.744600
1	-2.748972	3.762400	-0.371874
1	-2.155365	2.951184	-1.819417
6	-3.310089	1.667356	-0.500199
1	-3.580840	1.610899	0.558804
1	-4.236445	1.806597	-1.071210
6	-3.623158	-0.789688	-0.633058
1	-4.531497	-0.653732	-1.232948
1	-3.917681	-0.759150	0.420702
6	-2.937567	-2.115710	-0.963811
1	-2.734340	-2.181251	-2.040024
1	-3.586846	-2.959216	-0.708183
6	-0.361757	-3.494544	-0.960445
1	0.570159	-3.698682	-0.428412
6	-1.687172	-2.933858	1.565644
1	-0.770714	-2.985332	2.158597
1	-2.481972	0.380644	-1.860197
6	3.182486	-1.410476	-0.683928
6	4.208976	-1.099241	-1.580789
6	4.826303	0.149869	-1.527825
6	4.415420	1.082409	-0.570108
6	3.391308	0.766278	0.321701
6	2.758135	-0.485644	0.275462
6	1.638792	-0.820272	1.255760
1	2.717953	-2.393431	-0.724200
1	4.528076	-1.834190	-2.314230
1	5.627158	0.393860	-2.219229
1	4.903764	2.051295	-0.512727
1	3.087125	1.489398	1.073627
1	1.282542	-1.836737	1.010224
1	0.555538	3.007587	-1.918771
1	0.518602	4.333675	-0.725893
1	-0.647517	4.153632	1.734396
1	-1.617067	2.756625	2.279702
1	-0.113116	-3.157565	-1.969889
1	-0.943653	-4.419292	-1.019973
1	-2.398480	-2.303745	2.105788
1	-2.102467	-3.940226	1.457795
8	0.588980	0.122000	1.154606
6	2.123937	-0.840408	2.711932
1	2.492614	0.145699	3.008744
1	1.299600	-1.110123	3.379526
1	2.935636	-1.562850	2.842377

***cis*-I-TS2**

27	-0.468960	0.132846	-0.218229
15	-1.653122	2.036778	0.020199
15	0.704932	-1.695591	-0.950923
7	-1.660465	-0.178080	-1.837657
1	-2.439664	-0.615320	-1.337149
6	-2.671931	2.393734	1.483013
1	-3.174960	3.360831	1.395922
6	-0.694163	3.571810	-0.216235
1	0.015189	3.684567	0.608151
6	-2.800161	1.959966	-1.424827
1	-3.751978	1.533380	-1.086636
1	-3.025191	2.949596	-1.833573
6	-2.162978	1.065248	-2.474980
1	-2.870374	0.821254	-3.278235
1	-1.300195	1.556447	-2.941312
6	-1.172371	-1.172469	-2.825890
1	-0.411108	-0.674368	-3.438684
1	-1.988952	-1.463980	-3.498658
6	-0.587653	-2.356429	-2.084067
1	-0.189622	-3.104275	-2.777252
1	-1.352862	-2.844051	-1.467880
6	2.160374	-1.528005	-2.037174
1	3.013437	-1.159373	-1.461727
6	1.098569	-3.057772	0.184202
1	1.189616	-4.008861	-0.347843
1	1.961788	-0.802043	-2.829794
1	2.425816	-2.486884	-2.492590
1	-0.123605	3.526916	-1.147934
1	-1.343371	4.451797	-0.240193
1	-3.420201	1.611202	1.625268
1	-2.027912	2.407422	2.365714
1	0.293218	-3.111555	0.921995
1	2.045190	-2.853694	0.691019
6	-3.715192	-1.222371	0.767440
6	-2.581135	-1.307856	1.778662
6	-2.666814	-2.597057	2.581982
8	-1.329932	-1.246108	1.145627
1	-2.698324	-0.456771	2.482455

1	-3.608887	-2.679168	3.132865
1	-2.586050	-3.460074	1.911036
1	-1.844927	-2.654931	3.300533
1	-0.383864	-0.394655	1.763500
1	-3.625175	-2.029046	0.027475
1	-4.701167	-1.313892	1.233638
1	-3.697535	-0.259621	0.237623
8	0.328003	0.405612	1.619241
6	1.643748	-0.011423	2.000454
1	1.640087	-1.110058	2.097711
6	2.663805	0.369928	0.958414
6	3.912588	-0.258918	0.964695
6	2.417660	1.364505	0.007667
6	4.893102	0.096102	0.042819
1	4.118453	-1.031166	1.704738
6	3.394159	1.716130	-0.922252
1	1.456272	1.876378	0.012032
6	4.634843	1.083736	-0.907094
1	5.858980	-0.400148	0.063314
1	3.190694	2.496253	-1.651337
1	5.398754	1.361671	-1.626791
6	1.960265	0.601621	3.355328
1	1.953626	1.692849	3.283771
1	1.220016	0.296713	4.098916
1	2.947962	0.289643	3.704678

***trans*-I-TS2**

27	0.418843	-0.149479	-0.200954
15	-0.696035	1.757027	-0.751430
15	1.638422	-2.050547	-0.119139
7	1.212921	0.117273	-2.064786
1	0.436187	-0.185829	-2.655251
6	-2.011349	1.760439	-2.015241
1	-2.230335	2.775503	-2.359759
6	-1.229204	2.955956	0.500000
1	-2.197837	2.657344	0.908986
6	0.758263	2.541406	-1.549425
1	0.497236	3.447593	-2.105775
1	1.383544	2.827622	-0.697322
6	1.507872	1.546486	-2.430355
1	1.279659	1.691700	-3.492512
1	2.586652	1.683873	-2.316301
6	2.353354	-0.783401	-2.402511
1	3.238640	-0.370135	-1.906401
1	2.546852	-0.757502	-3.482269
6	2.073720	-2.188403	-1.906132
1	2.928647	-2.846998	-2.090175
1	1.214391	-2.621894	-2.433181
6	3.233347	-2.165227	0.757549
1	3.059824	-2.123688	1.835138
6	0.806821	-3.607358	0.327736
1	1.476849	-4.466268	0.232105
1	3.883182	-1.327722	0.493429
1	3.739415	-3.105397	0.518150
1	-0.476560	2.956336	1.292322
1	-1.324583	3.958197	0.072919
1	-1.722517	1.157439	-2.880894
1	-2.923355	1.324398	-1.598415
1	-0.068785	-3.771953	-0.304597
1	0.464654	-3.539822	1.363624
6	3.556995	1.486650	0.638572
6	2.562443	1.180493	1.746815
6	2.670403	2.189752	2.879488
8	1.253673	1.184038	1.241898
1	2.811613	0.178421	2.154048
1	3.674965	2.213724	3.313320
1	2.435822	3.193193	2.506460
1	1.960863	1.955345	3.677721
1	0.341882	0.276863	1.829123
1	3.421608	2.509555	0.266019
1	4.596658	1.389205	0.968296
1	3.396590	0.801694	-0.204764
8	-0.335746	-0.542063	1.638837
6	-1.678147	-0.233629	2.030825
1	-1.719303	0.828364	2.324504
6	-2.648117	-0.448404	0.895417
6	-3.858675	0.248860	0.884407
6	-2.395961	-1.371432	-0.126169
6	-4.799649	0.031141	-0.119383
1	-4.070176	0.962186	1.680222
6	-3.330156	-1.583769	-1.138046
1	-1.466227	-1.941048	-0.106518
6	-4.535932	-0.885011	-1.135962
1	-5.737749	0.578266	-0.109045
1	-3.127385	-2.311985	-1.919195
1	-5.268498	-1.058220	-1.918153
6	-2.030062	-1.093427	3.234249

1	-1.994535	-2.152246	2.960972
1	-1.324209	-0.921005	4.049902
1	-3.037907	-0.869816	3.594139

***cis*-I-TS2$_{shuttle}$**

27	-0.012712	-0.600095	0.134240
15	-0.649748	-0.678646	-2.112076
15	0.648151	-0.929897	2.328424
7	0.279193	-2.611657	-0.041103
6	-2.403976	-0.708668	-2.674069
1	-2.854200	0.275660	-2.535916
6	0.198702	0.413789	-3.317726
1	0.096494	0.036986	-4.339701
6	-0.062941	-2.405231	-2.474710
1	-0.551465	-2.829166	-3.357613
1	1.012688	-2.361100	-2.673086
6	-0.340045	-3.256169	-1.235232
1	-1.416116	-3.337708	-1.047863
1	0.050429	-4.274760	-1.355943
6	0.040009	-3.378798	1.217157
1	0.291031	-4.436711	1.066938
1	-1.031851	-3.323564	1.434664
6	0.861944	-2.782916	2.366473
1	1.924297	-3.012365	2.234074
1	0.556562	-3.215775	3.323749
6	2.238154	-0.174020	2.851390
1	2.226181	0.881889	2.566557
6	-0.508464	-0.539216	3.706905
1	-0.067608	-0.808719	4.671132
1	1.287064	-2.586311	-0.206340
1	2.396783	-0.277861	3.928400
1	3.062336	-0.648264	2.314535
1	-0.236354	1.415902	-3.267704
1	1.250446	0.470639	-3.033425
1	-2.980565	-1.417575	-2.075062
1	-2.464647	-0.990436	-3.729665
1	-0.719531	0.532978	3.698152
1	-1.452465	-1.076643	3.585850
6	1.644108	4.388717	-0.229816
6	2.476314	3.119016	-0.395058
1	2.519848	2.872584	-1.469083
6	3.903504	3.312638	0.119693
1	4.491376	2.397619	-0.000039
1	4.412286	4.115670	-0.423560
1	3.889125	3.571651	1.183679
8	1.865533	2.026014	0.301642
1	0.536899	1.805796	0.464780
6	3.423017	-0.585875	-0.698505
1	3.974542	-0.105208	0.130516
6	3.619343	-2.098684	-0.544056
1	3.245772	-2.460839	0.421158
1	3.118727	-2.646934	-1.353328
1	4.680580	-2.363133	-0.590261
6	4.058796	-0.108248	-2.011608
1	3.588130	-0.604638	-2.868713
1	3.931869	0.971254	-2.133401
1	5.131817	-0.326893	-2.041339
8	2.059563	-0.191459	-0.639527
1	2.043843	1.005982	-0.199513
1	2.114300	5.229261	-0.749505
1	0.637927	4.263712	-0.643314
1	1.556312	4.653659	0.829588
8	-0.419335	1.292432	0.603667
6	-1.539009	2.120338	0.256957
1	-1.356820	2.564901	-0.734098
6	-1.648174	3.246866	1.294888
1	-0.718787	3.818135	1.349796
1	-2.459854	3.931663	1.033264
1	-1.862096	2.825472	2.281679
6	-2.834608	1.331417	0.190118
6	-3.909822	1.843425	-0.550606
6	-3.019494	0.137656	0.896511
6	-5.134587	1.176328	-0.588389
1	-3.789450	2.774728	-1.099532
6	-4.242582	-0.539277	0.853077
1	-2.208875	-0.252007	1.504658
6	-5.304334	-0.021819	0.110650
1	-5.956154	1.590764	-1.164907
1	-4.371764	-1.460849	1.414378
1	-6.257454	-0.540651	0.082866

***trans*-I-TS2$_{shuttle}$**

27	-0.041343	-0.562422	0.201794
15	0.743050	-0.355515	2.368784
15	-0.917733	-1.213180	-1.886479
7	-0.447804	-2.526992	0.746884

6	2.556494	-0.200168	2.589000
1	2.875206	0.698885	2.054962
6	0.058873	0.910612	3.511510
1	0.457070	0.779000	4.521932
6	0.247857	-2.004029	3.077118
1	0.887849	-2.318620	3.907561
1	-0.770619	-1.906322	3.473545
6	0.284162	-3.035524	1.947918
1	1.313017	-3.231692	1.638686
1	-0.149944	-3.989883	2.272055
6	-0.433113	-3.504773	-0.381789
1	-0.774590	-4.486980	-0.029878
1	0.603744	-3.607234	-0.705889
6	-1.318626	-2.998644	-1.518714
1	-2.374718	-3.042523	-1.224538
1	-1.206430	-3.629754	-2.405952
6	-2.455092	-0.615611	-2.707778
1	-2.309115	0.407080	-3.062816
6	0.285997	-1.259905	-3.272149
1	-0.155157	-1.737754	-4.152030
1	-1.427746	-2.422367	1.027056
1	-2.692636	-1.253035	-3.565094
1	-3.291943	-0.616568	-2.007531
1	0.342246	1.898820	3.141780
1	-1.031685	0.857494	3.546831
1	3.064040	-1.058246	2.145445
1	2.817561	-0.125852	3.648698
1	0.581999	-0.238035	-3.519678
1	1.183915	-1.791071	-2.961295
6	2.239848	4.190911	-0.868449
6	2.884005	2.806236	-0.840887
1	2.944191	2.438050	-1.878169
6	4.297769	2.856704	-0.258185
1	4.748376	1.859599	-0.235403
1	4.947323	3.507690	-0.852629
1	4.270135	3.242686	0.766670
8	2.085531	1.898618	-0.074400
1	0.699652	1.856346	0.017290
6	3.225498	-1.025730	-0.807203
1	3.860108	-0.656206	0.019317
6	3.178449	-2.550161	-0.685577
1	2.728195	-2.861526	0.261707
1	2.603292	-2.993945	-1.506979
1	4.186433	-2.975659	-0.725741
6	3.919891	-0.626945	-2.118639
1	3.375323	-1.017980	-2.984617
1	3.974639	0.459710	-2.220751
1	4.942097	-1.019287	-2.156298
8	1.941373	-0.425183	-0.721070
1	2.116716	0.807173	-0.446272
1	2.861003	4.896261	-1.429290
1	1.256490	4.161018	-1.349001
1	2.121785	4.579711	0.149150
8	-0.280276	1.444213	0.187324
6	-1.357715	2.259700	-0.285682
1	-1.231640	2.433251	-1.365995
6	-1.317092	3.611233	0.442935
1	-0.358529	4.110901	0.288063
1	-2.110674	4.267927	0.075187
1	-1.467704	3.461812	1.516184
6	-2.700817	1.583271	-0.066796
6	-3.803403	1.980086	-0.835821
6	-2.895898	0.612863	0.923950
6	-5.061844	1.414127	-0.630973
1	-3.676151	2.737894	-1.605362
6	-4.153717	0.035181	1.126831
1	-2.063854	0.329230	1.561782
6	-5.241063	0.432333	0.347735
1	-5.902849	1.737182	-1.237113
1	-4.290703	-0.706838	1.909353
1	-6.220376	-0.007371	0.508897

I-TS4

27	-0.055988	-0.401973	-0.608736
15	-2.366245	-0.491780	-0.511358
15	2.229103	-0.795996	-0.466829
7	-0.093737	-0.650032	1.360389
6	-3.343383	0.894697	-1.207151
1	-4.380391	0.858418	-0.860447
6	-3.232995	-2.028691	-1.041361
1	-3.156074	-2.143737	-2.125991
6	-2.547013	-0.406691	1.328161
1	-2.520774	0.653587	1.596324
1	-3.498157	-0.827371	1.668006
6	-1.354034	-1.135339	1.955333
1	-1.333095	-0.956742	3.039763
1	-1.443844	-2.222088	1.815630

6	1.095553	-1.249727	1.991511
1	1.065917	-2.343397	1.882982
1	1.076340	-1.040548	3.070412
6	2.381507	-0.687598	1.374764
1	3.264408	-1.218141	1.744982
1	2.493817	0.371460	1.630969
6	2.751173	-2.509460	-0.904197
1	2.692882	-2.649077	-1.987148
6	3.542210	0.276027	-1.177619
1	3.349995	1.319194	-0.917697
1	2.087394	-3.237196	-0.429885
1	3.778662	-2.701387	-0.580418
1	-2.771312	-2.901172	-0.570920
1	-4.291345	-1.994931	-0.765921
1	-2.876995	1.829416	-0.888947
1	-3.333966	0.847579	-2.299521
1	3.540437	0.184730	-2.267267
1	4.527196	-0.015758	-0.801229
1	-0.075048	0.585633	1.168853
1	1.667848	2.366797	0.476234
6	0.624884	2.645521	0.228454
6	0.616946	3.235416	-1.182074
8	-0.203612	1.491890	0.269302
1	0.961798	2.496575	-1.915657
1	-0.397741	3.540609	-1.459525
1	1.267537	4.113045	-1.253116
6	0.147091	3.655698	1.274586
1	0.162582	3.215239	2.276806
1	0.783429	4.546590	1.286035
1	-0.879288	3.968574	1.055794

I-TS4$_{shuttle}$

27	0.442661	-0.822699	0.270058
15	2.614513	-0.069356	0.115195
15	-1.616550	-1.890205	-0.045168
7	0.292659	-0.368166	-1.670757
6	3.263900	1.139433	1.330183
1	4.170316	1.627537	0.960687
6	3.959702	-1.308878	-0.109487
1	4.098684	-1.874990	0.815521
6	2.463832	0.804789	-1.508127
1	2.012574	1.782114	-1.306090
1	3.435538	0.971409	-1.983560
6	1.537326	-0.032855	-2.395333
1	1.291445	0.522483	-3.311587
1	2.045077	-0.953536	-2.715980
6	-0.611583	-1.192560	-2.502839
1	-0.147179	-2.165213	-2.718217
1	-0.771007	-0.698372	-3.471408
6	-1.954075	-1.374463	-1.789146
1	-2.598212	-2.088086	-2.311979
1	-2.468451	-0.410778	-1.730503
6	-1.466764	-3.728744	-0.088823
1	-1.277992	-4.110146	0.918407
6	-3.177765	-1.577063	0.873258
1	-3.395200	-0.506626	0.858161
1	-0.627946	-4.020548	-0.726867
1	-2.381164	-4.189872	-0.474312
1	3.696777	-2.012057	-0.904348
1	4.903168	-0.818217	-0.367403
1	2.489069	1.882248	1.529016
1	3.495009	0.624791	2.266868
1	-3.078126	-1.903637	1.911409
1	-4.008280	-2.118741	0.410482
6	-1.232457	2.931507	-2.590030
6	-1.105389	2.868615	-1.067022
1	-0.183192	3.400424	-0.773393
6	-2.289662	3.543315	-0.375490
1	-2.192092	3.488026	0.713247
1	-2.358180	4.599859	-0.653317
1	-3.225416	3.050226	-0.659768
8	-1.021624	1.505627	-0.639841
1	-0.328791	0.661157	-1.299540
6	-0.801109	0.679581	2.663234
1	-1.850691	0.456870	2.421087
6	-0.239264	-0.453516	3.518419
1	-0.269813	-1.406768	2.971984
1	0.800267	-0.247650	3.794914
1	-0.816307	-0.580188	4.439413
6	-0.735258	2.028422	3.378162
1	0.299279	2.273874	3.639133
1	-1.128064	2.828080	2.743866
1	-1.326716	2.007556	4.299005
8	-0.048412	0.749884	1.441675
1	-0.580978	1.253608	0.570374
1	-1.290977	3.968500	-2.934593
1	-0.371104	2.467674	-3.084217

1	-2.139539	2.412851	-2.919576

I-TS3

27	1.476520	0.397346	-0.434342
15	2.510147	-1.660864	-0.148802
15	0.683466	2.584179	-0.255816
7	0.643433	0.083193	1.333011
6	2.244547	-2.947623	-1.427679
1	2.517537	-3.939239	-1.054792
6	4.295589	-1.760625	0.294698
1	4.906971	-1.444054	-0.554803
6	1.572683	-2.199842	1.355624
1	0.649223	-2.663834	0.997660
1	2.127050	-2.939215	1.941347
6	1.243582	-0.956919	2.189270
1	0.535430	-1.218427	2.987910
1	2.146118	-0.567359	2.681653
6	0.191157	1.259467	2.097586
1	1.039760	1.702554	2.638100
1	-0.534160	0.936652	2.857046
6	-0.457313	2.295798	1.172018
1	-0.679284	3.221925	1.711652
1	-1.398337	1.903550	0.771127
6	1.941366	3.789202	0.350623
1	2.656905	4.007980	-0.446759
6	-0.259495	3.525210	-1.523025
1	-1.088531	2.921969	-1.899184
1	2.491232	3.367367	1.196151
1	1.469517	4.725083	0.665001
1	4.511807	-1.099000	1.137951
1	4.573165	-2.783753	0.565434
1	1.188481	-2.928236	-1.704942
1	2.847754	-2.724134	-2.311934
1	0.397680	3.770809	-2.361763
1	-0.652094	4.453950	-1.098330
1	-0.151186	-0.369220	0.483537
1	-1.506474	0.667026	-1.758617
6	-1.507138	-0.390347	-1.441846
6	-1.600438	-1.248109	-2.708956
8	-0.294532	-0.692534	-0.758232
1	-0.731826	-1.070646	-3.352199
1	-1.628727	-2.310462	-2.447190
1	-2.505682	-1.013782	-3.277475
6	-2.708645	-0.588013	-0.526414
6	-3.718196	0.379502	-0.449282
6	-4.832004	0.189762	0.373361
6	-4.947066	-0.973758	1.134317
6	-3.945449	-1.946350	1.065702
6	-2.836595	-1.754301	0.242181
1	-3.642511	1.284034	-1.049975
1	-5.607778	0.948633	0.416901
1	-5.811646	-1.124979	1.773423
1	-4.033767	-2.857668	1.650328
1	-2.064143	-2.516012	0.184946

I-TS3$_{shuttle}$

27	0.059137	0.637683	-0.541563
15	-0.795428	2.651987	0.233339
15	0.563772	-1.300458	-1.728997
7	-1.803639	0.273179	-1.176292
6	-0.441230	3.218806	1.942319
1	-1.144270	3.997540	2.251907
6	-0.656692	4.167400	-0.808356
1	0.383197	4.504552	-0.832543
6	-2.581612	2.183919	0.188803
1	-2.778204	1.564498	1.070483
1	-3.242541	3.055643	0.229714
6	-2.791699	1.372256	-1.089355
1	-3.806193	0.950152	-1.109201
1	-2.707066	2.023625	-1.970952
6	-1.914604	-0.412873	-2.486106
1	-1.584793	0.257387	-3.292381
1	-2.968943	-0.650196	-2.685179
6	-1.087177	-1.697569	-2.466869
1	-0.998102	-2.142089	-3.462521
1	-1.557390	-2.424086	-1.798655
6	1.713326	-1.041636	-3.146737
1	2.710934	-0.805237	-2.767813
6	1.106571	-2.877667	-0.959735
1	0.405285	-3.123572	-0.158631
1	1.369258	-0.200958	-3.755993
1	1.770796	-1.935302	-3.775391
1	-0.967510	3.951071	-1.833806
1	-1.278693	4.975015	-0.410616
1	-0.517741	2.358448	2.609886
1	0.574850	3.619212	2.001701

1	2.111923	-2.775831	-0.547049
1	1.101358	-3.679913	-1.703946
6	-4.076723	-2.385383	0.562365
6	-2.997203	-1.772528	1.456983
1	-3.418787	-0.868223	1.933775
6	-2.567201	-2.734049	2.565225
1	-1.807888	-2.275025	3.207247
1	-3.415379	-3.015660	3.197401
1	-2.144055	-3.646301	2.130789
8	-1.860671	-1.416577	0.671849
1	-1.990183	-0.557470	-0.274225
6	1.149332	-0.718623	2.016282
1	1.015563	-1.809413	1.966276
6	1.304356	-0.321942	3.491024
1	1.454738	0.758127	3.583163
1	0.403711	-0.597556	4.046903
1	2.160830	-0.825897	3.949037
8	-0.002577	-0.085420	1.463358
1	-0.843157	-0.774622	1.271968
1	-4.969384	-2.645252	1.140254
1	-4.382514	-1.686726	-0.224998
1	-3.701968	-3.297093	0.084134
6	2.390627	-0.368114	1.205471
6	3.522086	-1.193503	1.233572
6	2.434028	0.783020	0.401766
6	4.651655	-0.886505	0.472162
1	3.518291	-2.088456	1.850941
6	3.561832	1.090666	-0.372507
1	1.638472	1.532583	0.484939
6	4.674685	0.252412	-0.340491
1	5.517670	-1.540693	0.510267
1	3.574606	1.994607	-0.974940
1	5.556728	0.487923	-0.927379

***cis*-I-TS6**

27	-0.024096	0.224951	0.113723
15	-2.285308	-0.302995	0.504294
15	2.255219	-0.375262	0.508564
7	-0.048617	-1.334177	-1.216453
6	-2.518267	-1.458937	1.927241
1	-2.438329	-0.897250	2.862034
6	-3.790774	0.755761	0.598802
1	-3.712430	1.431821	1.453993
6	-2.543450	-1.359813	-1.003070
1	-3.412884	-2.019070	-0.907034
1	-2.731970	-0.684897	-1.846153
6	-1.279031	-2.183975	-1.245179
1	-1.164795	-2.937547	-0.459377
1	-1.340344	-2.721291	-2.199518
6	1.180442	-2.185018	-1.288619
1	1.219727	-2.698985	-2.256918
1	1.081564	-2.957492	-0.519045
6	2.446947	-1.364738	-1.054266
1	2.593368	-0.645215	-1.867965
1	3.322835	-2.021910	-1.027001
6	3.789033	0.648189	0.551344
1	3.795699	1.277807	1.444803
6	2.551502	-1.594405	1.866659
1	2.523651	-1.072771	2.827474
1	-0.029553	1.635127	0.826988
1	-0.059430	-0.730471	-2.043577
6	-1.248706	3.177305	-0.384112
6	0.085880	2.435509	-0.396209
1	-3.894235	1.356492	-0.307100
1	-4.684806	0.136341	0.717217
1	-3.498835	-1.943333	1.889555
1	-1.740563	-2.226993	1.931282
1	3.834030	1.291684	-0.330238
1	4.675385	0.006678	0.566026
1	1.766904	-2.355639	1.878718
1	3.523567	-2.086131	1.761719
8	0.273824	1.565456	-1.350865
6	1.269162	3.304926	0.022320
1	1.409312	4.065620	-0.754248
1	1.085488	3.816655	0.970572
1	2.183696	2.720632	0.094397
1	-1.167057	4.014740	-1.086578
1	-2.050638	2.527599	-0.730900
1	-1.494143	3.584758	0.600084

***trans*-I-TS6**

27	-0.028629	0.152831	0.195374
15	2.290661	-0.428408	0.537275
15	-2.308178	-0.384557	0.541318
7	-0.061967	-1.504266	-0.974750
6	3.732335	0.643928	0.115063

1	3.869409	1.410611	0.881784
6	2.855663	-1.271408	2.080804
1	2.932374	-0.535753	2.886232
6	2.371483	-1.772448	-0.767702
1	3.327363	-1.750278	-1.299219
1	2.308953	-2.747335	-0.267888
6	1.207812	-1.608567	-1.749649
1	1.303685	-0.688335	-2.331225
1	1.158541	-2.457407	-2.443371
6	-1.293305	-1.477166	-1.816685
1	-1.282551	-2.307804	-2.533496
1	-1.271175	-0.537460	-2.374520
6	-2.528199	-1.555145	-0.909319
1	-2.667337	-2.574357	-0.530076
1	-3.429846	-1.302242	-1.474346
6	-2.605137	-1.437227	2.031254
1	-2.564528	-0.812657	2.927889
6	-3.808740	0.688506	0.521535
1	-3.751315	1.417677	1.333640
1	-0.041412	1.567223	0.894421
1	-0.116861	-2.339418	-0.386025
6	-1.280320	3.084089	-0.353952
6	0.065057	2.362095	-0.352791
1	2.127325	-2.028671	2.383634
1	3.831243	-1.747988	1.945344
1	4.645596	0.044300	0.054226
1	3.558147	1.135706	-0.844712
1	-1.828348	-2.202016	2.117885
1	-3.582809	-1.926468	1.985775
1	-3.881294	1.230318	-0.423549
1	-4.709399	0.081164	0.652145
8	0.269727	1.482839	-1.291934
6	1.226284	3.257825	0.071911
1	1.012936	3.784697	1.005538
1	2.149441	2.693639	0.175124
1	1.369021	4.006100	-0.716363
1	-1.199254	3.931070	-1.045129
1	-2.065603	2.426626	-0.721996
1	-1.548200	3.477356	0.630204

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27	-1.377446	0.000592	0.508794
15	-1.580610	2.234171	0.433033
15	-1.640116	-2.224075	0.337024
7	-1.442492	0.045110	-1.594879
6	-3.225212	2.936955	0.878801
1	-3.387276	2.810006	1.952388
6	-0.387583	3.403602	1.204462
1	-0.477526	3.338529	2.291923
6	-1.421138	2.520602	-1.407307
1	-1.910414	3.443873	-1.735141
1	-0.352303	2.622773	-1.630103
6	-2.001422	1.309461	-2.147465
1	-3.088146	1.267553	-2.014552
1	-1.810311	1.384830	-3.226304
6	-2.041630	-1.176289	-2.199340
1	-1.856215	-1.210471	-3.281244
1	-3.126152	-1.107276	-2.059725
6	-1.495478	-2.434860	-1.514499
1	-0.430857	-2.558172	-1.746861
1	-2.012930	-3.328424	-1.879107
6	-0.490701	-3.475343	1.044739
1	-0.576092	-3.464140	2.134422
6	-3.308044	-2.890013	0.754459
1	-3.461861	-2.814145	1.834064
1	-1.454859	-0.022709	2.003587
1	-0.436009	0.032358	-1.775132
6	3.363212	0.103792	-1.187183
6	4.616819	0.141617	-1.785798
6	5.769060	0.039515	-0.998660
6	5.662106	-0.099426	0.387000
6	4.406555	-0.135290	0.989017
6	3.240315	-0.034687	0.208150
6	1.890445	-0.070868	0.820318
1	2.463204	0.182398	-1.786772
1	4.702457	0.250237	-2.862481
1	6.748697	0.068598	-1.465954
1	6.556120	-0.179087	0.997027
1	4.339779	-0.242986	2.066074
1	0.632097	3.127090	0.925461
1	-0.579567	4.434569	0.892842
1	-3.290415	4.000248	0.629243
1	-4.018262	2.396759	0.354625
1	0.538677	-3.226291	0.775800
1	-0.723492	-4.480239	0.680211
1	-4.083271	-2.295006	0.263996
1	-3.413117	-3.935618	0.449548

8	0.878209	-0.006048	0.102372
6	1.745173	-0.185920	2.318277
1	2.202333	-1.113507	2.679913
1	2.258833	0.639346	2.822678
1	0.685722	-0.173000	2.576629

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27	-1.537057	-0.000619	-0.473055
15	-1.659725	2.247650	-0.339111
15	-1.655882	-2.249174	-0.339347
7	-1.712192	-0.000887	1.623818
6	-0.188092	3.246309	-0.820488
1	-0.055665	3.191947	-1.904185
6	-3.070285	3.207626	-1.030654
1	-3.010861	3.187480	-2.122006
6	-1.790033	2.466479	1.517601
1	-1.321945	3.394851	1.860447
1	-2.855206	2.532668	1.773058
6	-1.157055	1.250999	2.207863
1	-0.077919	1.228568	2.034529
1	-1.326871	1.286933	3.292345
6	-1.155162	-1.251986	2.207760
1	-1.324999	-1.288300	3.292226
1	-0.076046	-1.227878	2.034511
6	-1.786205	-2.468366	1.517316
1	-2.851319	-2.536175	1.772585
1	-1.316779	-3.396059	1.860172
6	-3.064786	-3.211372	-1.031202
1	-3.005259	-3.191006	-2.122545
6	-0.182587	-3.245595	-0.820412
1	-0.049245	-3.190006	-1.903935
1	-1.603595	-0.000636	-1.967788
1	-2.717845	-0.001654	1.809966
6	3.258304	0.001640	1.106042
6	4.524982	0.001716	1.678047
6	5.659819	0.001652	0.859758
6	5.522192	0.001521	-0.530150
6	4.253488	0.001471	-1.105362
6	3.104570	0.001522	-0.293191
6	1.739275	0.001436	-0.874498
1	2.371468	0.001706	1.729886
1	4.634091	0.001830	2.758113
1	6.649670	0.001710	1.305958
1	6.402751	0.001468	-1.164485
1	4.163404	0.001373	-2.186118
1	-4.016346	2.745876	-0.736183
1	-3.055353	4.247481	-0.690963
1	-0.306913	4.294088	-0.528958
1	0.704521	2.836603	-0.342654
1	-4.011646	-2.751216	-0.736797
1	-3.048189	-4.251238	-0.691630
1	0.709169	-2.835445	-0.341337
1	-0.300507	-4.293797	-0.530034
8	0.747046	0.001105	-0.127052
6	1.560296	0.001716	-2.373356
1	2.037371	0.880951	-2.819587
1	2.036392	-0.878026	-2.819672
1	0.494985	0.002218	-2.606320

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27	-0.004846	-0.247024	-0.518574
15	2.222879	-0.558990	-0.496315
15	-2.238379	-0.513425	-0.498659
7	-0.014135	-1.068240	1.417614
6	2.857748	-1.980694	-1.483181
1	2.758040	-1.749195	-2.546833
6	3.471839	0.760125	-0.791106
1	3.436040	1.057338	-1.842395
6	2.465298	-1.067817	1.285249
1	3.367096	-1.670928	1.434553
1	2.585910	-0.149774	1.872990
6	1.220465	-1.831167	1.752095
1	1.151875	-2.797054	1.239739
1	1.272829	-2.039000	2.829013
6	-1.264148	-1.806531	1.750399
1	-1.321855	-2.013561	2.827195
1	-1.214150	-2.773392	1.237781
6	-2.492932	-1.018292	1.282344
1	-2.595817	-0.098246	1.870278
1	-3.406785	-1.603313	1.430329
6	-3.456941	0.834203	-0.791880
1	-3.414850	1.131514	-1.842906
6	-2.905667	-1.919165	-1.487129
1	-2.799616	-1.689314	-2.550517
1	0.000105	0.239385	-1.932992
1	-0.005917	-0.197151	1.953519
6	0.046251	3.969168	1.437896

6	0.038806	2.913373	0.360810
1	3.238215	1.633582	-0.177528
1	4.482185	0.414549	-0.553447
1	3.907933	-2.189503	-1.257915
1	2.263986	-2.875717	-1.278482
1	-3.202924	1.701380	-0.177468
1	-4.474801	0.511559	-0.554087
1	-2.333866	-2.828402	-1.282519
1	-3.960751	-2.102700	-1.262797
8	0.010176	1.718023	0.663296
6	0.066750	3.367869	-1.073884
1	-0.815050	3.984681	-1.284530
1	0.937019	4.011092	-1.248121
1	0.089737	2.507932	-1.744218
1	-0.801087	4.651426	1.304913
1	0.001220	3.513638	2.427797
1	0.951356	4.582127	1.355392

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27	-0.003806	-0.427067	-0.563144
15	-2.253244	-0.603879	-0.493121
15	2.244451	-0.625740	-0.487438
7	-0.010521	-1.309865	1.343099
6	-3.282363	0.925183	-0.482665
1	-3.208784	1.414989	-1.457138
6	-3.177246	-1.727460	-1.621600
1	-3.154292	-1.311643	-2.632329
6	-2.477784	-1.339457	1.217047
1	-3.404708	-1.004944	1.693723
1	-2.552162	-2.428572	1.105997
6	-1.261483	-0.979144	2.080450
1	-1.234045	0.094766	2.283486
1	-1.298919	-1.505440	3.043530
6	1.241723	-0.991842	2.083741
1	1.271566	-1.518789	3.046729
1	1.224454	0.082201	2.287401
6	2.456512	-1.364044	1.223240
1	2.519900	-2.453821	1.111848
1	3.385633	-1.039353	1.702414
6	3.161577	-1.758158	-1.612736
1	3.147436	-1.341570	-2.623310
6	3.289578	0.892548	-0.472623
1	3.227723	1.381898	-1.448131
1	-0.002203	0.038069	-1.984707
1	-0.015348	-2.319281	1.178664
6	0.007558	3.866969	1.214269
6	0.020762	2.765312	0.183159
1	-2.694639	-2.707904	-1.649754
1	-4.218395	-1.847396	-1.307818
1	-4.332197	0.694919	-0.278351
1	-2.911760	1.613658	0.280229
1	2.668906	-2.733498	-1.643625
1	4.200040	-1.889168	-1.294499
1	2.921236	1.585981	0.286864
1	4.335565	0.651612	-0.260921
8	0.002261	1.584471	0.538434
6	0.056282	3.160289	-1.269029
1	-0.829902	3.758709	-1.511860
1	0.921105	3.805451	-1.462186
1	0.093349	2.273255	-1.902546
1	-0.844404	4.534971	1.043877
1	-0.043384	3.453428	2.222162
1	0.907732	4.484680	1.114849

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15	2.188158	-0.170562	-0.039369
15	-2.188151	-0.170437	-0.039361
7	0.000044	1.751159	-0.268964
6	3.146104	-0.535779	1.501126
1	3.044901	-1.600050	1.732655
6	3.265255	-0.942767	-1.328796
1	3.241107	-2.029487	-1.205468
6	2.457310	1.661637	-0.298776
1	3.377129	2.026048	0.171207
1	2.546629	1.837529	-1.377901
6	1.230710	2.387196	0.253869
1	1.194192	2.293173	1.343807
1	1.256121	3.459387	0.004427
6	-1.230669	2.387319	0.253622
1	-1.256016	3.459465	0.003985
1	-1.194270	2.293513	1.343581
6	-2.457236	1.661711	-0.299050
1	-2.546393	1.837419	-1.378220
1	-3.377098	2.026265	0.170735
6	-3.265384	-0.942867	-1.328554
1	-3.240919	-2.029584	-1.205258

6	-3.145926	-0.535526	1.501258
1	-3.045145	-1.599903	1.732502
1	0.000151	-0.458547	-1.618626
1	0.000143	1.839387	-1.284608
1	2.855946	-0.710245	-2.314566
1	4.304000	-0.601891	-1.264505
1	4.208833	-0.288313	1.403759
1	2.706161	0.022988	2.330308
1	-2.856394	-0.710216	-2.314427
1	-4.304204	-0.602279	-1.263988
1	-2.705540	0.022827	2.330478
1	-4.208567	-0.287572	1.404179
1	-0.000030	-0.119737	1.499318
6	-0.000105	-2.093583	0.119511
8	-0.000259	-3.252892	0.232085
26	0.000021	-0.364777	-0.049293

Fe-TS$_O$

15	0.404005	2.115441	0.291863
15	-2.728116	-0.980661	0.371846
7	-1.243842	0.597400	-1.582182
6	-0.236083	3.756017	0.858085
1	-0.361712	3.730231	1.944304
6	2.147199	2.198454	0.894152
1	2.147435	2.169688	1.987776
6	0.535363	2.296768	-1.551427
1	0.838264	3.301729	-1.865451
1	1.286927	1.577175	-1.893335
6	-0.825119	1.911306	-2.130543
1	-1.587423	2.648493	-1.854238
1	-0.782522	1.870391	-3.228976
6	-2.586790	0.219054	-2.082793
1	-2.583376	0.150677	-3.180850
1	-3.281201	1.018844	-1.802988
6	-3.031564	-1.105268	-1.460971
1	-2.416178	-1.924606	-1.848329
1	-4.076461	-1.327835	-1.704195
6	-2.797366	-2.733016	0.965611
1	-2.748657	-2.736110	2.058754
6	-4.331608	-0.341446	1.036156
1	-4.236710	-0.207343	2.117429
1	0.168575	-0.736794	0.096400
1	-0.555538	-0.096754	-1.936201
1	2.709830	1.339050	0.528913
1	2.636121	3.122139	0.567303
1	0.443593	4.573544	0.594329
1	-1.219755	3.932864	0.418030
1	-1.939668	-3.291554	0.588153
1	-3.722057	-3.230425	0.655089
1	-4.534100	0.639292	0.600467
1	-5.164131	-1.022204	0.828489
6	3.470338	-0.705868	-1.232547
6	4.748269	-0.452830	-0.729498
6	5.045012	-0.740312	0.603868
6	4.056040	-1.283233	1.430657
6	2.781924	-1.538164	0.926389
6	2.473600	-1.248640	-0.410772
6	1.130276	-1.567865	-1.042562
1	3.222441	-0.499201	-2.268556
1	5.512763	-0.036051	-1.379909
1	6.038099	-0.543786	0.998333
1	4.277595	-1.501989	2.471651
1	2.012076	-1.930842	1.583272
8	0.865532	-1.074873	-2.170810
6	0.572871	-2.952554	-0.709724
1	0.558906	-3.170992	0.359094
1	-0.433142	-3.049419	-1.120287
1	1.212764	-3.694589	-1.205783
1	-2.043831	1.447982	0.725341
6	-0.699296	0.146844	2.191037
8	-0.511423	-0.010545	3.329074
26	-0.975447	0.377029	0.488030

Fe-TSI-a

15	-4.561525	-2.489316	0.026755
15	-0.151007	3.077535	0.090537
7	-1.673543	0.616334	0.645363
6	-3.188424	-3.737084	-0.180703
1	-3.603505	-4.631438	-0.655746
6	-4.795789	-1.968173	-1.750991
1	-5.292316	-2.782303	-2.287883
6	-3.636756	-1.010949	0.736563
6	-2.396292	-0.506783	-0.012683
1	-1.663871	-1.303728	-0.132013
1	-2.646795	-0.155880	-1.016552
6	-2.499366	1.846749	0.739112

1	-3.352977	1.708337	1.415774
1	-2.900873	2.029394	-0.263555
6	-1.652462	3.039293	1.184667
1	-1.304718	2.899583	2.214415
1	-2.234000	3.967431	1.148031
6	1.038204	4.173702	0.977489
1	1.938306	4.290036	0.366908
6	-0.661630	4.142827	-1.333225
1	-0.965410	5.146791	-1.017634
1	-1.423870	0.332025	1.591771
1	-5.458207	-1.097697	-1.791493
1	-3.863385	-1.728315	-2.271279
1	-2.348436	-3.381392	-0.785335
1	-2.815004	-4.033601	0.804603
1	1.326485	3.689961	1.912954
1	0.616043	5.163529	1.179320
1	0.179430	4.223378	-2.027920
1	-1.480821	3.655929	-1.867524
26	0.261931	0.975701	-0.199834
1	0.865806	1.046604	1.278075
6	3.203705	-1.709500	-1.056367
6	4.527510	-1.919223	-1.428889
6	5.507583	-2.109056	-0.450593
6	5.159280	-2.092304	0.902255
6	3.833200	-1.888363	1.277374
6	2.842086	-1.690622	0.301383
6	1.408426	-1.490150	0.652369
1	2.429083	-1.555210	-1.798906
1	4.798260	-1.929663	-2.480341
1	6.541976	-2.268872	-0.741679
1	5.920597	-2.237047	1.663026
1	3.575802	-1.873719	2.331059
8	0.574221	-1.267716	-0.239149
6	0.971666	-1.723348	2.085683
1	1.209518	-2.752782	2.380854
1	1.481589	-1.044013	2.771096
1	-0.103719	-1.568798	2.165727
1	-4.393604	-0.223292	0.834876
1	-3.368653	-1.299391	1.763232
1	-0.434593	0.939802	-1.597568
6	1.735278	1.296539	-1.074307
8	2.674170	1.561110	-1.708644

Fe-TSI-b

15	0.715606	1.847509	0.435024
15	-2.576254	-1.186426	0.345986
7	-1.824455	1.344515	-1.007621
6	0.587121	2.728070	2.059855
1	1.017010	2.088309	2.835756
6	2.508536	2.157609	0.063562
1	3.138240	1.593089	0.754396
6	-0.052282	3.056724	-0.764112
1	0.145724	4.101681	-0.499010
1	0.413095	2.871921	-1.740567
6	-1.549160	2.791762	-0.835677
1	-2.025147	3.089663	0.104336
1	-2.019756	3.375879	-1.641888
6	-3.288839	1.109367	-1.001887
1	-3.767122	1.610102	-1.857660
1	-3.679001	1.580356	-0.093227
6	-3.604091	-0.379489	-0.985385
1	-3.302380	-0.842273	-1.933153
1	-4.679942	-0.547849	-0.858510
6	-3.001035	-2.967915	-0.001497
1	-2.572003	-3.618260	0.765695
6	-3.589368	-0.933914	1.875616
1	-4.595492	-1.357401	1.782975
1	0.157707	-0.868461	1.151299
1	-1.446528	1.040790	-1.907625
6	2.988825	-0.905290	-1.342120
6	4.376748	-0.766502	-1.267667
6	5.027207	-0.865999	-0.036575
6	4.278211	-1.108935	1.119005
6	2.892344	-1.250862	1.040516
6	2.229154	-1.143442	-0.189516
6	0.741873	-1.435525	-0.352687
1	2.469171	-0.831580	-2.292507
1	4.950943	-0.583675	-2.172581
1	6.106839	-0.759364	0.023944
1	4.775515	-1.188138	2.082430
1	2.313416	-1.430973	1.942847
1	2.745616	1.821908	-0.947143
1	2.738839	3.224445	0.157841
1	1.113621	3.688793	2.052093
1	-0.465249	2.877203	2.308769
1	-2.599451	-3.269109	-0.972406
1	-4.087097	-3.109926	-0.009192

1	-3.074542	-1.408850	2.715720
1	-3.649760	0.133540	2.096088
8	0.139206	-0.907786	-1.390163
6	0.485608	-2.925523	-0.086323
1	1.065152	-3.506384	-0.815178
1	0.805834	-3.227938	0.914656
1	-0.564092	-3.169403	-0.215993
1	-1.236337	0.658379	1.477371
26	-0.646564	0.036044	0.210741

Full model

Cy-1

27	-0.012024	-0.017068	0.245042
15	2.251060	0.323185	0.360833
15	-2.280669	-0.329904	0.324599
7	-0.030524	-0.017244	2.325322
6	3.440935	-1.032243	-0.302510
1	3.305058	-0.979036	-1.391390
6	4.926969	-0.778937	0.030252
1	5.066349	-0.767570	1.121570
1	5.248041	0.200654	-0.343463
6	5.821228	-1.885498	-0.575180
1	5.776744	-1.824576	-1.672418
1	6.865579	-1.705633	-0.292849
6	5.376454	-3.288478	-0.121075
1	5.538458	-3.389887	0.962705
1	5.996013	-4.054195	-0.602751
6	3.888902	-3.534345	-0.440204
1	3.574049	-4.515823	-0.064814
1	3.745713	-3.551826	-1.530516
6	2.991449	-2.434000	0.168129
1	1.942715	-2.608012	-0.108790
1	3.055783	-2.493805	1.265481
6	2.953363	2.006859	-0.236251
1	3.948054	2.112415	0.219555
6	3.093549	2.023447	-1.775929
1	2.111678	1.820659	-2.226915
1	3.770615	1.228885	-2.112053
6	3.619380	3.389551	-2.269836
1	4.647290	3.535100	-1.906022
1	3.672021	3.384140	-3.365231
6	2.735156	4.552046	-1.781266
1	1.741094	4.475111	-2.246749
1	3.159497	5.510362	-2.103522
6	2.584749	4.529493	-0.248511
1	1.910437	5.328759	0.083040
1	3.560847	4.726308	0.218720
6	2.052360	3.166387	0.245957
1	1.035032	3.012994	-0.146290
1	1.980904	3.177868	1.342072
6	2.458970	0.333037	2.268633
1	3.415211	-0.105472	2.569499
1	2.461570	1.376848	2.602959
6	1.296913	-0.439026	2.904776
1	1.395458	-1.510678	2.706971
1	1.292899	-0.300866	3.995191
6	-1.179145	-0.825666	2.875950
1	-1.231417	-0.711593	3.967916
1	-0.951625	-1.874555	2.662386
6	-2.509194	-0.420951	2.228448
1	-2.824300	0.568426	2.579619
1	-3.297108	-1.129269	2.503349
6	-3.407186	1.111252	-0.258796
1	-3.367080	1.044934	-1.354664
6	-2.798301	2.468948	0.157894
1	-2.747497	2.533021	1.256353
1	-1.770868	2.550133	-0.222748
6	-3.651580	3.644244	-0.368063
1	-3.222749	4.593612	-0.024205
1	-3.605481	3.656565	-1.466787
6	-5.119654	3.523280	0.082984
1	-5.175864	3.631892	1.176754
1	-5.712337	4.341395	-0.343135
6	-5.721237	2.165419	-0.327503
1	-5.778010	2.107589	-1.424344
1	-6.748564	2.074075	0.045325
6	-4.875676	0.982892	0.198879
1	-5.308235	0.036433	-0.148311
1	-4.921559	0.971993	1.298063
6	-3.053846	-1.939926	-0.375494
1	-4.086235	-1.977914	0.001193
6	-2.288708	-3.179906	0.140735
1	-1.230790	-3.097367	-0.153667
1	-2.320097	-3.224764	1.237716
6	-2.875604	-4.483406	-0.444567
1	-2.290058	-5.340290	-0.089063

1	-3.898368	-4.621594	-0.064146
6	-2.900854	-4.448905	-1.984138
1	-3.362672	-5.363918	-2.373603
1	-1.868932	-4.429328	-2.365601
6	-3.659091	-3.211052	-2.499005
1	-4.720269	-3.290940	-2.220390
1	-3.624653	-3.170341	-3.594378
6	-3.076892	-1.902569	-1.920198
1	-3.668619	-1.050566	-2.276754
1	-2.052298	-1.758175	-2.290821
1	-0.001904	0.008821	-1.271025
1	-0.187516	0.969669	2.561441

Cy-O-2

27	0.025058	0.029440	0.107453
15	2.368067	0.328351	0.290427
15	-2.310259	0.280953	0.325355
7	0.042698	0.172033	2.312550
6	2.500426	0.405463	2.208424
1	3.454074	-0.008319	2.549291
1	2.490087	1.463592	2.494135
6	1.324284	-0.322897	2.878702
1	1.378815	-1.401159	2.695266
1	1.368295	-0.171514	3.969474
6	-1.212551	-0.367900	2.896226
1	-1.246641	-0.220486	3.987881
1	-1.232135	-1.447732	2.713284
6	-2.421973	0.321641	2.246225
1	-2.442383	1.379752	2.533474
1	-3.354743	-0.123832	2.599252
1	0.051074	1.525840	-0.000825
1	0.024705	1.193395	2.358184
6	-0.262849	-3.235275	0.580573
8	-0.054039	-2.036519	-0.277315
6	0.090340	-2.444736	-1.705448
6	-0.369298	-3.904421	-1.742281
6	0.007119	-4.432862	-0.337967
1	0.426474	-3.160717	1.423385
1	-1.294999	-3.212070	0.944298
1	-0.526129	-1.765241	-2.297607
1	1.142599	-2.323404	-1.979988
1	-1.452196	-3.963776	-1.897852
1	0.117152	-4.467640	-2.542993
1	-0.579773	-5.309466	-0.051016
1	1.066040	-4.711567	-0.306391
6	2.921380	2.081453	-0.314703
6	4.094463	2.769736	0.416700
6	3.127750	2.076633	-1.846858
1	2.010993	2.659910	-0.107308
6	4.281935	4.209209	-0.118246
1	5.027548	2.214818	0.269000
1	3.913961	2.804412	1.498374
6	3.343006	3.511548	-2.377775
1	4.003262	1.463367	-2.105371
1	2.257860	1.624132	-2.341664
6	4.496220	4.222476	-1.644072
1	5.131293	4.681439	0.390778
1	3.392286	4.807022	0.130580
1	3.538246	3.479926	-3.456892
1	2.414837	4.086064	-2.241028
1	4.590626	5.254845	-2.002338
1	5.445967	3.720266	-1.882660
6	3.717547	-0.962761	-0.242453
6	5.185900	-0.539110	-0.019048
6	3.436834	-2.324666	0.435672
1	3.551989	-1.073628	-1.324399
6	6.169038	-1.638578	-0.485692
1	5.357206	-0.333954	1.048096
1	5.404407	0.384892	-0.561565
6	4.419346	-3.416178	-0.043045
1	3.541401	-2.216496	1.525980
1	2.405417	-2.634439	0.240801
6	5.881989	-2.993506	0.184532
1	7.196884	-1.317831	-0.276248
1	6.091437	-1.749521	-1.577581
1	4.207475	-4.357861	0.480049
1	4.257581	-3.605440	-1.115072
1	6.563766	-3.760345	-0.202262
1	6.074848	-2.916941	1.265179
6	-3.406372	-1.214075	-0.269837
6	-4.517264	-1.689216	0.690091
6	-3.959122	-0.958075	-1.692457
1	-2.664778	-2.019078	-0.347673
6	-5.236691	-2.936672	0.124833
1	-5.252969	-0.889912	0.847504
1	-4.099530	-1.933898	1.674998
6	-4.673831	-2.211538	-2.244692

1	-4.676860	-0.127425	-1.669043
1	-3.148922	-0.657838	-2.371252
6	-5.785987	-2.688505	-1.292397
1	-6.046540	-3.231381	0.803458
1	-4.528290	-3.779170	0.096824
1	-5.087130	-1.991713	-3.236715
1	-3.939413	-3.020431	-2.382989
1	-6.252367	-3.601525	-1.681706
1	-6.577884	-1.926136	-1.248039
6	-3.246070	1.889049	-0.208860
6	-4.663417	2.025721	0.394178
6	-2.402356	3.150637	0.081686
1	-3.334976	1.787259	-1.299473
6	-5.366733	3.305049	-0.115668
1	-4.594823	2.070598	1.490966
1	-5.277315	1.152288	0.149220
6	-3.111220	4.424015	-0.429732
1	-2.241464	3.246971	1.167040
1	-1.413485	3.054239	-0.376932
6	-4.526600	4.565433	0.159274
1	-6.353696	3.390774	0.355694
1	-5.541853	3.212850	-1.197994
1	-2.504163	5.304071	-0.183079
1	-3.174732	4.383509	-1.527421
1	-5.024522	5.449410	-0.257228
1	-4.455603	4.727171	1.245542

Cy-O-3

27	0.019341	0.228888	-0.619776
15	-2.334055	-0.051371	-0.791443
15	2.375844	-0.140252	-0.553215
7	0.094228	-0.456042	-2.342665
6	-2.359782	-0.200884	-2.676539
1	-3.262063	-0.698394	-3.043708
1	-2.332460	0.817429	-3.077795
6	-1.092750	-0.958011	-3.070162
1	-1.236923	-2.041800	-2.900276
1	-0.926627	-0.842695	-4.152660
6	1.317279	-1.057413	-2.920458
1	1.273165	-0.978435	-4.017882
1	1.374828	-2.138875	-2.694400
6	2.578065	-0.354223	-2.421126
1	2.639484	0.650518	-2.850134
1	3.486020	-0.901868	-2.685066
6	0.320515	1.222004	2.349207
8	-0.051419	1.515321	0.934682
6	-0.392742	2.961197	0.777171
6	0.137071	3.613707	2.054734
6	-0.030880	2.501120	3.115640
1	-0.247233	0.343390	2.661583
1	1.390891	0.999934	2.368775
1	0.083714	3.305776	-0.141365
1	-1.478787	3.039467	0.687580
1	1.193336	3.882042	1.942097
1	-0.416875	4.520720	2.310597
1	0.619416	2.648614	3.981794
1	-1.065822	2.465949	3.473038
6	-3.635716	1.308903	-0.364700
6	-4.934579	1.269131	-1.203606
6	-3.950618	1.369789	1.147026
1	-3.098060	2.229457	-0.640614
6	-5.828375	2.486779	-0.873169
1	-5.492132	0.348884	-0.991269
1	-4.702653	1.263648	-2.275072
6	-4.850558	2.582435	1.474008
1	-4.469547	0.450127	1.449339
1	-3.022501	1.415621	1.732239
6	-6.141551	2.569728	0.633171
1	-6.757551	2.424999	-1.452629
1	-5.319420	3.408414	-1.193312
1	-5.092186	2.585234	2.544218
1	-4.294969	3.511522	1.272903
1	-6.738658	3.464361	0.846536
1	-6.755876	1.705108	0.925513
6	-2.893864	-1.797202	-0.183630
6	-2.521328	-2.059693	1.294221
6	-4.369972	-2.155165	-0.456513
1	-2.263944	-2.453879	-0.803806
6	-2.818557	-3.526217	1.682373
1	-3.096533	-1.390231	1.948923
1	-1.457936	-1.836809	1.460441
6	-4.653486	-3.625969	-0.077757
1	-5.023543	-1.505020	0.140357
1	-4.624343	-1.987367	-1.510130
6	-4.283226	-3.908209	1.390695
1	-2.588347	-3.680753	2.744027
1	-2.149918	-4.190149	1.114074

1	-5.711669	-3.853803	-0.254936
1	-4.073532	-4.288858	-0.736905
1	-4.449131	-4.966156	1.626733
1	-4.948394	-3.331246	2.050650
6	2.830785	-1.846776	0.253324
6	3.898680	-2.681012	-0.489547
6	3.189112	-1.674551	1.747698
1	1.879240	-2.395811	0.195360
6	4.107312	-4.046153	0.206363
1	4.853914	-2.140871	-0.513888
1	3.599500	-2.847034	-1.530964
6	3.405249	-3.042591	2.431977
1	4.109871	-1.081708	1.841881
1	2.397305	-1.121331	2.270665
6	4.467402	-3.879209	1.694348
1	4.892720	-4.605201	-0.316774
1	3.185929	-4.641046	0.118204
1	3.698486	-2.887517	3.477790
1	2.453250	-3.593872	2.448886
1	4.571411	-4.861353	2.170867
1	5.445852	-3.383355	1.779694
6	3.694234	1.165549	-0.027189
6	5.140652	0.805210	-0.436978
6	3.300520	2.558082	-0.575353
1	3.638462	1.197993	1.070565
6	6.138536	1.898545	0.008866
1	5.193815	0.693952	-1.529467
1	5.436634	-0.155639	-0.003254
6	4.300831	3.644535	-0.123437
1	2.286894	2.817779	-0.250206
1	3.282171	2.529232	-1.674285
6	5.743165	3.286412	-0.527541
1	7.146623	1.630503	-0.330241
1	6.174481	1.928427	1.108238
1	4.012210	4.611340	-0.554544
1	4.247050	3.756216	0.970416
1	5.825288	3.291416	-1.624639
1	6.439867	4.048008	-0.157440

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27	0.019341	0.228888	-0.619776
15	-2.334055	-0.051371	-0.791443
15	2.375844	-0.140252	-0.553215
7	0.094228	-0.456042	-2.342665
6	-2.359782	-0.200884	-2.676539
1	-3.262063	-0.698394	-3.043708
1	-2.332460	0.817429	-3.077795
6	-1.092750	-0.958011	-3.070162
1	-1.236923	-2.041800	-2.900276
1	-0.926627	-0.842695	-4.152660
6	1.317279	-1.057413	-2.920458
1	1.273165	-0.978435	-4.017882
1	1.374828	-2.138875	-2.694400
6	2.578065	-0.354223	-2.421126
1	2.639484	0.650518	-2.850134
1	3.486020	-0.901868	-2.685066
6	0.320515	1.222004	2.349207
8	-0.051419	1.515321	0.934682
6	-0.392742	2.961197	0.777171
6	0.137071	3.613707	2.054734
6	-0.030880	2.501120	3.115640
1	-0.247233	0.343390	2.661583
1	1.390891	0.999934	2.368775
1	0.083714	3.305776	-0.141365
1	-1.478787	3.039467	0.687580
1	1.193336	3.882042	1.942097
1	-0.416875	4.520720	2.310597
1	0.619416	2.648614	3.981794
1	-1.065822	2.465949	3.473038
6	-3.635716	1.308903	-0.364700
6	-4.934579	1.269131	-1.203606
6	-3.950618	1.369789	1.147026
1	-3.098060	2.229457	-0.640614
6	-5.828375	2.486779	-0.873169
1	-5.492132	0.348884	-0.991269
1	-4.702653	1.263648	-2.275072
6	-4.850558	2.582435	1.474008
1	-4.469547	0.450127	1.449339
1	-3.022501	1.415621	1.732239
6	-6.141551	2.569728	0.633171
1	-6.757551	2.424999	-1.452629
1	-5.319420	3.408414	-1.193312
1	-5.092186	2.585234	2.544218
1	-4.294969	3.511522	1.272903
1	-6.738658	3.464361	0.846536
1	-6.755876	1.705108	0.925513
6	-2.893864	-1.797202	-0.183630

6	-2.521328	-2.059693	1.294221
6	-4.369972	-2.155165	-0.456513
1	-2.263944	-2.453879	-0.803806
6	-2.818557	-3.526217	1.682373
1	-3.096533	-1.390231	1.948923
1	-1.457936	-1.836809	1.460441
6	-4.653486	-3.625969	-0.077757
1	-5.023543	-1.505020	0.140357
1	-4.624343	-1.987367	-1.510130
6	-4.283226	-3.908209	1.390695
1	-2.588347	-3.680753	2.744027
1	-2.149918	-4.190149	1.114074
1	-5.711669	-3.853803	-0.254936
1	-4.073532	-4.288858	-0.736905
1	-4.449131	-4.966156	1.626733
1	-4.948394	-3.331246	2.050650
6	2.830785	-1.846776	0.253324
6	3.898680	-2.681012	-0.489547
6	3.189112	-1.674551	1.747698
1	1.879240	-2.395811	0.195360
6	4.107312	-4.046153	0.206363
1	4.853914	-2.140871	-0.513888
1	3.599500	-2.847034	-1.530964
6	3.405249	-3.042591	2.431977
1	4.109871	-1.081708	1.841881
1	2.397305	-1.121331	2.270665
6	4.467402	-3.879209	1.694348
1	4.892720	-4.605201	-0.316774
1	3.185929	-4.641046	0.118204
1	3.698486	-2.887517	3.477790
1	2.453250	-3.593872	2.448886
1	4.571411	-4.861353	2.170867
1	5.445852	-3.383355	1.779694
6	3.694234	1.165549	-0.027189
6	5.140652	0.805210	-0.436978
6	3.300520	2.558082	-0.575353
1	3.638462	1.197993	1.070565
6	6.138536	1.898545	0.008866
1	5.193815	0.693952	-1.529467
1	5.436634	-0.155639	-0.003254
6	4.300831	3.644535	-0.123437
1	2.286894	2.817779	-0.250206
1	3.282171	2.529232	-1.674285
6	5.743165	3.286412	-0.527541
1	7.146623	1.630503	-0.330241
1	6.174481	1.928427	1.108238
1	4.012210	4.611340	-0.554544
1	4.247050	3.756216	0.970416
1	5.825288	3.291416	-1.624639
1	6.439867	4.048008	-0.157440

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27	-0.042547	-0.406383	-0.452048
15	2.425004	0.113655	-0.509636
15	-2.417640	0.273070	-0.576803
7	0.004692	-0.048737	-2.435222
6	2.498797	-0.126047	-2.394506
1	3.417775	0.275953	-2.827773
1	2.461559	-1.201346	-2.596460
6	1.270260	0.545312	-2.997007
1	1.263808	1.622502	-2.791694
1	1.261810	0.415927	-4.087773
6	-1.181697	0.664915	-3.026975
1	-1.152644	0.550371	-4.119337
1	-1.076679	1.734149	-2.807014
6	-2.497203	0.124762	-2.473374
1	-2.613370	-0.931023	-2.736972
1	-3.346515	0.674245	-2.891028
1	-0.121837	-2.017341	-0.861186
1	-0.020370	-1.046160	-2.783227
6	1.137718	-4.005151	-1.408333
6	-0.044956	-3.252949	-2.005306
8	0.128382	-2.616180	-3.115571
6	-1.414391	-3.860318	-1.721572
1	-1.544670	-4.117251	-0.666583
1	-2.210692	-3.183122	-2.037829
1	-1.508502	-4.783362	-2.311296
1	2.055264	-3.423105	-1.515014
1	0.981267	-4.258369	-0.356395
1	1.268618	-4.941535	-1.969259
6	-0.029557	0.034649	2.622234
8	-0.140528	-0.906750	1.474907
6	-0.250417	-2.314337	1.959007
6	-0.475497	-2.184678	3.468032
6	0.242029	-0.863371	3.832020
1	0.778252	0.730337	2.391830
1	-0.976045	0.576366	2.700642

1	-1.074525	-2.775466	1.416169
1	0.685066	-2.818982	1.706244
1	-1.544936	-2.114946	3.695097
1	-0.071221	-3.040532	4.015173
1	-0.136504	-0.424932	4.759192
1	1.317532	-1.031790	3.951692
6	3.798880	-1.089183	0.123586
6	5.234134	-0.773627	-0.350944
6	3.752472	-1.299146	1.653564
1	3.485751	-2.032675	-0.349457
6	6.207828	-1.894988	0.079226
1	5.568887	0.175285	0.089137
1	5.265820	-0.652473	-1.440500
6	4.729458	-2.416138	2.083796
1	4.026150	-0.367496	2.166543
1	2.731301	-1.549231	1.965396
6	6.164871	-2.129816	1.601560
1	7.225818	-1.638334	-0.238598
1	5.940378	-2.825630	-0.442761
1	4.709646	-2.525044	3.175616
1	4.388845	-3.374753	1.664160
1	6.826721	-2.960612	1.874023
1	6.550915	-1.238385	2.118506
6	-3.740654	-0.969392	0.088521
6	-4.032747	-0.753060	1.590589
6	-5.050007	-1.070438	-0.726233
1	-3.205139	-1.924812	-0.014569
6	-4.934250	-1.879870	2.142866
1	-4.538946	0.211158	1.734592
1	-3.094909	-0.709703	2.159064
6	-5.943988	-2.203220	-0.170387
1	-5.599772	-0.122993	-0.674244
1	-4.834773	-1.258647	-1.784723
6	-6.237099	-2.010931	1.330030
1	-5.161542	-1.687373	3.198933
1	-4.385388	-2.833277	2.105351
1	-6.880670	-2.242360	-0.739658
1	-5.441927	-3.170041	-0.324189
1	-6.834647	-2.848764	1.708867
1	-6.844039	-1.103929	1.469191
6	-2.968905	2.111768	-0.300768
6	-4.459453	2.422905	-0.555551
6	-2.514346	2.649483	1.074834
1	-2.379588	2.637503	-1.069633
6	-4.729188	3.940662	-0.437722
1	-5.077807	1.896912	0.183473
1	-4.769054	2.065399	-1.545136
6	-2.798638	4.162325	1.202792
1	-3.045363	2.114336	1.875277
1	-1.442504	2.457776	1.215046
6	-4.279876	4.487734	0.930576
1	-5.796946	4.136017	-0.595179
1	-4.190865	4.468970	-1.238733
1	-2.508788	4.509700	2.202436
1	-2.168575	4.708088	0.484237
1	-4.442206	5.571216	0.976539
1	-4.901725	4.043153	1.722075
6	2.955268	1.976795	-0.263271
6	3.364536	2.274689	1.197445
6	4.008596	2.529252	-1.249769
1	2.008841	2.506707	-0.455011
6	3.576065	3.788855	1.418303
1	4.300322	1.748988	1.430093
1	2.606517	1.899388	1.897601
6	4.222456	4.044936	-1.025932
1	4.963063	2.005307	-1.112826
1	3.699742	2.362263	-2.288333
6	4.610847	4.359967	0.430624
1	3.895115	3.968545	2.452528
1	2.616845	4.312417	1.288017
1	4.994305	4.409797	-1.714650
1	3.295480	4.581095	-1.280060
1	4.708964	5.443275	0.569870
1	5.597850	3.924634	0.646495

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27	0.404795	-0.442322	0.871855
15	-1.863794	-1.091858	0.518437
15	0.757225	1.827246	0.527104
7	-0.376228	0.130672	2.918275
6	-2.005424	-1.709187	2.320650
1	-2.998981	-2.107875	2.545474
1	-1.276753	-2.517955	2.409652
6	-1.663170	-0.564491	3.282836
1	-2.460735	0.185858	3.267311
1	-1.610941	-0.945490	4.311301
6	-0.437503	1.619637	3.071605
1	-0.465162	1.906515	4.133719

1	-1.382986	1.949122	2.627187
6	0.738492	2.312853	2.375519
1	1.687401	1.976631	2.804077
1	0.676768	3.395934	2.514176
1	1.934342	-0.323071	1.262404
1	0.387991	-0.237003	3.485952
6	4.939497	-2.809752	-1.796582
6	5.379301	-2.327601	-0.557086
6	4.460545	-2.083081	0.466852
6	3.086488	-2.314504	0.261382
6	2.655292	-2.804393	-0.986203
6	3.575406	-3.049721	-2.007082
1	5.655174	-3.004946	-2.588096
1	6.435623	-2.149311	-0.386849
1	4.820545	-1.710270	1.419088
1	1.601807	-3.009336	-1.131159
1	3.233011	-3.437215	-2.960705
6	2.084292	-2.108167	1.348314
6	2.545547	-2.184850	2.791828
1	2.903400	-3.204293	2.986727
1	3.359228	-1.494402	3.020553
1	1.705250	-1.993083	3.460690
8	0.815554	-2.374933	1.103188
6	-2.299099	-2.596880	-0.610698
6	-1.590955	-2.451888	-1.978871
6	-1.968045	-3.960423	0.038901
1	-3.385786	-2.542794	-0.768669
6	-1.949533	-3.619777	-2.922561
1	-0.504573	-2.435247	-1.813112
1	-1.851471	-1.497060	-2.451611
6	-2.329958	-5.123541	-0.911512
1	-2.515855	-4.080416	0.981212
1	-0.898126	-3.996754	0.278954
6	-1.634487	-4.983012	-2.278419
1	-1.406636	-3.507639	-3.869586
1	-3.021013	-3.571847	-3.167955
1	-2.057481	-6.076202	-0.440601
1	-3.420092	-5.146531	-1.059475
1	-0.546312	-5.081062	-2.144793
1	-1.943074	-5.796994	-2.945614
6	2.468751	2.371702	-0.185468
6	3.584251	2.428134	0.880427
6	2.869822	1.439579	-1.353423
1	2.315640	3.387250	-0.575336
6	4.931911	2.849865	0.250543
1	3.696413	1.436139	1.343971
1	3.323071	3.133645	1.678201
6	4.214526	1.867897	-1.979257
1	2.089004	1.426420	-2.123197
1	2.955038	0.413390	-0.971451
6	5.331220	1.934346	-0.921025
1	5.711073	2.846395	1.023034
1	4.851045	3.886645	-0.108076
1	4.485562	1.165388	-2.776926
1	4.099612	2.854175	-2.453332
1	5.530184	0.920800	-0.542621
1	6.263759	2.290889	-1.375120
6	-0.508851	3.023909	-0.318827
6	-0.351385	4.504471	0.093939
6	-0.446326	2.870571	-1.857102
1	-1.490335	2.666095	0.022881
6	-1.400213	5.394582	-0.613381
1	0.654969	4.859202	-0.171978
1	-0.454851	4.622200	1.179197
6	-1.500344	3.759305	-2.553009
1	-0.585556	1.819894	-2.142590
1	0.549022	3.168338	-2.214754
6	-1.346865	5.235875	-2.144042
1	-1.237726	6.441815	-0.330407
1	-2.404106	5.123848	-0.252814
1	-1.408295	3.651772	-3.640813
1	-2.508172	3.410082	-2.284945
1	-0.385969	5.619947	-2.517754
1	-2.130496	5.842515	-2.613515
6	-3.370553	0.107213	0.321513
6	-3.579251	0.502585	-1.158728
6	-4.685121	-0.430859	0.931860
1	-3.071982	1.008589	0.877441
6	-4.725090	1.526917	-1.310179
1	-3.833788	-0.392564	-1.742837
1	-2.652387	0.905965	-1.583651
6	-5.839569	0.584398	0.765528
1	-4.557963	-0.657730	1.996881
1	-4.961353	-1.373017	0.436651
6	-6.037013	0.993539	-0.705534
1	-4.863586	1.769146	-2.371227
1	-4.446188	2.464298	-0.805149
1	-6.763648	0.154127	1.170709

1	-5.620736	1.480166	1.366296
1	-6.376005	0.122179	-1.285199
1	-6.827082	1.749855	-0.784692

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27	-0.029652	-0.506093	-0.561758
15	-2.350495	-0.632617	-0.780834
15	2.350774	-0.381992	-0.705371
7	0.027893	-1.032457	-2.550394
6	-2.476110	-1.157223	-2.612246
1	-3.326952	-1.816445	-2.799073
1	-2.619797	-0.256924	-3.220862
6	-1.165287	-1.858780	-2.976361
1	-1.082043	-2.819659	-2.459209
1	-1.108614	-2.051185	-4.056740
6	1.326280	-1.679339	-2.963631
1	1.321159	-1.859446	-4.047578
1	1.369221	-2.652171	-2.463558
6	2.509405	-0.801376	-2.562234
1	2.491059	0.144353	-3.117434
1	3.455667	-1.294143	-2.794633
1	-0.034228	-0.123623	-3.028855
6	0.445169	2.975265	2.400903
6	-0.193536	4.197801	2.648674
6	-1.553982	4.223389	2.972262
6	-2.269903	3.019881	3.049681
6	-1.628210	1.802638	2.799984
6	-0.261320	1.764949	2.471741
6	0.437322	0.431941	2.229015
1	1.506625	2.962175	2.164756
1	0.370225	5.123879	2.595227
1	-2.049886	5.167423	3.173271
1	-3.322156	3.032668	3.317689
1	-2.181020	0.870898	2.866972
1	1.456708	0.652015	1.871781
8	-0.277085	-0.357403	1.249604
6	0.543498	-0.404412	3.515038
1	-0.455843	-0.648816	3.888873
1	1.070643	-1.342791	3.312293
1	1.079498	0.143965	4.297880
6	-3.246094	1.057903	-0.627357
6	-2.449753	2.149286	-1.377764
6	-4.729895	1.044564	-1.052167
1	-3.178579	1.273306	0.447623
6	-3.097354	3.539141	-1.192172
1	-2.416964	1.915202	-2.454173
1	-1.414521	2.170797	-1.011055
6	-5.366355	2.441401	-0.865985
1	-4.813240	0.750381	-2.109350
1	-5.291118	0.305965	-0.467985
6	-4.578617	3.532265	-1.615550
1	-2.537777	4.285160	-1.770253
1	-3.015156	3.830183	-0.135644
1	-6.407633	2.416128	-1.209671
1	-5.393471	2.683321	0.206564
1	-5.027835	4.515389	-1.430746
1	-4.649349	3.353525	-2.699382
6	-3.330263	-1.895602	0.300631
6	-4.479418	-2.614576	-0.438039
6	-2.374219	-2.914503	0.963138
1	-3.759318	-1.262118	1.090819
6	-5.258820	-3.527840	0.536104
1	-4.064164	-3.238033	-1.243889
1	-5.163953	-1.897380	-0.906199
6	-3.149950	-3.837233	1.927955
1	-1.902587	-3.529998	0.179600
1	-1.573855	-2.381662	1.485504
6	-4.327933	-4.542199	1.228110
1	-6.054888	-4.048910	-0.009856
1	-5.753210	-2.904778	1.295943
1	-2.464409	-4.577421	2.359116
1	-3.530493	-3.237420	2.768426
1	-4.895597	-5.140023	1.951418
1	-3.937483	-5.246324	0.477621
6	3.295170	-1.774145	0.274763
6	4.301371	-2.589028	-0.566101
6	3.961614	-1.214994	1.554159
1	2.479597	-2.441167	0.586517
6	4.933560	-3.720195	0.278384
1	5.097141	-1.929669	-0.940951
1	3.811315	-3.031277	-1.442761
6	4.583648	-2.355305	2.390837
1	4.754199	-0.505768	1.279406
1	3.233016	-0.667551	2.162260
6	5.587034	-3.179094	1.563244
1	5.670446	-4.258699	-0.329968
1	4.152688	-4.447735	0.545406

1	5.073717	-1.930570	3.275329
1	3.782536	-3.012705	2.759647
1	5.980961	-4.008491	2.162539
1	6.447403	-2.546679	1.297936
6	3.309602	1.278484	-0.520815
6	4.710779	1.281677	-1.174019
6	2.439359	2.441627	-1.052642
1	3.424999	1.404237	0.563728
6	5.408283	2.645920	-0.968353
1	4.616847	1.090440	-2.252813
1	5.335215	0.480610	-0.761198
6	3.146500	3.800953	-0.860144
1	2.241724	2.295007	-2.126328
1	1.468933	2.450314	-0.540807
6	4.548735	3.809143	-1.497972
1	6.385203	2.634381	-1.466781
1	5.603754	2.793664	0.103960
1	2.526612	4.600025	-1.284864
1	3.234321	4.009383	0.216403
1	5.046857	4.765839	-1.300662
1	4.453847	3.724728	-2.591184

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7	-0.204445	-0.702267	-0.715289
5	-2.469475	-0.201734	-0.856865
5	2.120012	-0.269455	-0.993659
7	-0.254065	-0.740576	-2.748082
1	-0.156263	-1.764073	-2.765614
6	-2.725709	-0.887268	-2.588829
1	-2.703577	-1.978728	-2.489991
1	-3.681268	-0.589973	-3.032895
6	-1.556184	-0.396628	-3.419135
1	-1.563890	-0.829758	-4.428332
1	-1.576855	0.693431	-3.533039
6	0.893338	-0.111582	-3.476932
1	0.757494	0.974113	-3.397417
1	0.840347	-0.373935	-4.542600
6	2.209960	-0.541289	-2.865940
1	3.044070	0.009862	-3.309485
1	2.398116	-1.607286	-3.038799
6	0.541969	-4.032516	-2.199367
6	-0.054758	-3.963135	-0.800607
6	1.038755	-4.051105	0.260370
8	-0.830829	-2.747221	-0.650117
1	-0.748409	-4.808038	-0.672080
1	1.695675	-3.171764	0.185817
1	0.612360	-4.075077	1.269546
1	1.654016	-4.949060	0.137865
1	-0.776217	-2.194206	0.624909
1	1.293253	-3.237876	-2.316253
1	1.043392	-4.988105	-2.384119
1	-0.236508	-3.911421	-2.962414
8	-0.562909	-1.246000	1.174475
6	0.266143	-1.368563	2.366402
1	1.169996	-1.944241	2.114101
6	0.664784	-0.000903	2.851790
6	1.817886	0.162303	3.632445
6	-0.138112	1.114059	2.581549
6	2.162883	1.421431	4.130084
1	2.445538	-0.699703	3.851474
6	0.206882	2.374722	3.073661
1	-1.031018	0.974788	1.981775
6	1.358491	2.531350	3.850521
1	3.055749	1.536619	4.736158
1	-0.424235	3.231716	2.854392
1	1.626492	3.508744	4.238811
6	-0.547215	-2.136446	3.406133
1	-1.440020	-1.566634	3.681384
1	-0.862658	-3.109478	3.013651
1	0.044670	-2.303895	4.311044
6	3.756612	-1.087460	-0.445441
6	5.009802	-0.438119	-1.051476
6	3.886093	-1.214729	1.076952
1	3.655699	-2.104240	-0.865008
6	6.259514	-1.250661	-0.682221
1	5.113379	0.583291	-0.657161
1	4.922906	-0.352992	-2.142158
6	5.136700	-2.023794	1.442020
1	2.990705	-1.692834	1.491680
1	3.947828	-0.216033	1.531105
6	6.396395	-1.398530	0.835884
1	7.149456	-0.771564	-1.105208
1	6.189639	-2.247097	-1.142644
1	5.227810	-2.095751	2.531938
1	5.020921	-3.052113	1.067340
1	6.560732	-0.407147	1.283347
1	7.277120	-2.001762	1.080395
6	-3.662646	-1.141991	0.273372

6	-3.801273	-0.470745	1.646961
6	-5.035642	-1.433163	-0.351613
1	-3.130115	-2.097435	0.405677
6	-4.632787	-1.358329	2.582228
1	-4.300782	0.504195	1.537534
1	-2.808271	-0.285163	2.073039
6	-5.861843	-2.315821	0.595399
1	-4.922964	-1.929770	-1.323140
1	-5.574385	-0.492189	-0.530066
6	-6.004644	-1.668240	1.975981
1	-4.741560	-0.872955	3.558799
1	-4.088984	-2.299454	2.755206
1	-6.846906	-2.508101	0.155825
1	-5.366645	-3.292325	0.698954
1	-6.578725	-0.734238	1.881400
1	-6.577846	-2.320535	2.643701
6	-2.926988	1.642527	-1.030917
6	-4.428378	1.940848	-1.144924
6	-2.271409	2.489362	0.070622
1	-2.451352	1.923619	-1.986864
6	-4.654771	3.438803	-1.397448
1	-4.928399	1.652790	-0.209138
1	-4.885103	1.345642	-1.945974
6	-2.508425	3.982332	-0.181303
1	-1.194742	2.273369	0.122977
1	-2.696843	2.211059	1.047104
6	-4.004031	4.290849	-0.303471
1	-5.728745	3.645760	-1.459217
1	-4.225693	3.708357	-2.373997
1	-2.056534	4.574018	0.623807
1	-1.996866	4.275307	-1.111215
1	-4.495581	4.083638	0.658431
1	-4.158028	5.355422	-0.509775
6	2.235857	1.651468	-0.849418
6	2.761616	2.096956	0.523931
6	2.991949	2.369268	-1.977237
1	1.172460	1.950210	-0.909585
6	2.617820	3.615692	0.679882
1	3.825295	1.827271	0.608712
1	2.233471	1.579878	1.331929
6	2.856136	3.891122	-1.814087
1	2.613344	2.078504	-2.964383
1	4.054701	2.090150	-1.948664
6	3.348820	4.357124	-0.441951
1	2.995216	3.921968	1.662245
1	1.547035	3.875938	0.661085
1	3.404559	4.398057	-2.615814
1	1.797091	4.168316	-1.932435
1	4.428823	4.165130	-0.359753
1	3.215407	5.439435	-0.338749

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27	0.134810	-0.083064	-0.455587
15	2.458988	-0.049337	-0.617499
15	-2.284168	-0.148996	-0.663335
7	0.160049	-0.238621	-2.512714
6	2.665205	-0.212327	-2.504760
1	3.552778	0.301528	-2.881399
1	2.776814	-1.275668	-2.747820
6	1.398010	0.360453	-3.142772
1	1.337347	1.442392	-2.987068
1	1.382196	0.175289	-4.225620
6	-1.094447	0.267148	-3.175204
1	-1.046254	0.075039	-4.256202
1	-1.115134	1.352216	-3.032356
6	-2.322735	-0.396015	-2.561557
1	-2.318697	-1.473293	-2.766533
1	-3.238381	0.013405	-2.997523
1	0.201292	-1.257283	-2.654945
6	-0.169106	-1.511886	2.805930
6	-0.387912	-0.030543	2.472262
1	-1.458840	0.133425	2.273564
8	0.380708	0.344566	1.305961
6	0.033261	0.886317	3.626466
1	1.090296	0.730319	3.869619
1	-0.103212	1.936546	3.349961
1	-0.560887	0.682374	4.525204
1	-0.735131	-1.808839	3.697073
1	-0.483367	-2.150942	1.971053
1	0.893979	-1.697768	2.998037
6	3.430620	-1.505453	0.165624
6	2.674700	-2.831301	-0.085767
6	4.904306	-1.604714	-0.287134
1	3.396942	-1.290305	1.241430
6	3.391167	-4.017397	0.596402
1	2.620317	-3.028627	-1.168387
1	1.644584	-2.750194	0.284639
6	5.612035	-2.797623	0.395606

1	4.947213	-1.739634	-1.378275
1	5.441785	-0.677551	-0.058338
6	4.862484	-4.120707	0.151615
1	2.856375	-4.948584	0.371823
1	3.346596	-3.883111	1.687080
1	6.643022	-2.868363	0.028243
1	5.675261	-2.607768	1.477157
1	5.360166	-4.939618	0.684538
1	4.903726	-4.372259	-0.919027
6	-3.452878	-1.568415	-0.020798
6	-3.898171	-1.368019	1.445248
6	-4.669780	-1.866451	-0.928512
1	-2.780651	-2.439890	-0.054423
6	-4.679322	-2.600936	1.955016
1	-4.542612	-0.481234	1.516074
1	-3.033661	-1.189667	2.091890
6	-5.438182	-3.106397	-0.414076
1	-5.349783	-1.006012	-0.936310
1	-4.358107	-2.039197	-1.964810
6	-5.880559	-2.930844	1.050199
1	-5.012900	-2.418920	2.983875
1	-4.001024	-3.466348	1.992247
1	-6.307208	-3.286616	-1.058648
1	-4.793349	-3.993899	-0.498616
1	-6.382687	-3.838822	1.404783
1	-6.619319	-2.117988	1.112912
6	-3.087639	1.606389	-0.486449
6	-4.585743	1.689025	-0.845418
6	-2.802998	2.248886	0.889620
1	-2.522671	2.180256	-1.239326
6	-5.068882	3.157846	-0.820752
1	-5.168716	1.111676	-0.116123
1	-4.783435	1.252814	-1.832639
6	-3.295904	3.713380	0.916198
1	-3.321646	1.683037	1.675692
1	-1.731147	2.202643	1.111284
6	-4.785943	3.821747	0.540124
1	-6.141161	3.193238	-1.048986
1	-4.558586	3.720612	-1.616868
1	-3.121040	4.139402	1.911648
1	-2.697057	4.308634	0.209971
1	-5.094881	4.873670	0.517170
1	-5.393984	3.332859	1.315816
6	3.227252	1.637155	-0.072577
6	3.574259	1.603249	1.433801
6	4.415628	2.134854	-0.922561
1	2.387699	2.334535	-0.201940
6	4.047922	2.992889	1.912042
1	4.378535	0.875019	1.612254
1	2.695675	1.280026	2.000121
6	4.887084	3.522801	-0.428182
1	5.251779	1.425288	-0.856303
1	4.139406	2.207229	-1.982364
6	5.232194	3.509266	1.073111
1	4.325709	2.938017	2.971790
1	3.211114	3.703623	1.842800
1	5.754158	3.843423	-1.018684
1	4.090393	4.258985	-0.612398
1	5.519872	4.515567	1.400640
1	6.106770	2.862607	1.239736

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27	0.242657	-1.160527	0.597484
15	-1.941089	-0.196431	0.442536
15	1.935171	0.408532	0.466303
7	0.040704	-0.599478	2.765577
6	-2.408467	-0.851149	2.176124
1	-3.415905	-0.548625	2.475724
1	-2.383475	-1.940192	2.097081
6	-1.382420	-0.359058	3.204283
1	-1.501464	0.718505	3.360167
1	-1.566722	-0.838587	4.174783
6	0.960245	0.535094	3.104004
1	1.150213	0.579043	4.186896
1	0.437461	1.458293	2.832150
6	2.287375	0.449349	2.344207
1	2.811993	-0.478221	2.589999
1	2.936893	1.283998	2.622692
1	1.529162	-2.025652	0.798997
1	0.393022	-1.459846	3.186997
6	0.991547	-4.175618	-0.662948
6	0.361079	-3.644103	0.600380
6	0.747855	-4.297828	1.904745
1	0.342018	-5.319968	1.910484
1	1.831819	-4.373727	2.017168
1	0.317884	-3.764630	2.754348
8	-0.727216	-2.945666	0.528855
6	-3.201822	-0.963730	-0.807202

6	-2.491410	-1.244850	-2.151929
6	-3.908672	-2.233706	-0.282098
1	-3.964591	-0.189031	-0.968518
6	-3.479456	-1.798880	-3.200518
1	-1.690781	-1.976283	-1.974687
1	-2.014042	-0.332788	-2.533533
6	-4.899866	-2.779418	-1.334666
1	-4.447683	-2.017741	0.648367
1	-3.156405	-2.999250	-0.055275
6	-4.207295	-3.054283	-2.682901
1	-2.942421	-2.023697	-4.130681
1	-4.220579	-1.023317	-3.445671
1	-5.368765	-3.695014	-0.953012
1	-5.710483	-2.050232	-1.483169
1	-3.480043	-3.870819	-2.558181
1	-4.941518	-3.397321	-3.421955
6	3.586367	-0.083581	-0.407915
6	4.524115	-0.921370	0.487564
6	3.280414	-0.825200	-1.730910
1	4.089997	0.864962	-0.641194
6	5.817722	-1.305762	-0.266797
1	4.003462	-1.837730	0.804437
1	4.788913	-0.367289	1.395923
6	4.576683	-1.204458	-2.478873
1	2.640720	-0.213837	-2.378522
1	2.712628	-1.736830	-1.496637
6	5.517723	-2.036445	-1.588350
1	6.445363	-1.928946	0.382214
1	6.394696	-0.393419	-0.478187
1	4.324462	-1.757251	-3.392385
1	5.093649	-0.288102	-2.800116
1	5.048929	-3.008272	-1.369790
1	6.451802	-2.252434	-2.120584
6	1.663228	2.259459	-0.040924
6	2.692027	3.237926	0.567996
6	1.620148	2.392966	-1.581423
1	0.666694	2.502992	0.354202
6	2.411917	4.692879	0.123493
1	3.706312	2.955183	0.250054
1	2.676088	3.189731	1.663199
6	1.334663	3.847977	-2.013359
1	0.866157	1.716924	-2.004338
1	2.589638	2.091681	-2.001357
6	2.361105	4.824141	-1.409421
1	3.181300	5.354214	0.540359
1	1.451505	5.020459	0.549225
1	1.344193	3.911785	-3.108444
1	0.323711	4.135111	-1.689343
1	3.356381	4.612273	-1.827774
1	2.115599	5.854842	-1.691971
6	-2.413865	1.679762	0.497208
6	-2.316004	2.304197	-0.914112
6	-3.795786	1.957797	1.129924
1	-1.642224	2.142185	1.131108
6	-2.632596	3.815675	-0.885263
1	-3.033531	1.809155	-1.583088
1	-1.319084	2.134495	-1.338080
6	-4.113652	3.470657	1.146601
1	-3.839025	1.570145	2.154534
1	-4.575578	1.434258	0.558026
6	-4.012325	4.090458	-0.258723
1	-2.588080	4.219583	-1.904318
1	-1.858775	4.339320	-0.303266
1	-5.115871	3.627844	1.563694
1	-3.408869	3.980124	1.821024
1	-4.796142	3.665542	-0.903209
1	-4.197957	5.170113	-0.209836
1	0.562263	-5.167253	-0.869224
1	0.769493	-3.527364	-1.512061
1	2.071966	-4.298071	-0.559186

I-1$_{bent}$

27	0.392896	0.189866	-0.195286
15	1.103121	-1.535528	1.229988
15	1.659185	1.993713	0.018029
7	2.127065	-0.612788	-1.488490
6	2.507903	-1.467655	2.429516
1	2.237427	-0.831044	3.276292
6	-0.126860	-2.571938	2.137037
1	0.309240	-3.520573	2.464058
6	1.708316	-2.671226	-0.118233
1	2.191765	-3.567580	0.287302
1	0.814515	-2.989060	-0.664534
6	2.671517	-1.928574	-1.053990
1	3.609673	-1.739129	-0.523357
1	2.925541	-2.562481	-1.913114
6	3.175913	0.417244	-1.713393

1	3.655852	0.300906	-2.694139
1	3.955965	0.250526	-0.963870
6	2.639340	1.847447	-1.556621
1	1.956114	2.098130	-2.374096
1	3.470672	2.560930	-1.582513
6	0.894875	3.666831	-0.062902
1	0.337205	3.858730	0.858007
6	2.945700	2.224516	1.329977
1	3.562774	3.106196	1.130047
1	-0.075884	1.166996	-1.229030
1	1.592720	-0.738137	-2.345293
1	1.654844	4.445058	-0.179623
1	0.195870	3.705255	-0.900658
1	-0.486380	-2.030635	3.016669
1	-0.981800	-2.778727	1.488947
1	3.396955	-1.041729	1.958397
1	2.755831	-2.464805	2.805664
1	2.457109	2.352046	2.300071
1	3.593782	1.347097	1.391959
6	-4.757374	1.564912	1.055516
6	-5.259703	0.829817	-0.021281
6	-4.431568	-0.051695	-0.709858
6	-3.079155	-0.195777	-0.343272
6	-2.588940	0.549329	0.746702
6	-3.421752	1.418986	1.442371
1	-5.407073	2.245777	1.596841
1	-6.296693	0.941562	-0.320701
1	-4.836447	-0.615087	-1.543188
1	-1.560019	0.419771	1.076193
1	-3.036625	1.978177	2.289258
6	-2.192154	-1.116032	-1.079052
8	-0.952058	-1.091199	-0.957264
6	-2.775841	-2.136687	-2.025455
1	-3.577641	-2.711321	-1.553143
1	-3.204979	-1.635027	-2.900599
1	-1.987396	-2.808847	-2.364187

I-5$_{bent}$

27	-0.102472	-0.523959	-0.129315
15	-0.534816	1.699483	-0.743580
15	2.036297	-1.010669	-0.437627
7	0.624647	0.496838	1.807188
6	0.684016	2.912507	-1.419332
1	0.920364	2.655498	-2.455467
6	-2.068825	2.127957	-1.677185
1	-2.304845	3.193288	-1.597014
6	-0.893409	2.316218	0.977542
1	-1.052404	3.400503	0.998354
1	-1.828449	1.834471	1.280996
6	0.241892	1.931263	1.936492
1	1.126339	2.532091	1.703924
1	-0.037155	2.179625	2.968193
6	2.071075	0.245565	2.055426
1	2.291103	0.180562	3.129054
1	2.618797	1.115449	1.679791
6	2.587054	-1.011657	1.338814
1	2.171192	-1.916374	1.792978
1	3.678249	-1.064205	1.425257
6	2.506840	-2.670158	-1.081040
1	2.234930	-2.741800	-2.137927
6	3.248239	0.093836	-1.295255
1	4.270604	-0.280989	-1.186354
1	0.075234	-1.926294	0.383116
1	0.077859	-0.052463	2.466344
1	3.582530	-2.843732	-0.984287
1	1.959872	-3.439624	-0.532570
1	-1.938545	1.876392	-2.733429
1	-2.907784	1.548091	-1.285118
1	1.612821	2.884017	-0.844557
1	0.284417	3.930831	-1.392402
1	3.004548	0.143391	-2.360086
1	3.199039	1.107254	-0.890574
6	-2.691831	-2.574221	-0.809023
6	-2.927516	-1.452833	0.160753
8	-2.043849	-0.624039	0.422304
6	-4.272054	-1.333658	0.817453
1	-5.067516	-1.359905	0.064125
1	-4.432530	-2.204344	1.465624
1	-4.342352	-0.421251	1.410108
1	-1.653728	-2.910993	-0.733016
1	-3.383240	-3.405175	-0.654793
1	-2.849447	-2.194096	-1.827274

I-4$_{Agostic}$

27	-0.352559	-0.269330	-0.304636
15	-0.213820	1.975931	-0.548912

15	1.780864	-1.107551	-0.451333
7	0.153147	0.054764	1.845492
6	1.010527	2.914221	-1.555503
1	0.906284	3.990182	-1.386761
6	-1.822123	2.745949	-0.982895
1	-1.801153	3.825080	-0.805404
6	0.129859	2.479826	1.212079
1	1.208431	2.645204	1.307693
1	-0.353187	3.435531	1.441153
6	-0.354635	1.406290	2.201376
1	-0.061254	1.686321	3.222463
1	-1.445321	1.343702	2.169867
6	1.589052	-0.165750	2.155114
1	1.744449	-0.314843	3.231500
1	2.137800	0.740249	1.881820
6	2.137698	-1.357225	1.360521
1	1.634517	-2.282129	1.667565
1	3.208023	-1.492012	1.549478
6	2.001445	-2.774137	-1.208396
1	1.875831	-2.701974	-2.292231
6	3.241053	-0.175395	-1.084555
1	4.158890	-0.754559	-0.947013
1	-1.114319	-1.894323	-0.111518
1	-0.393485	-0.627841	2.367428
1	2.995598	-3.177963	-0.995340
1	1.244884	-3.462107	-0.822621
1	-2.037890	2.559599	-2.038187
1	-2.609929	2.274317	-0.393803
1	0.839358	2.708628	-2.615630
1	2.030772	2.614294	-1.307278
1	3.112729	0.033489	-2.149901
1	3.345293	0.776182	-0.557764
6	-2.831506	-2.145479	-1.405498
6	-2.248144	-1.504017	-0.141935
8	-2.189820	-0.131315	-0.202440
6	-2.867449	-2.033880	1.155886
1	-2.772764	-3.120505	1.239672
1	-2.410755	-1.567808	2.033622
1	-3.932073	-1.780604	1.163358
1	-3.888273	-1.872268	-1.484848
1	-2.317945	-1.775868	-2.297002
1	-2.759214	-3.237011	-1.377548

I-TS6$_{bent}$

27	-0.413311	-0.247089	-0.279526
15	0.226305	1.963534	-0.571995
15	1.447203	-1.476922	-0.450647
7	0.201560	0.089570	1.860426
6	1.553363	2.629967	-1.666407
1	1.704122	3.699717	-1.493854
6	-1.184024	3.096291	-0.914784
1	-0.884256	4.142502	-0.805689
6	0.783063	2.414905	1.150445
1	1.870316	2.287056	1.193847
1	0.584913	3.470728	1.362838
6	0.085368	1.531835	2.197181
1	0.492443	1.744937	3.195637
1	-0.983178	1.763277	2.219886
6	1.537101	-0.493766	2.145960
1	1.669130	-0.673507	3.221100
1	2.293666	0.241767	1.858024
6	1.759445	-1.790321	1.356039
1	1.048795	-2.560150	1.676876
1	2.768998	-2.177335	1.531469
6	1.368994	-3.142283	-1.229199
1	0.519005	-3.695540	-0.824243
6	3.056290	-0.820953	-1.079235
1	3.849914	-1.565841	-0.966450
1	-0.965700	-1.658629	-0.037185
1	-0.489049	-0.419837	2.407196
1	1.224431	-3.033308	-2.307708
1	2.290113	-3.705703	-1.054169
1	-1.539252	2.931198	-1.935433
1	-2.008043	2.869900	-0.236356
1	1.265818	2.482372	-2.711155
1	2.496194	2.106660	-1.494949
1	2.962111	-0.565082	-2.137988
1	3.343527	0.080909	-0.532908
6	-3.133885	-1.519099	-1.405578
6	-2.695538	-0.846701	-0.121561
8	-2.300663	0.363296	-0.151044
6	-3.216564	-1.430196	1.173996
1	-3.065377	-2.509573	1.234240
1	-2.769820	-0.932938	2.036042
1	-4.298496	-1.245112	1.205088
1	-4.193062	-1.274072	-1.561872
1	-2.570253	-1.137474	-2.258657

1	-3.047531	-2.606141	-1.352555

I-TS1$_{bent}$

27	-0.264767	-0.006215	0.145191
15	-1.617522	-1.636877	-0.759031
15	-0.918897	1.947754	-0.742896
7	-1.955089	0.289996	1.606253
6	-2.334744	-1.706091	-2.457059
1	-3.037534	-2.539029	-2.552578
6	-0.964924	-3.341841	-0.523578
1	-1.741670	-4.089854	-0.707301
6	-3.105075	-1.548784	0.361487
1	-3.854903	-0.918469	-0.128923
1	-3.560740	-2.536942	0.484023
6	-2.720425	-0.976848	1.735532
1	-3.623338	-0.839941	2.347206
1	-2.069780	-1.682571	2.259411
6	-2.784968	1.470654	1.258649
1	-3.352232	1.827713	2.128432
1	-3.521263	1.156174	0.513259
6	-1.925827	2.602246	0.678269
1	-1.220458	2.970999	1.431566
1	-2.555426	3.445593	0.374842
6	0.341322	3.244428	-1.086481
1	1.007107	3.343550	-0.226423
6	-2.048888	2.090320	-2.197772
1	-2.321301	3.134460	-2.379055
1	0.701154	0.940385	0.890177
1	-1.495056	0.472654	2.495364
1	0.943073	2.945278	-1.949077
1	-0.127351	4.209360	-1.300472
1	-0.137743	-3.513536	-1.217717
1	-0.577249	-3.444342	0.491190
1	-1.529268	-1.843696	-3.183876
1	-2.853573	-0.775236	-2.695548
1	-1.554310	1.695937	-3.089510
1	-2.962604	1.514562	-2.030189
6	4.976451	-0.158905	-1.211831
6	4.037256	-1.179997	-1.370480
6	2.939161	-1.257956	-0.515488
6	2.768575	-0.315414	0.511665
6	3.723669	0.701980	0.670318
6	4.817571	0.780230	-0.188690
1	5.833387	-0.098746	-1.875724
1	4.166715	-1.921841	-2.152692
1	2.217202	-2.060890	-0.612813
1	3.615730	1.442987	1.456040
1	5.549712	1.571094	-0.058004
6	1.577515	-0.447822	1.419221
8	0.711487	-1.371377	1.158856
6	1.705536	0.005766	2.863524
1	2.133108	1.002894	2.971297
1	0.732910	-0.031949	3.356590
1	2.371169	-0.702707	3.370925

I-TS5$_{shuttle}$

27	0.480756	-0.434294	-0.098121
15	0.292774	-1.903132	1.922698
15	1.385772	-1.643958	-1.881174
7	-1.263812	-1.390134	-0.710340
6	1.220951	-3.500652	2.056312
1	2.259814	-3.293850	2.328966
6	0.162837	-1.395470	3.697462
1	1.161621	-1.224203	4.106326
6	-1.445468	-2.463379	1.548676
1	-1.690889	-3.401391	2.059218
1	-2.135178	-1.700012	1.924988
6	-1.624893	-2.630904	0.042235
1	-0.980401	-3.435814	-0.324600
1	-2.658768	-2.911892	-0.194947
6	-1.381577	-1.611677	-2.199580
1	-2.208108	-1.003105	-2.576034
1	-1.651941	-2.657744	-2.369352
6	-0.085544	-1.278791	-2.955465
1	-0.032971	-0.204143	-3.166931
1	-0.051665	-1.801230	-3.918032
6	2.807972	-0.954887	-2.817968
1	3.742286	-1.260381	-2.340857
6	1.645155	-3.469220	-2.011165
1	2.512944	-3.756880	-1.411178
1	-1.722907	0.622153	2.017307
1	-1.953890	-0.676641	-0.464395
6	-3.138254	1.529045	-0.939506
6	-4.322445	1.334026	-1.654509
6	-5.412234	0.700749	-1.051126
6	-5.312786	0.265472	0.271863
6	-4.127558	0.460180	0.984766

6	-3.025766	1.093231	0.390354
6	-1.754739	1.353852	1.194974
1	-2.292984	2.027674	-1.404179
1	-4.399366	1.687912	-2.678781
1	-6.333459	0.552976	-1.606289
1	-6.157123	-0.222484	0.749727
1	-4.063863	0.131454	2.020280
1	-0.399370	-0.461987	3.780646
1	-0.331517	-2.167355	4.295623
1	0.784713	-4.161419	2.812035
1	1.224191	-4.016679	1.092658
1	2.756186	0.135187	-2.798002
1	2.807150	-1.310818	-3.852452
1	0.776083	-4.017023	-1.639129
1	1.825424	-3.762680	-3.049928
8	-0.584462	1.208192	0.392884
6	-1.793782	2.753363	1.828533
1	-1.849248	3.522801	1.051882
1	-2.675922	2.856400	2.466855
1	-0.899367	2.929347	2.432537
6	1.295838	3.879531	-0.334121
1	0.405864	4.491504	-0.136593
8	1.214203	2.758225	0.570010
1	0.223560	2.121245	0.508959
6	2.536701	4.698512	0.006097
1	3.448631	4.122078	-0.185282
1	2.578332	5.607646	-0.601820
1	2.526491	4.987230	1.060299
6	1.268306	3.421567	-1.793854
1	0.370695	2.827916	-1.997404
1	1.266511	4.282546	-2.469256
1	2.148637	2.811223	-2.023347
6	3.277550	0.173798	0.785088
1	3.310973	-0.924230	0.726023
8	2.111669	0.606184	0.068729
1	1.813713	1.796870	0.301229
6	4.529781	0.742049	0.110900
1	4.532615	1.835658	0.168538
1	5.434631	0.379267	0.609325
1	4.580759	0.458151	-0.942916
6	3.209687	0.592496	2.256532
1	2.292746	0.228232	2.724738
1	4.065907	0.198422	2.813955
1	3.216863	1.683147	2.346398

I-TS5

27	-0.828753	0.072935	-0.285333
15	0.228091	-1.785062	-1.118435
15	-3.011828	-0.599930	-0.022435
7	-0.645761	-0.992106	1.716237
6	-0.616828	-3.272613	-1.810541
1	-1.166351	-2.996568	-2.714700
6	1.601504	-1.553447	-2.320824
1	1.200996	-1.189607	-3.271107
6	1.034186	-2.358626	0.452017
1	1.440011	-3.371066	0.348521
1	1.871578	-1.679130	0.637777
6	0.031578	-2.310017	1.613854
1	-0.746542	-3.064137	1.455159
1	0.537241	-2.577315	2.551425
6	-1.906466	-1.019100	2.512495
1	-1.747818	-0.586647	3.505948
1	-2.188819	-2.064128	2.671602
6	-3.055964	-0.274893	1.804491
1	-2.922389	0.804914	1.907855
1	-4.021355	-0.555874	2.240223
6	-4.459679	0.292055	-0.730003
1	-4.528542	0.078416	-1.800437
6	-3.580903	-2.351420	-0.181386
1	-3.617037	-2.645499	-1.232972
1	1.905370	1.445780	-1.520872
1	0.006434	-0.315056	2.106816
6	3.485009	0.417377	1.312843
6	4.675143	-0.197845	1.704957
6	5.698116	-0.405598	0.776395
6	5.525140	0.009255	-0.544780
6	4.332182	0.622050	-0.935375
6	3.297219	0.828683	-0.013965
6	2.031606	1.562359	-0.434785
1	2.696124	0.590758	2.038680
1	4.808590	-0.507260	2.737681
1	6.624498	-0.881913	1.082337
1	6.317253	-0.142478	-1.271959
1	4.210128	0.951617	-1.965319
1	2.322759	-0.832076	-1.936164
1	2.115392	-2.503268	-2.497161
1	0.123864	-4.034374	-2.071155

1	-1.320163	-3.701474	-1.096624
1	-4.357260	1.368489	-0.598387
1	-5.382683	-0.040239	-0.245759
1	-2.917725	-3.036228	0.350708
1	-4.585520	-2.448948	0.241193
8	0.885126	1.013986	0.237224
6	2.155480	3.060223	-0.124706
1	2.235443	3.219363	0.955121
1	3.054142	3.469733	-0.594167
1	1.293405	3.617285	-0.503620
6	-1.617161	3.070209	-0.216347
1	-0.787385	3.781096	-0.092410
8	-1.242098	1.872339	0.493604
1	-0.009631	1.740746	0.491617
6	-1.789474	2.822454	-1.716774
1	-2.620021	2.138985	-1.917887
1	-1.992471	3.759177	-2.245743
1	-0.877116	2.392205	-2.147109
6	-2.842269	3.703053	0.440347
1	-2.654929	3.871739	1.504343
1	-3.071171	4.667910	-0.023406
1	-3.730341	3.069907	0.349233

I-4$_{vacant}$

27	0.107744	0.404610	0.234843
15	-2.118745	0.802142	0.564368
15	0.546388	-1.775138	0.577477
7	-0.507714	-0.088312	-1.807052
6	-3.475325	-0.414816	0.843595
1	-3.394988	-0.831037	1.851269
6	-2.564355	2.211966	1.662553
1	-2.489590	1.900074	2.707890
6	-2.382079	1.443583	-1.166482
1	-3.434457	1.678495	-1.362499
1	-1.819418	2.382344	-1.236106
6	-1.852782	0.427614	-2.192878
1	-2.538047	-0.423298	-2.249775
1	-1.830798	0.877870	-3.191405
6	-0.307578	-1.537319	-2.083950
1	-0.096428	-1.713994	-3.146102
1	-1.251587	-2.045653	-1.862677
6	0.812640	-2.148978	-1.225205
1	1.778750	-1.706312	-1.488618
1	0.872782	-3.227603	-1.408761
6	2.100202	-2.275993	1.422312
1	1.987955	-2.140060	2.501375
6	-0.682641	-3.013308	1.170222
1	-0.887312	-2.846669	2.231247
1	2.834065	0.909097	1.315271
1	0.223362	0.445041	-2.277898
6	2.951132	2.880578	0.474842
6	2.858129	1.359879	0.307686
1	-1.866786	3.038032	1.501497
1	-3.583505	2.559628	1.468974
1	-4.454076	0.062282	0.737376
1	-3.404832	-1.236362	0.126530
1	2.928603	-1.653209	1.079875
1	2.331043	-3.326529	1.221540
1	-1.622170	-2.915869	0.621477
1	-0.300667	-4.030670	1.040955
8	1.649565	1.049524	-0.379199
6	4.053028	0.797450	-0.464903
1	4.100012	1.244986	-1.463047
1	4.993692	1.011416	0.052502
1	3.974022	-0.288346	-0.586409
1	2.946375	3.369732	-0.504440
1	2.101816	3.256961	1.053430
1	3.873689	3.158179	0.994294

I-2$_{vacant}$

27	-0.843148	-0.432194	0.323411
15	-0.241549	1.713522	0.662205
15	-3.121060	-0.621249	0.442887
7	-1.217989	0.064605	-1.780861
6	-1.436524	3.047646	1.095483
1	-1.747617	2.936083	2.137723
6	1.248604	2.137647	1.648213
1	1.024898	2.023294	2.712456
6	0.226153	2.012311	-1.112136
1	0.398934	3.076944	-1.306391
1	1.171510	1.482550	-1.271455
6	-0.862801	1.482569	-2.060322
1	-1.774399	2.074531	-1.931401
1	-0.544821	1.615342	-3.102161
6	-2.562511	-0.340783	-2.282287
1	-2.490537	-0.814983	-3.267416

1	-3.161287	0.565208	-2.415866
6	-3.273037	-1.282078	-1.294333
1	-2.790914	-2.267156	-1.294472
1	-4.318866	-1.431052	-1.586468
6	-3.788487	-1.959696	1.518147
1	-3.794860	-1.622910	2.558433
6	-4.393623	0.707456	0.566298
1	-4.378400	1.139895	1.570197
1	1.616079	-1.424120	1.710119
1	-0.498161	-0.543815	-2.170224
6	3.285012	-0.564766	-1.134334
6	4.445754	0.107565	-1.520689
6	5.382554	0.501154	-0.561515
6	5.152505	0.215970	0.785147
6	3.988456	-0.454895	1.169635
6	3.041926	-0.851243	0.216253
6	1.800401	-1.625861	0.641410
1	2.562526	-0.882104	-1.880461
1	4.624799	0.317180	-2.571543
1	6.286474	1.021728	-0.862692
1	5.877390	0.513927	1.536983
1	3.819455	-0.680027	2.220788
1	2.072324	1.469743	1.387626
1	1.548611	3.173140	1.460283
1	-0.977019	4.032936	0.970479
1	-2.325985	2.988516	0.464848
1	-3.147354	-2.842333	1.448577
1	-4.807751	-2.232658	1.228893
1	-4.188817	1.504225	-0.153051
1	-5.392432	0.305690	0.371540
8	0.668827	-1.258576	-0.131378
6	2.004010	-3.141938	0.479841
1	2.175127	-3.387900	-0.572124
1	2.871362	-3.474335	1.057493
1	1.118828	-3.682359	0.828983

O-TS1$_{bent}$

27	0.173983	-0.035643	-0.296160
15	-0.223490	2.168101	-0.168826
15	2.416530	-0.535022	-0.878012
7	0.733642	0.164797	1.639433
6	1.170720	3.368719	-0.208509
1	1.574638	3.429966	-1.222319
6	-1.529647	2.992889	-1.162434
1	-1.749336	3.985183	-0.756770
6	-0.820388	2.128879	1.585874
1	-0.985009	3.128660	2.003069
1	-1.783704	1.608849	1.566737
6	0.211505	1.332791	2.401500
1	1.042186	1.994488	2.673359
1	-0.238026	0.991265	3.342483
6	2.188400	-0.014853	1.865107
1	2.361592	-0.363408	2.892621
1	2.693580	0.957504	1.778016
6	2.823556	-1.006109	0.878972
1	2.419250	-2.010046	1.049188
1	3.905910	-1.054793	1.041077
6	2.886058	-2.023428	-1.863059
1	2.753659	-1.815412	-2.928440
6	3.712925	0.692306	-1.352174
1	4.714629	0.263410	-1.251838
1	0.264598	-1.757734	0.035446
1	0.104354	-0.864835	1.962727
1	3.928820	-2.304297	-1.686874
1	2.240756	-2.863733	-1.594835
1	-1.191892	3.101285	-2.196791
1	-2.438091	2.387853	-1.155303
1	1.969625	3.054430	0.466461
1	0.825522	4.362402	0.093384
1	3.564884	0.998498	-2.391581
1	3.644559	1.581925	-0.721973
6	-3.984428	0.018325	-1.188865
6	-2.903792	-0.385877	-1.970214
6	-1.835624	-1.077326	-1.376571
6	-1.848082	-1.361230	0.008552
6	-2.925919	-0.911740	0.789068
6	-3.991289	-0.243355	0.190097
1	-4.826188	0.528058	-1.647681
1	-2.895790	-0.192931	-3.038693
1	-1.041605	-1.484134	-2.005725
1	-2.913555	-1.125536	1.852990
1	-4.839806	0.067920	0.792448
6	-0.706323	-2.156166	0.654132
6	-0.703645	-3.643485	0.259006
1	-1.574901	-4.120371	0.717169
1	-0.755519	-3.789752	-0.823582
1	0.194462	-4.123353	0.654444

8	-0.520298	-1.940101	1.957595

O-1$_{bent}$

27	-0.105292	-0.243777	-1.021392
15	1.935456	-0.629404	0.076772
15	-2.005173	-0.505930	0.064028
7	0.115278	1.787492	-0.304620
6	2.129213	-0.898919	1.891184
1	1.855154	-1.928923	2.134306
6	3.248950	-1.695769	-0.655326
1	4.228018	-1.483682	-0.215961
6	2.541783	1.113395	-0.211374
1	3.487517	1.309714	0.306804
1	2.740244	1.205967	-1.286973
6	1.476992	2.131874	0.223380
1	1.419752	2.154220	1.315404
1	1.766612	3.139130	-0.094388
6	-0.970043	2.023952	0.697396
1	-1.148997	3.098675	0.827585
1	-0.602168	1.645919	1.656403
6	-2.287716	1.313746	0.346990
1	-2.714159	1.719370	-0.576102
1	-3.012907	1.484246	1.150364
6	-3.520499	-1.124990	-0.768493
1	-3.425685	-2.200446	-0.941339
6	-2.092109	-1.274972	1.741505
1	-3.065354	-1.090655	2.207286
1	-1.176886	0.189178	-1.952975
1	-0.074888	2.369870	-1.118369
1	-4.407271	-0.944148	-0.154087
1	-3.633187	-0.630709	-1.735341
1	3.002390	-2.746231	-0.478770
1	3.300874	-1.536777	-1.735777
1	1.470016	-0.231244	2.451237
1	3.162519	-0.725180	2.206345
1	-1.942713	-2.354552	1.653794
1	-1.306603	-0.874109	2.386911