

Supporting Information

Oxidation Triggers Extensive Conjugation and Unusual Stabilization of Two Di-heme Dication Diradical Intermediates: Role of Bridging Group for Electronic Communication

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Experimental Section

Trans-1,2-bis[(chloro){5-(2,3,7,8,12,13,17,18-octaethylporphyrinato)}iron(III)]ethene (*trans*-**1**), *cis*-1,2-bis[(chloro){5-(2,3,7,8,12,13,17,18-octaethylporphyrinato)}iron(III)]ethene (*cis*-**1**) and 1,2-bis[(chloro){5-(2,3,7,8,12,13,17,18-octaethylporphyrinato)}iron(III)]ethane (**4**), has been synthesized following the reported procedure.¹⁻³ Reagents and solvents are purchased from commercial sources and purified by standard procedures before use.

Synthesis of *trans*-**2**:

To a dichloromethane (25 mL) solution of *trans/cis*-**1** (100 mg, 0.079 mmol), a solution of 59 mg (0.167 mmol) Fe(ClO₄)₃ in 2 mL CH₃CN was added and the resulting solution was stirred in air at room temperature for 30 minutes. During the progress of the reaction, the colour of the solution changed from bright red to dark red. The solution was then evaporated to complete dryness. The resulting solid was then dissolved in a minimum volume of CH₂Cl₂, filtered off to remove unreacted oxidant and then carefully layered with n-hexane. On standing for 6-7 days in air at room temperature, dark red needle crystals were obtained, which was then isolated by filtration, washed well with n-hexane, and dried in vacuum. Yield 98 mg (76%). Conductivity (CH₂Cl₂, 10⁻⁴ M solution at 295 K): $\Lambda_M = 41 \text{ } \Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$. UV-vis [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 326 (3.9 × 10⁴), 389 (4.2 × 10⁴), 477 (3.7 × 10⁴), 1150 (4.0 × 10³). ¹H NMR (CDCl₃, 295 K): *meso-H*:

26.5, 32.4, 37.9, 41.8; CH_3 : 6.1, 6.4, 6.5, 6.7, 7.0, 8.1; CH_2 : 39.5, 40.2, 43.2, 44.6, 46.8, 50.3, 52.2, 53.9, 54.7, 56.4, 56.8, 58.9, 60.2, 63.9, 67.1; $\text{CH}_2(\text{b})$: 78.6, 88.3 ppm.

Synthesis of *trans*-3:

Trans/cis-1 (100 mg, 0.079 mmol) was dissolved in CH_2Cl_2 (25 mL) and a solution of 58 mg (0.358 mmol) FeCl_3 in 2 mL CH_3CN was added to it. The solution was stirred in air at room temperature for 30 minutes. During the progress of the reaction, the colour of the solution has changed from bright red to wine red. The resulting solution was then evaporated to complete dryness. The solid thus obtained was dissolved in a minimum volume of CH_2Cl_2 , filtered off to remove unreacted oxidant and then carefully layered with n-hexane on the top. On standing for 8-10 days in air at room temperature, dark red crystals were obtained. The crystalline solid was then isolated by filtration, washed well with n-hexane, and dried in vacuum. Yield 110 mg (84%). Conductivity (CH_2Cl_2 , 10^{-4} M solution at 295 K): $\Lambda_{\text{M}} = 42 \text{ } \Omega^{-1}\text{cm}^2\text{mol}^{-1}$. UV-vis [λ_{max} , nm (ϵ , $\text{M}^{-1}\text{cm}^{-1}$)]: 317 (4.1×10^4), 365 (4.1×10^4), 488 (8.2×10^3), 1210 (2.0×10^3).

Instrumentation

UV-vis spectra were recorded on a PerkinElmer UV/Vis spectrometer. Electron paramagnetic resonance (EPR) spectra were obtained on a Bruker EMX EPR spectrometer. EPR spectral simulations were carried out using the EasySpin software.⁴ Elemental (C, H and N) analyses were performed on a Perkin-Elmer 2400II elemental analyzer. ^1H NMR spectra were recorded on a JEOL 500 MHz instrument. The spectra for paramagnetic molecules were recorded over a 100-kHz bandwidth with 64 K data points and a 5-ms 90° pulse. The residual ^1H resonances of the solvents were used as a secondary reference. Cyclic voltammetric studies were performed on a BAS Epsilon electrochemical workstation in dichloromethane with 0.1 M tetrabutylammonium hexafluorophosphate (TBAH) as supporting electrolyte and the reference electrode was Ag/AgCl and the auxiliary electrode was a Pt wire. The concentration of the compounds was in the order of 10^{-3} M. The ferrocene/ferrocenium couple occurs at $E_{1/2} = +0.45$ (65) V versus Ag/AgCl under the same experimental conditions. ^{57}Fe Mössbauer spectra were recorded using a Wissel 1200 spectrometer and a proportional counter. $^{57}\text{Co}(\text{Rh})$ in a constant acceleration mode was used as the radioactive source. WinNormos for Igor Pro software has

been used for the simulation of the Mossbauer spectra. Isomer shifts (δ) are given related to α -iron foil at room temperature.

X-ray Structure Solution and Refinement.

Single-crystal X-ray data were collected at 100 K on a Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low temperature apparatus and intensity data were collected using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å). The data integration and reduction were processed with SAINT software.⁵ An absorption correction was applied.⁶ The structure was solved by the direct method using SHELXS-97 and was refined on F^2 by full-matrix least-squares technique using the SHELXL-2014 program package.⁷ Non-hydrogen atoms were refined anisotropically. In the refinement, hydrogen was treated as riding atoms using SHELXL default parameters.

Magnetic measurements:

Magnetic susceptibility data were collected using a Quantum Design MPMS SQUID magnetometer over the temperature range 5 to 300 K. The magnetic data were fitted, using the software PHI,⁸ to a model considering antiferromagnetic coupling between the unpaired spin ($S = 1/2$) of the porphyrin π -cation radicals with the high-spin ($S = 5/2$) iron(III) centers, antiferromagnetic interaction between the radical spins ($S = 1/2$) on the two porphyrin units of *trans*-**2/3** and interaction between two iron centers in *trans*-**2/3**. Presence of small amount of mononuclear iron(III) impurity and temperature-independent paramagnetism have also been taken into account. Intermolecular interactions as well as interaction with the FeCl_4^- counterions, particularly in *trans*-**3**, have been excluded to keep the fitting model simple.

Two sets of data were collected over the temperature range of 5 to 300 K, by using two different applied magnetic fields of 0.1 and 1 T and corrected for diamagnetism using Pascal's constant.⁹ The plots are shown in Figure 10 (see text). The value of g has been kept fixed at 2.00. The parameters obtained after fitting the magnetic data for *trans*-**2** are: $J_{\text{Fe-r}} = -124.36 \text{ cm}^{-1}$, $J_{\text{Fe-Fe}} = -0.05 \text{ cm}^{-1}$, $J_{\text{r-r}} = -16.67 \text{ cm}^{-1}$, $D = 4.0 \text{ cm}^{-1}$, while the values for *trans*-**3** are: $J_{\text{Fe-r}} = -149.88 \text{ cm}^{-1}$,

$J_{\text{Fe-Fe}} = -0.13 \text{ cm}^{-1}$, $J_{\text{r-r}} = -8.41 \text{ cm}^{-1}$, $D = 6.0 \text{ cm}^{-1}$. The D values are similar to those observed for other iron(III)porphyrin π -cation radical complexes reported in the literature.^{10,11}

Computational Details.

All geometry optimizations were initiated from the crystal structure coordinates of the *U* form of *trans*-2, while for the *P'* and *P* forms the same was rotated to a desired orientation and then optimized. For *U*, *P'* and *P* forms of *trans*-2, hydrogen atoms were added to give the molecular formula $\text{C}_{74}\text{N}_8\text{H}_{92}\text{Fe}_2\text{Cl}_4\text{O}_{18}$ and a total atom count of 198. However, for *trans*-2 (without counterion), the counterions were being removed leaving us with a molecular formula of $[\text{C}_{74}\text{N}_8\text{H}_{92}\text{Fe}_2\text{Cl}_2\text{O}_{10}]^{2+}$ and a total atom count of 188. All structures were optimized using the Gaussian 09, revision B.01, package.¹² Geometry optimizations were carried out without any constraints and frequency calculations were also carried out on all optimised structures. Free energies were taken from the Gaussian frequencies and contain, zero-point, thermal and entropic corrections to the energy.

Geometry optimizations have been carried out using the unrestricted hybrid density functional method B3LYP,¹³ along with unrestricted density functional method B97D,¹⁴ which incorporates a force-field-like pairwise dispersion correction developed by Grimme. The basis set was LanL2DZ for iron atom and 6-31G** for carbon, nitrogen, chlorine, oxygen and hydrogen atoms. *U* form of *trans*-2 was optimized as charge neutral species for three different spin multiplicities: (a) tridectet (13) state (considering the radical centers of the two porphyrin units ferromagnetically coupled to the respective iron center), (b) undectet (11) state (where the two radical spins are antiferromagnetically coupled to each other) and (c) nonet (9) state (where the radical spins are antiferromagnetically coupled to the respective iron center). The *P'* and *P* forms of *trans*-2 were also optimized as charge neutral species with nonet spin multiplicity. All three conformations, namely, *U*, *P* and *P'* of *trans*-2 were also optimized after removal of the counterions with a total charge of +2 and nonet (9) spin multiplicity. Self-consistent reaction field (SCRF) method was applied in all the optimizations to consider solvent effect (chloroform was used as solvent) and frequency corrections ensured that there are no imaginary frequencies. Visualization of the molecular orbitals and the corresponding diagrams were done using the Chem Craft software.¹⁵

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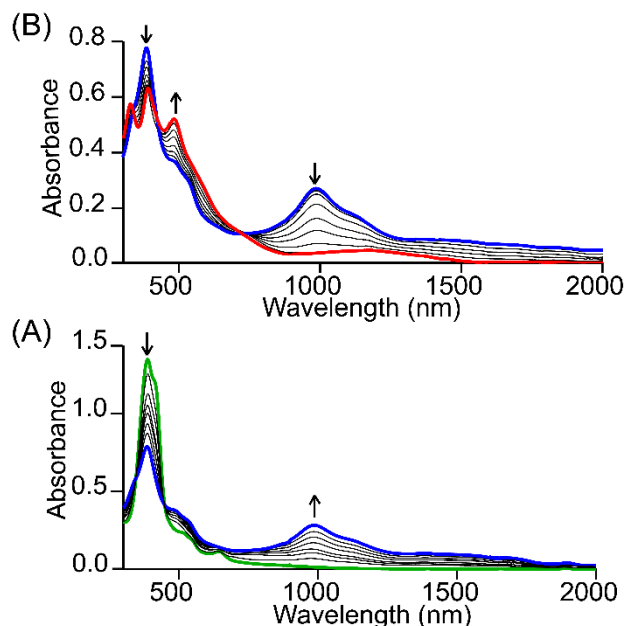


Figure S1. UV-vis-NIR spectral change (in CH_2Cl_2 at 295 K) of 1.2×10^{-5} (M) solution of *trans*-**1** (green line) upon gradual addition, (A) 0 to 1.0 eq., and (B) 1.0 to 2.0 eq. of $\text{Fe}(\text{ClO}_4)_3$.

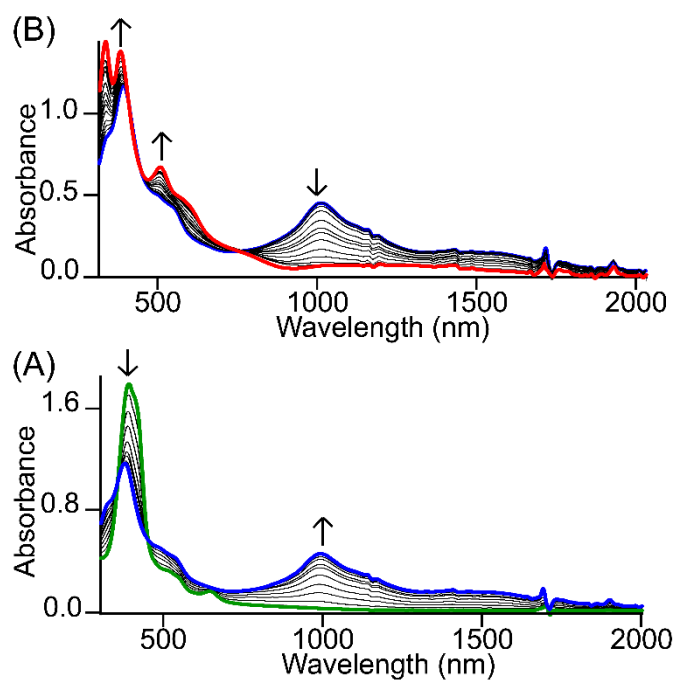


Figure S2. UV-vis-NIR spectral change (in CH_2Cl_2 at 295 K) of 1.1×10^{-5} (M) solution of *trans*-1 (green line) upon gradual addition, (A) 0 to 2.0 eq., and (B) 2.0 to 4.0 eq. of FeCl_3 .

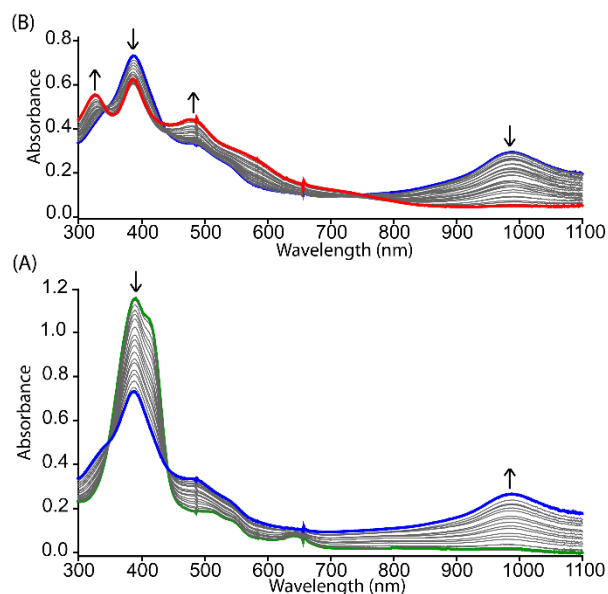


Figure S3. UV-vis-NIR spectral change (in CH_2Cl_2 at 255 K) of 1.2×10^{-5} (M) solution of *trans*-1 (green line) upon gradual addition, (A) 0 to 1.0 eq., and (B) 1.0 to 2.0 eq. of $\text{Fe}(\text{ClO}_4)_3$.

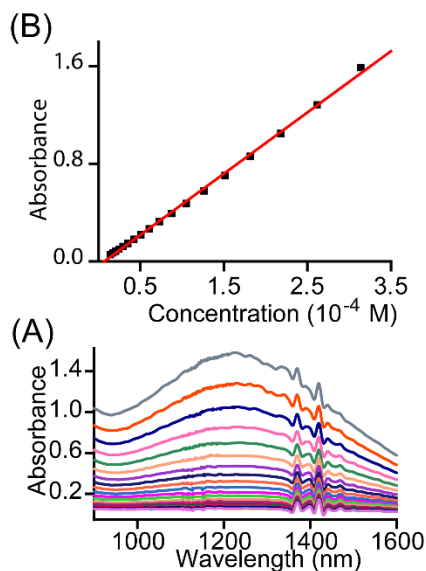


Figure S4. (A) Gradual change in the absorbance of the NIR band (in CH_2Cl_2 at 295 K) of *trans*-3 with change in concentration and (B) plot of absorbance of the NIR band as function of concentration.

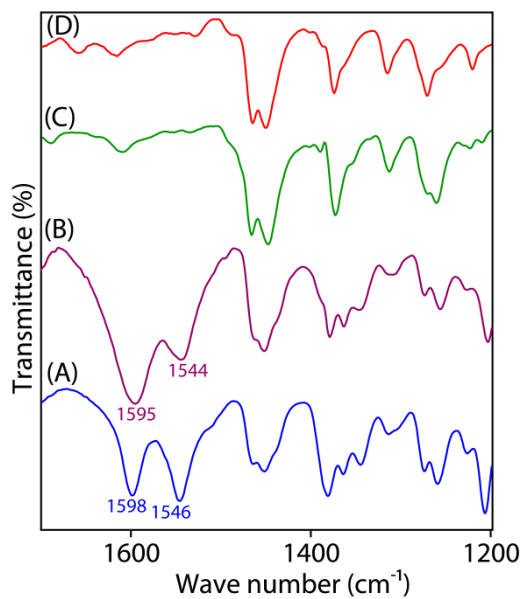


Figure S5. IR spectra (selected portions only) of solid polycrystalline samples of (A) *trans*-2, (B) *trans*-3, (C) *cis*-1, and (D) *trans*-1. The π -cation radical marker bands in *trans*-2 and *trans*-3 have been labeled.

Table S1. Selected Bond Distances ($\text{\AA}$) and Angles ($^\circ$)

	<i>trans</i> -2	<i>trans</i> -3
Fe1-N1	2.058(4)	2.056(3)
Fe1-N2	2.009(4)	2.034(3)
Fe1-N3	2.014(4)	2.029(3)
Fe1-N4	2.028(4)	2.059(3)
Fe1-O1	2.093(3)	-
Fe1-O2	2.187(3)	-
Fe1-Cl1	-	2.2249(11)
C20-C37	1.374(6)	1.364(4)
C37-C37A	1.435(9)	1.432(7)
Fe2-N101	2.060(4)	-
Fe2-N102	2.011(4)	-
Fe2-N103	2.026(4)	-
Fe2-N104	2.037(4)	-
Fe2-O101	2.095(3)	-
Fe2-O102	2.178(3)	-
C120-C137	1.371(6)	-
C137-C137A	1.433(9)	-
N1-Fe1-N2	89.67(14)	88.16(11)
N1-Fe1-N3	176.53(14)	156.31(12)
N1-Fe1-N4	89.60(14)	86.75(11)
N2-Fe1-N3	90.77(14)	88.07(12)
N2-Fe1-N4	178.95(15)	158.27(12)
N3-Fe1-N4	89.91(14)	88.16(11)
O1-Fe1-N1	88.45(13)	-
O1-Fe1-N2	89.92(14)	-
O1-Fe1-N3	94.99(14)	-
O1-Fe1-N4	90.82(14)	-
O2-Fe1-N1	86.46(13)	-
O2-Fe1-N2	87.75(13)	-
O2-Fe1-N3	90.12(13)	-
O2-Fe1-N4	91.45(13)	-
O1-Fe1-O2	174.41(13)	-
Cl1-Fe1-N1	-	99.76(8)
Cl1-Fe1-N2	-	103.42(9)
Cl1-Fe1-N3	-	103.87(10)
Cl1-Fe1-N4	-	98.26(9)
N101-Fe2-N102	90.30(15)	-
N101-Fe2-N103	177.63(15)	-
N101-Fe2-N104	89.41(15)	-
N102-Fe2-N103	90.67(15)	-
N102-Fe2-N104	179.47(15)	-
N103-Fe2-N104	89.64(15)	-
O101-Fe2-N101	87.78(13)	-

O101-Fe2-N102	89.61(14)	-
O101-Fe2-N103	94.38(14)	-
O101-Fe2-N104	89.94(14)	-
O102-Fe2-N101	87.78(13)	-
O102-Fe2-N102	88.09(13)	-
O102-Fe2-N103	90.09(13)	-
O102-Fe2-N104	92.34(13)	-
O101-Fe2-O102	174.99(13)	

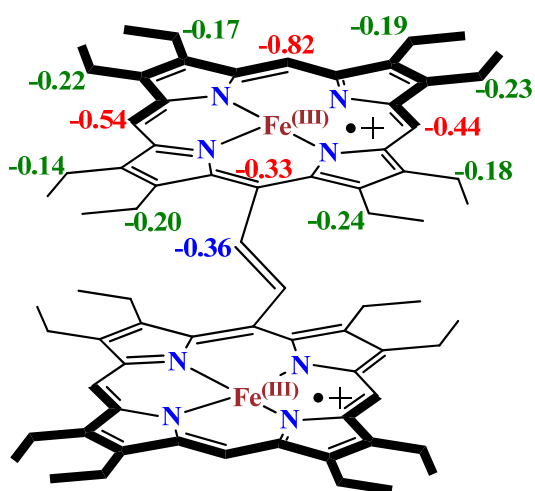


Figure S6. Mulliken spin densities ($\times 10^{-2}$) on the porphyrin methylene (green), meso (red) and bridging (blue) carbons for *trans*-2, as obtained from its optimized structure, using the unrestricted B97D functional and nonet spin multiplicity.

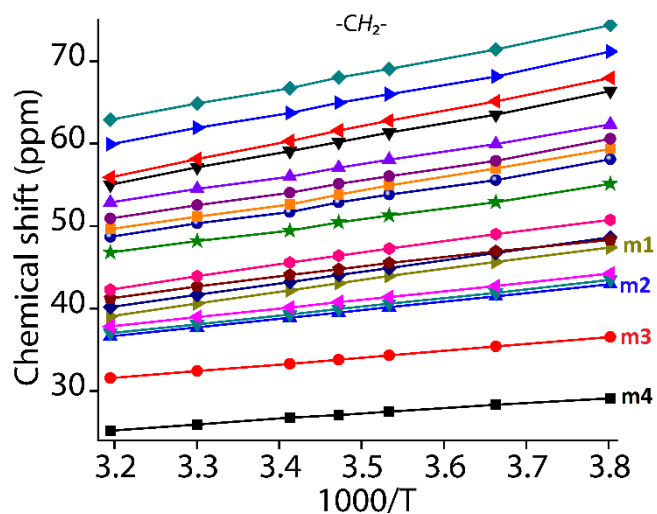
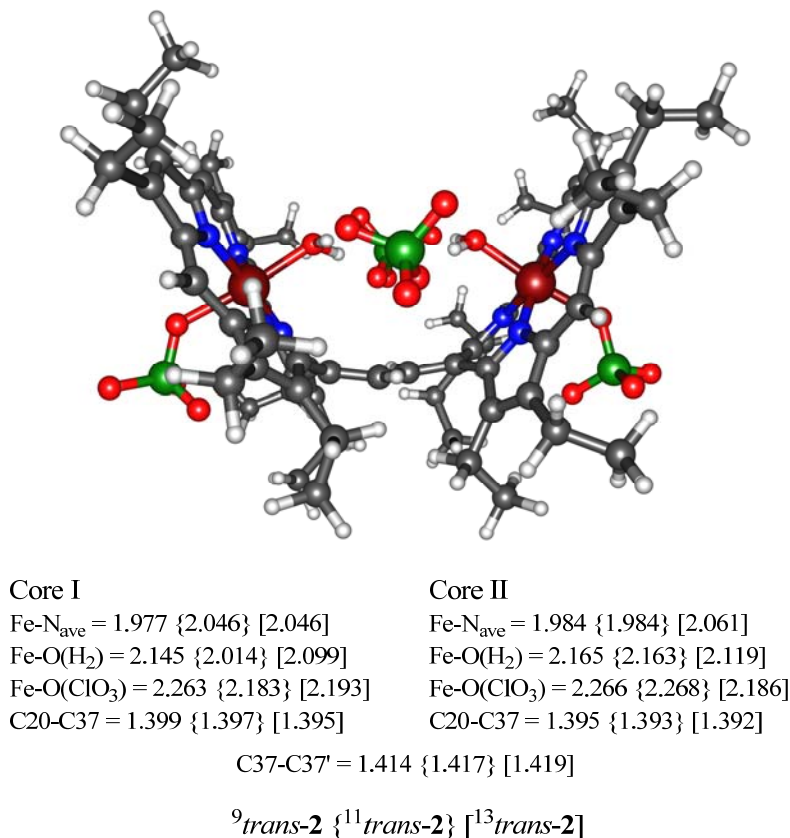
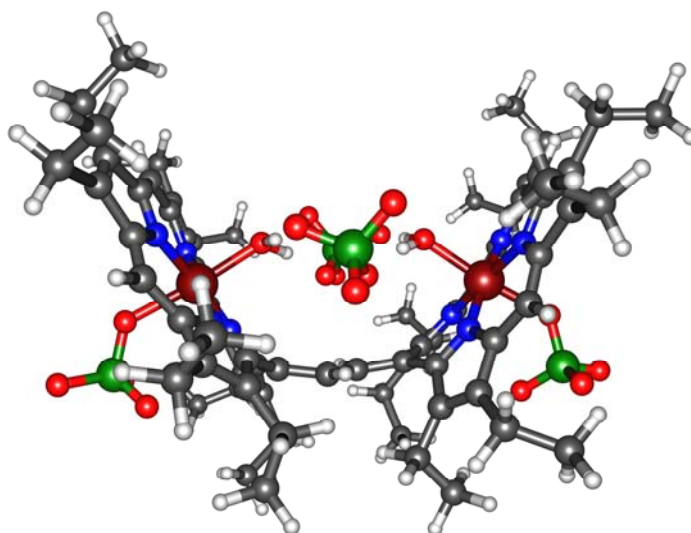


Figure S7. Curie plots of methylene and meso proton signals of *trans*-2.**Table S2.** Parameters used to simulate X-band EPR spectra of *trans*-2 and *trans*-3.

		$g_{\perp}$	$g_{\parallel}$	g_{iso}	$A_{\perp}^a$	$A_{\parallel}^a$	A_{iso}^a
<i>trans</i> -2		5.470	1.945	-	55.0	56.7	-
<i>trans</i> -3	component 1	5.750	1.942	-	50.0	55.0	-
	component 2	-	-	2.016	-	-	104.98

^a Values in Gauss.**Figure S8.** Optimized geometries, in chloroform solution, of the nonet (9), undectet (11) and tridecet (13) states of *U* form of the charge neutral *trans*-2 calculated at unrestricted B3LYP level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.



Core I

$$\text{Fe-N}_{\text{ave}} = 1.985 \{2.057\} [2.051]$$

$$\text{Fe-O(H}_2\text{)} = 2.203 \{2.180\} [2.183]$$

$$\text{Fe-O(ClO}_3\text{)} = 2.261 \{2.191\} [2.193]$$

$$\text{C20-C37} = 1.386 \{1.386\} [1.407]$$

Core II

$$\text{Fe-N}_{\text{ave}} = 2.056 \{2.057\} [2.052]$$

$$\text{Fe-O(H}_2\text{)} = 2.188 \{2.180\} [2.184]$$

$$\text{Fe-O(ClO}_3\text{)} = 2.185 \{2.191\} [2.194]$$

$$\text{C20-C37} = 1.387 \{1.386\} [1.407]$$

$$\text{C37-C37A} = 1.425 \{1.427\} [1.403]$$

$${}^9\text{trans-2} \{ {}^{11}\text{trans-2} \} [{}^{13}\text{trans-2}]$$

Figure S9. Optimized geometries, in chloroform solution, of the nonet (9), undectet (11) and tridectet (13) states of *U* form of the charge neutral *trans-2* calculated at unrestricted B97D level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.

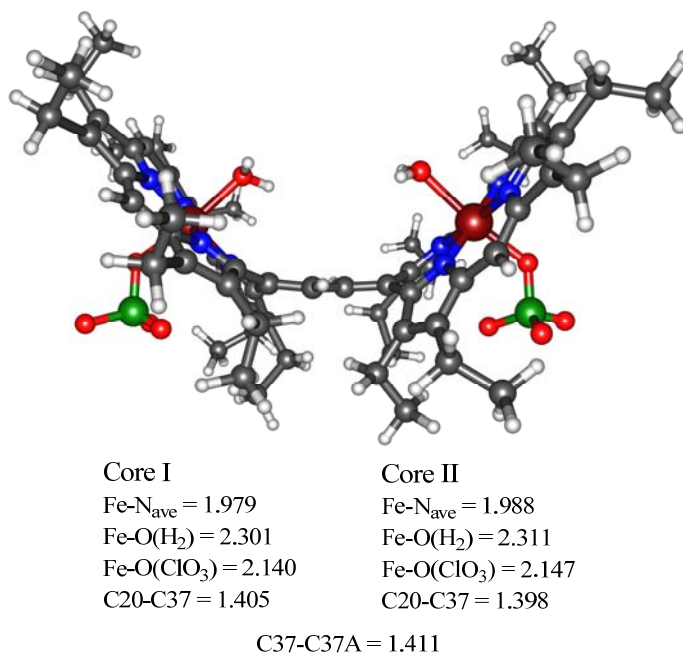


Figure S10. Optimized geometries, in chloroform solution, of the nonet (9) state of *U* form of *trans*-2 (without counteranion) with a total charge of +2, calculated at unrestricted B3LYP level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.

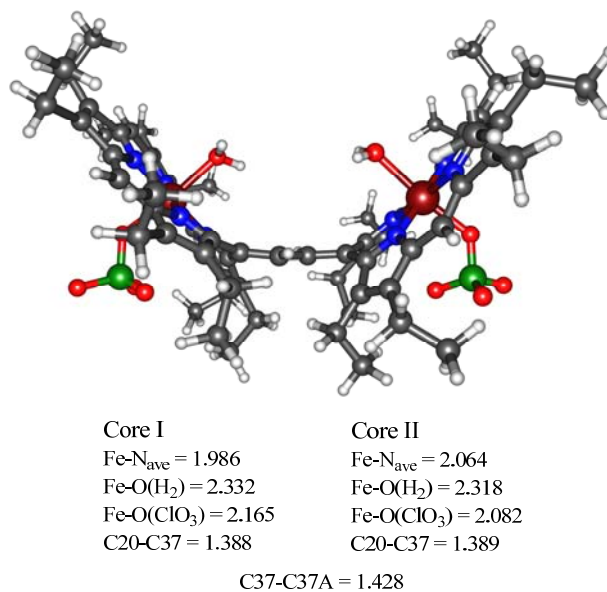


Figure S11. Optimized geometries, in chloroform solution, of the nonet (9) state of *U* form of *trans*-2 (without counteranion) with a total charge of +2, calculated at unrestricted B97D level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.

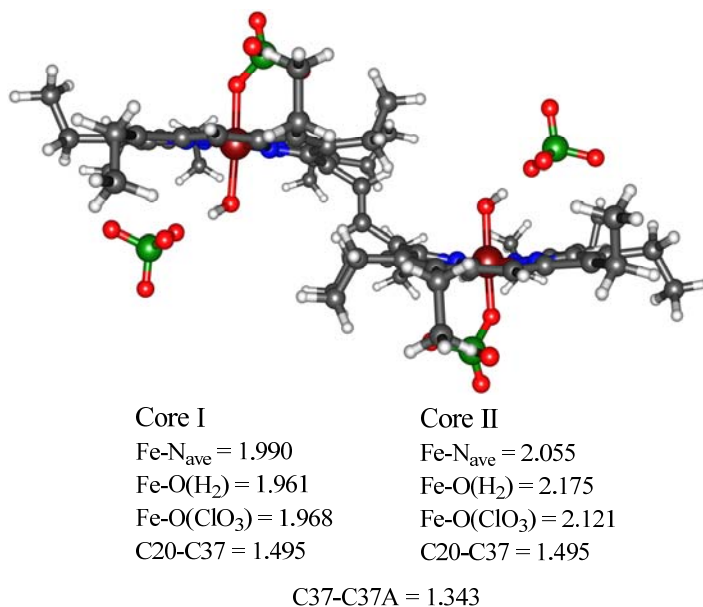


Figure S12. Optimized geometries, in chloroform solution, of the nonet (9) state of the *P* form of the charge neutral *trans*-2 calculated at unrestricted B3LYP level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.

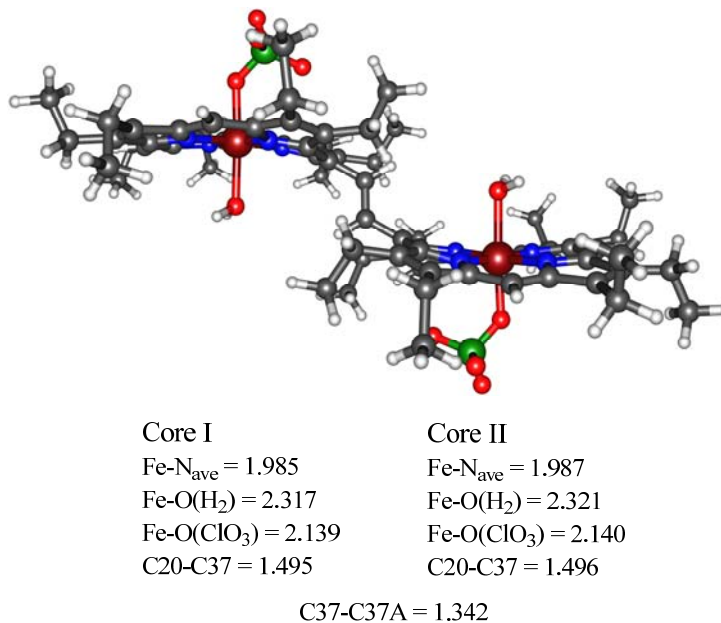
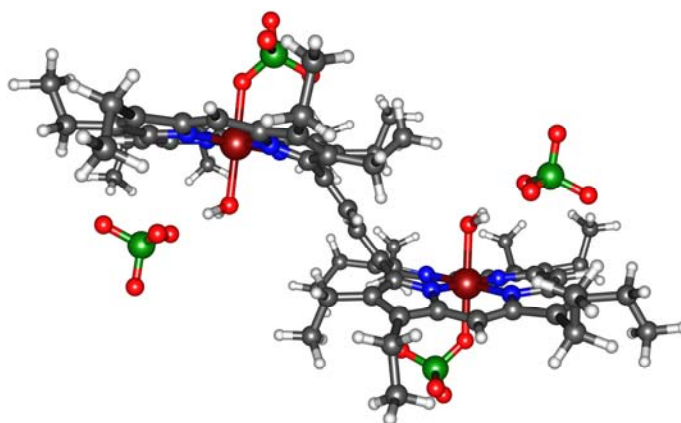
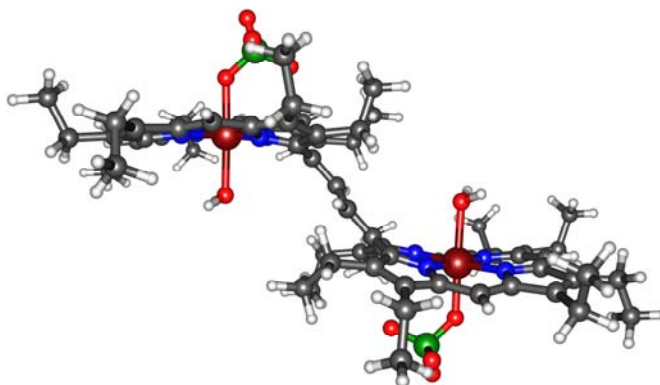


Figure S13. Optimized geometries, in chloroform solution, of the nonet (9) state of *P* form of *trans*-2 (without counteranion) with a total charge of +2, calculated at unrestricted B3LYP level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.



Core I	Core II
Fe-N _{ave} = 1.984	Fe-N _{ave} = 1.977
Fe-O(H ₂) = 2.204	Fe-O(H ₂) = 2.199
Fe-O(ClO ₃) = 2.223	Fe-O(ClO ₃) = 2.218
C20-C37 = 1.397	C20-C37 = 1.402
C37-C37A = 1.406	

Figure S14. Optimized geometries, in chloroform solution, of the nonet (9) state of the *P'* form of the charge neutral *trans*-2 calculated at unrestricted B3LYP level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.



Core I	Core II
Fe-N _{ave} = 1.988	Fe-N _{ave} = 1.979
Fe-O(H ₂) = 2.310	Fe-O(H ₂) = 2.301
Fe-O(ClO ₃) = 2.155	Fe-O(ClO ₃) = 2.142
C20-C37 = 1.399	C20-C37 = 1.405
C37-C37A = 1.404	

Figure S15. Optimized geometries, in chloroform solution, of the nonet (9) state of the *P'* form of *trans*-2 (without counteranion) with a total charge of +2, calculated at unrestricted B3LYP level of theory in gaussian, using LanL2DZ basis set for iron atom and 6-31G** for all other atoms. Bond lengths and non-bonding distances are given in Å.

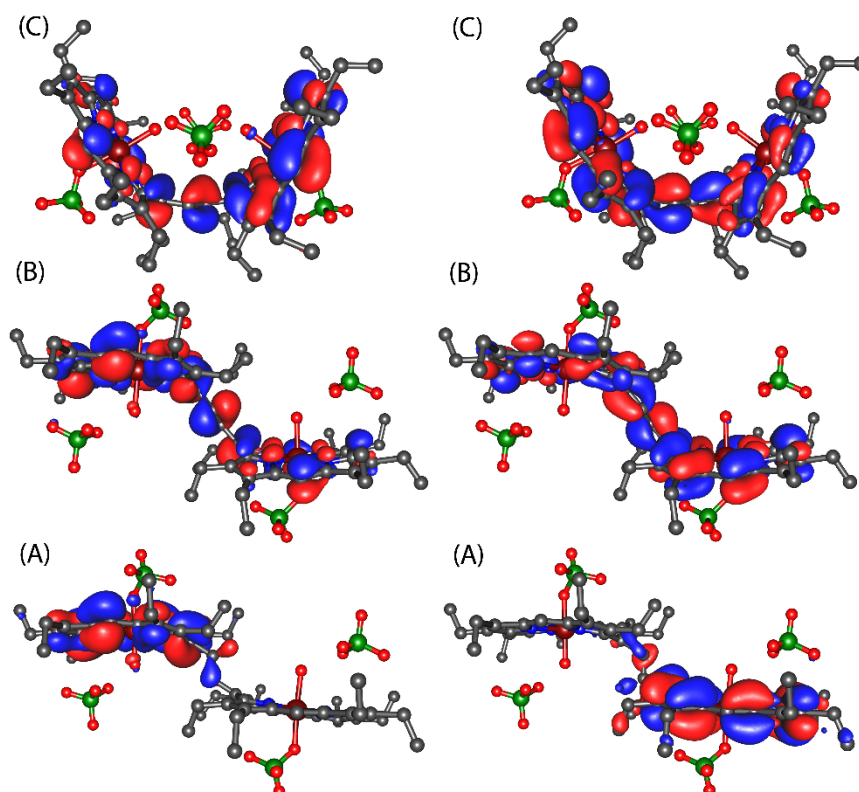


Figure S16. *Left:* HOMO and *Right:* LUMO of (A) *P*, (B) *P'* and (C) *U* conformations of nonet (9) state of *trans*-2 as obtained from respective optimized geometries.

Cartesian Coordinates:

⁹*trans*-2{UB3LYP} (*U* form)

26	4.115230778	0.098341904	0.233438080	6	5.905777170	3.391817411	2.250543854	6	7.781277915	-2.736605651	4.534720146
17	6.400601978	-0.102632960	-2.348991730	6	5.187089223	2.752572347	1.149222878	1	8.159681823	-2.929879640	5.542880165
8	2.366327593	0.182710768	1.472261167	6	4.731091869	3.410544528	0.015555865	1	8.116225047	-1.740409541	4.230256518
8	6.091602311	0.184082440	-0.866324531	1	4.978895325	4.458933835	-0.088443886	1	8.235116675	-3.462838083	3.853806602
8	5.361257220	0.545087418	-3.195271598	6	3.882054835	2.858608144	-0.934365395	6	6.737369162	2.546473668	4.549298418
8	6.394833152	-1.576083987	-2.551509621	6	3.217686795	3.613623452	-1.982212523	1	7.414323762	1.699348228	4.712387449
8	7.740782996	0.469566085	-2.625989027	6	2.302777988	2.768258129	-2.556616774	1	7.364703922	3.442977225	4.567178693
7	3.363512900	-1.214070418	-1.027460405	6	2.466751888	1.479695272	-1.883554754	6	5.716848244	2.616209667	5.704159844
7	4.828364490	-1.371290058	1.347112161	6	1.751374263	0.258106107	-2.151519731	1	6.236467123	2.693192230	6.663811355
7	4.979738918	1.421990805	1.419938465	6	1.788298701	-2.142027323	-4.305542898	1	5.080332492	1.726562173	5.732212694
7	3.444919157	1.551540206	-0.942653845	1	1.350727542	-3.128981824	-4.492027935	1	5.064073013	3.487416387	5.597703722
6	2.498675622	-0.975602231	-2.044123314	1	0.966074802	-1.425848603	-4.359514702	6	6.290116648	4.841638870	2.298670403
6	2.417164598	-2.119632526	-2.938354763	6	2.806882470	-1.819374730	-5.418597755	1	7.168419751	4.955140913	2.942310130
6	3.184309258	-3.106212957	-2.363435957	1	2.307202550	-1.790175994	-6.391832400	1	6.603060484	5.171179340	1.301392215
6	3.728081051	-2.545029919	-1.139623206	1	3.596215632	-2.574582818	-5.463603275	6	5.161677206	5.758504072	2.813943070
6	4.377609881	-3.257228697	-0.147385690	1	3.286350210	-0.851495058	-5.245490373	1	5.491045772	6.801803213	2.809962197
1	4.498187690	-4.323331075	-0.290922300	6	3.459333935	-4.492223768	-2.865181324	1	4.878030506	5.493867663	3.836631900
6	4.813493917	-2.711778803	1.056804331	6	5.406815412	-4.984382179	2.233217967	1	4.266024465	5.680220553	2.190773184
6	5.330999129	-3.486709486	2.181580322	1	6.174571007	-5.278908519	2.955311211	6	3.477982617	5.057581368	-2.301164664
6	5.651726634	-2.584681615	3.156519028	1	5.741798687	-5.370999585	1.263679530	1	3.294630739	5.226381920	-3.366870942
6	5.359249204	-1.260263543	2.607217565	6	4.063207707	-5.639183175	2.616495285	1	4.538177388	5.283851865	-2.142546372
6	5.657535465	-0.062999684	3.242569948	1	4.155375836	-6.729322599	2.606590816	6	2.609554364	6.027645790	-1.473576871
1	6.096680085	-0.112045718	4.230038211	1	3.264153389	-5.349574785	1.928242222	1	2.826379635	7.062317437	-1.755880006
6	5.543019021	1.188352393	2.644076358	1	3.755179954	-5.335727540	3.621329765	1	2.798755212	5.916852849	-0.402073879
6	6.096982351	2.425163393	3.198369032	6	6.242674955	-2.845794979	4.511251309	1	1.545227688	5.837299570	-1.634746486
				1	5.946799466	-3.846549534	4.840689934	6	1.434846643	3.093492287	-3.741656342
				1	5.813614919	-2.149633267	5.240907973	1	1.415119745	4.180787213	-3.856742059

1	0.396431731	2.804079116	-3.563304389	1	-5.603559598	-6.139836659	4.062938604	6	5.686121620	1.456132252	2.447804691
6	1.930668844	2.458749828	-5.05676679	1	-4.874466243	-4.699018262	4.792367875	6	6.183259515	2.756560582	2.912801286
1	1.291735582	2.766450015	-5.889109780	1	-4.378544932	-5.212923238	3.178181200	6	5.824621382	3.674691089	1.960552547
1	1.916900028	1.366692936	-5.004694891	6	-3.746127429	-5.405380971	-1.351650935	6	5.085287760	2.940093904	0.930882821
1	2.955637084	2.770554949	-5.276374125	1	-3.574406533	-5.766133961	-2.370827229	6	4.520855257	3.499094525	-0.217515959
0	0.369421440	0.298276909	-2.366232992	1	-4.811042746	-5.568678773	-1.152964003	1	4.691107300	4.557787511	-0.371884217
1	-0.081595637	1.281011138	-2.380520905	6	-2.901112211	-6.239874972	-0.367078133	6	3.706193756	2.862384649	-1.156918386
6	4.892525576	-4.689705970	-3.401512986	1	-3.131572141	-7.304255582	-0.475865941	6	3.053966281	3.512365682	-2.285200747
1	5.023649956	-5.720023043	-3.745399779	1	-3.100476384	-5.950697015	0.669076849	6	2.221841370	2.577892853	-2.854328597
1	5.640105213	-4.486057635	-2.630310341	1	-1.832194308	-6.094093096	-0.544873641	6	2.401141159	1.347697796	-2.076129293
1	5.096437821	-4.018047212	-4.239373676	6	-1.645014192	-3.796941416	-3.122225818	6	1.716489687	0.076100272	-2.243803560
1	1.677263582	-0.479367437	1.233022202	1	-1.645685326	-4.887196792	-3.031477375	6	1.752233731	-2.550394813	-4.150961863
1	1.936462324	1.066956782	1.500916962	1	-0.600361802	-3.500433322	-2.994853066	1	1.298272080	-3.542692100	-4.249148278
7	-3.374431001	1.007392972	-1.204703578	6	-2.123062531	-3.411629532	-4.534705546	1	0.947824458	-1.826711894	-4.298177286
7	-4.717353613	1.628373335	1.169677325	1	-1.484275904	-3.873469929	-5.294453355	6	2.803172154	-2.360113174	-5.265017966
7	-5.002841940	-1.113283298	1.714932001	1	-2.097903725	-2.328645405	-4.684245178	1	2.325362881	-2.409474663	-6.248372394
7	-3.560239808	-1.716676306	-0.635427595	1	-3.150810152	-3.746793759	-4.703093477	1	3.571180320	-3.136977300	-5.220260620
6	-2.583866370	0.560758706	-2.196739567	6	-0.506222994	-0.807563996	-2.265777788	1	3.306123918	-1.393476396	-5.170103813
6	-2.500694211	1.517282234	-3.277004167	1	-0.063709384	-1.776531820	-2.075441420	6	3.313349040	-4.781951021	-2.429273655
6	-3.219738410	2.622381356	-2.862388274	6	-4.914458449	4.011063311	-4.164822021	6	5.561970605	-4.787073298	2.584754308
6	-3.718513426	2.316369054	-1.543090775	1	-5.037711678	4.959733489	-4.696339212	1	6.405658584	-5.031116817	3.237661247
6	-4.287299073	3.199542461	-0.662015508	1	-5.656297190	3.964255233	-3.363333742	1	5.768897166	-5.280024903	1.627912792
1	-4.403260991	4.227111252	-0.986304296	1	-5.133939136	3.196131850	-4.859670622	6	4.261438827	-5.357114185	3.189351417
6	-4.672643867	2.894073015	0.656462602	26	-4.133682151	-0.046324667	0.289599889	1	4.326011496	-6.446330195	3.270891731
6	-5.082812481	3.861962408	1.637876697	17	-6.514568977	-0.205046720	-2.240648282	1	3.390741953	-5.106913139	2.576249752
6	-5.380037826	3.149449394	2.784776895	8	-2.297670904	-0.025692804	1.436184069	1	4.087558205	-4.948368725	4.189126560
6	-5.173449066	1.760311061	2.463367762	8	-6.144735941	-0.182239741	-0.745915719	6	6.697111050	-2.453011684	4.513912235
6	-5.494710960	0.691348766	3.291905042	8	-5.457798253	-0.928593892	-2.999699684	1	6.475262220	-3.430713230	4.952669639
1	-5.867147918	0.928159395	4.281529867	8	-6.629606766	1.199470258	-2.715019686	1	6.333545007	-1.709517459	5.232903532
6	-5.473704634	-0.648234700	2.923927074	8	-7.815827580	-0.911547521	-2.350157270	6	8.223530075	-2.305111199	4.345806974
6	-6.027264465	-1.731944732	3.697918583	1	-1.620549100	0.614284456	1.123100620	1	8.723822554	-2.401375304	5.314049635
6	-5.923331619	-2.863923041	2.910628601	1	-1.863902275	-0.899738989	1.529535561	1	8.486741357	-1.331301281	3.921645924
6	-5.267281463	-2.451376738	1.695818171	17	-0.043007877	2.997957727	1.128771305	1	8.618532421	-3.076290587	3.677806884
6	-4.878847386	-3.320468072	0.659966036	8	-0.458628725	1.754008650	0.370703202	6	6.921458550	2.979983291	4.199243990
1	-5.180971193	-4.357228434	0.748850891	8	-0.960593489	3.215190968	0.227586464	1	7.668020066	2.188117121	4.334652934
6	-4.054966946	-2.992517066	-0.388247470	8	-0.059792290	4.162024636	0.270872532	1	7.482665257	3.917329324	4.134342115
6	-3.441623997	-3.935716445	-1.294205956	8	1.364735425	2.776103701	1.633922256	6	5.995515630	3.026100342	5.432522843
6	-2.502748525	-3.235363432	-2.019886424	17	0.133528265	-2.871534404	1.281175469	1	6.584034286	3.177733558	6.342253095
6	-2.620000667	-1.853502344	-1.593277215	8	0.539289503	-1.612691188	0.538156577	1	5.429822187	2.096077751	5.544035836
6	-1.887504438	-0.711201348	-2.099936490	8	1.099799417	-3.133613860	2.379889390	1	5.275078228	3.845155728	5.350396651
1	-1.926503161	1.265468081	-4.645944879	8	0.104699766	-4.005156634	0.319708982	6	6.069894667	5.154613478	1.950763059
1	-1.510956074	2.196110931	-5.048301255	8	-1.243084513	-2.639211505	1.848083157	1	6.951079934	5.376029203	2.561217155
1	-1.095233495	0.558517984	-4.586046566	1	-3.284804632	4.750272465	-2.945628987	1	6.317251163	5.479333333	0.932797946
6	-2.979370842	0.714189045	-5.629186911	1	-2.763228437	3.985061673	-4.431170085	6	4.870651235	5.972679673	2.473647253
1	-2.517146702	0.481551505	-6.593911115	1	3.275930694	-5.209345026	-2.054915381	1	5.094452793	7.042717188	2.429352164
1	-3.777398566	1.441834470	-5.800732205	1	2.738981096	-4.735707052	-3.651924312	1	4.643650319	5.713323553	3.511784084
1	-3.444694738	-0.195037353	-5.237443926					1	3.970047729	5.786582217	1.881082734
6	-3.480139708	3.897922923	-3.608483051					6	3.259597697	4.943182433	-2.690751660
1	-5.092245917	5.352748896	1.449307856					3	3.118745615	5.034229109	-3.772304373
1	-5.826465512	5.796738822	2.129596235					1	4.299591718	5.230876529	-2.500112830
1	-5.435701664	5.600396017	0.438096429					6	2.310830103	5.922261676	-1.968599724
6	-3.712217339	5.995864569	1.696371638	26	4.098426019	0.145522826	0.194263911	1	2.505158308	6.947481264	-2.298168468
1	-3.758789958	7.077293629	1.533171173	17	6.242587746	-0.305012501	-2.405268704	1	2.440685209	5.878022722	-0.883569586
1	-2.951598451	5.578519459	1.030053580	8	2.414738522	0.268430023	1.450198969	1	1.265452163	5.681328915	-2.179653466
1	-3.377546818	5.818332005	2.722766513	8	5.946030148	0.199506053	-0.967118075	6	1.418398776	2.758930698	-4.112045216
6	-5.885451948	3.684260989	4.094845807	8	5.167680388	0.176542282	-3.312074104	1	1.367745560	3.828103494	-4.336996506
1	-5.480547901	4.689923218	4.249010237	8	6.285612979	-1.788588907	-2.375851021	1	0.382517939	2.443085473	-3.964463634
1	-5.497144169	3.076364523	4.919611063	7	7.555446285	0.267678736	-2.779146597	6	2.011570526	2.014281802	-5.324216982
6	-7.424532596	3.739134098	4.176705992	7	3.269906117	-1.330898969	-0.950410293	1	1.404310284	2.198115962	-6.215866676
1	-7.742926799	4.140871194	5.143709267	7	4.928104692	-1.273212775	1.413432189	1	2.044939220	0.934663433	-5.153253212
1	-7.863344046	2.743314143	4.059537772	7	5.014418745	1.611729684	1.269109979	1	3.031908523	2.351771155	-5.527827930
1	-7.836965301	4.377419875	3.389342867	7	3.319007347	1.540691522	-1.101958137	6	0.336162226	0.100464921	-2.457801728
6	-6.592108472	-1.615380308	5.084974297	6	2.440590698	-1.168490354	-2.005788280	1	-0.110393020	1.080777574	-2.558124209
1	-7.193249753	-0.702216934	5.166410098	6	2.348145460	-2.400420022	-2.777595605	6	4.742494385	-5.068162076	-2.936106559
1	-7.283742131	-2.446045479	5.260059982	6	3.071441984	-3.344328515	-2.078859212	1	4.852923718	-6.132764152	-3.163054155
6	-5.513651589	-1.614373093	6.187172252	6	3.621028224	-2.668986134	-0.913928014	1	5.493644085	-4.796196149	-2.189668896
1	-5.977251394	-1.531131099	7.175076589	6	4.306903286	-3.271413918	0.137517942	1	4.961687126	-4.498704813	-3.843231852
1	-4.819700383	-0.777053011	6.064497059	1	4.397584803	-4.350609797	0.101022048	1	1.717050927	-0.403165320	1.253614759
1	-4.926293662	-2.536973196	6.162340186	6	4.867479632	-2.630827242	1.248779143	1	1.978898376	1.153659564	1.479959802
6	-6.354214459	-4.265766195	3.239516870	6	5.502427158	-3.301190960	2.386030476	7	-3.372311234	0.918839763	-1.248160746
1	-7.198453205	-4.224011784	3.936027681	6	5.946665849	-2.312193226	3.221989842	7	-4.655986409	1.698359026	-1.113753566
1	-6.737906224	-4.755510701	2.337112521	6	5.591529229	-1.037226535	2.586578853	7	-4.984660854	-1.002510735	1.817092208
6	-5.235436830	-5.130468607	3.853966022	6	5.922338142	0.228231337	3.078936536	7	-3.582558043	-1.763427989	-0.515537380

¹¹*trans*-2{UB3LYP} (U form)

6	-2.613458173	0.401931095	-2.231547846
6	-2.543454066	1.292294462	-3.367513078
6	-3.231666743	2.433158901	-2.999474138
6	-3.701711064	2.212751508	-1.652945538
6	-4.229430927	3.156269595	-0.809736125
1	-4.331443770	4.166809817	-1.187687460
6	-4.589533246	2.932971782	0.531919414
6	-4.955054466	3.962958204	1.466898475
6	-5.251346058	3.320745964	2.654782466
6	-5.087070209	1.911433865	2.405305741
6	-5.424580210	0.897321723	3.294275201
1	-5.780772168	1.196736730	4.272994513
6	-5.436105796	-0.460615887	3.001106517
6	-5.999431118	-1.488831258	3.841566795
6	-5.918353966	-2.666368887	3.121726528
6	-5.267294163	-2.335284812	1.879463950
6	-4.896428475	-3.270584131	0.896585336
1	-5.205047171	-4.297025833	1.054126705
6	-4.081316819	-3.017071382	-0.178596060
6	-3.482587010	-4.022292706	-1.025551123
6	-2.551891787	-3.377062240	-1.810058178
6	-2.656520247	-1.969028765	-1.475459959
6	-1.924999710	-0.868296547	-2.069132723
6	-2.007397619	0.951940430	-4.732937687
1	-1.598488129	1.853544260	-5.202898293
1	-1.177692821	0.245032904	-6.650998067
6	-3.087792164	0.349032754	-5.653769258
1	-2.654461853	0.069626996	-6.619488474
1	-3.893659200	1.065340368	-5.836107228
1	-3.536736067	-0.541534480	-5.204212457
6	-3.489243472	3.668866625	-3.810474774
6	-4.931608808	5.441273530	1.197852590
1	-5.634519536	5.940394569	1.872954403
1	-5.297978734	5.643381826	0.184413490
6	-3.529681293	6.061171180	1.370311953
1	-3.556018587	7.133176811	1.150071150
1	-2.798993834	5.589819987	0.706358154
1	-3.168759707	5.930541448	2.394807129
6	-5.719597108	3.938200504	3.942258616
1	-5.282398993	4.937655648	4.036809551
1	-5.335772255	3.363238451	4.792386507
6	-7.254623254	4.044613032	4.044113362
1	-7.544589208	4.507457722	4.992581214
1	-7.725213384	3.057964279	3.988114751
1	-7.660906284	4.652116414	3.229637724
6	-6.549914525	-1.282258975	5.223818601
1	-7.141488545	-0.359746419	5.253603538
1	-7.247569480	-2.093618447	5.455975450
6	-5.460766832	-1.223578632	6.313962380
1	-5.913185545	-1.069284300	7.298498980
1	-4.757567840	-0.405655535	6.129427954
1	-4.885417979	-2.153596201	6.344728375
6	-6.363762351	-4.040694136	5.356174202
1	-7.204029993	-3.947860539	4.232558529
1	-6.756775891	-4.579662434	2.666483633
6	-5.251040505	-4.878757304	4.196962797
1	-5.629185482	-5.868527060	4.471483496
1	-4.878743212	-4.392900712	5.103801815
1	-4.400099872	-5.013666271	3.522076338
6	-3.780762213	-5.492997960	-0.966612642
1	-3.642891510	-5.928100565	-1.961696427
1	-4.836447308	-5.647571216	-0.717935298
6	-2.893551432	-6.245007198	0.047061832
1	-3.124103736	-7.314870930	0.035487322
1	-3.051841693	-5.870743360	1.062904512
1	-1.833134338	-6.114091974	-0.185526297
1	-1.706074346	-4.017546452	-2.877760354
1	-1.745596171	-5.101668659	-2.736183294
1	-0.652876267	-3.751884957	-2.750307982
6	-2.158166795	-3.685293202	-4.312043936
1	-1.530286395	-4.206715740	-5.041709416
1	-2.093126582	-2.612793669	-4.515248148
1	-3.195801289	-3.992214795	-4.473611688

6	-0.549057316	-0.986962195	-2.254216292
1	-0.111078118	-1.942893495	-1.998406898
6	-4.936330672	3.779042149	-4.333126696
1	-5.054967661	4.694149138	-4.921515387
1	-5.655052513	3.801569240	-3.509810438
1	-5.193274654	2.926019446	-4.966612047
26	-4.118663969	-0.034560831	0.319599979
17	-6.567681809	-0.316549862	-2.141099649
8	-2.272919950	0.014735829	1.446916440
8	-6.157376292	-0.188586403	-0.663007678
8	-5.592173026	-1.190163676	-2.848727166
8	-6.583568240	1.042728211	-2.743861545
8	-7.923658663	-0.921321911	-2.158238504
1	-1.585685606	0.623711843	1.096638482
1	-1.853129719	-0.858833476	1.588090262
17	-0.036397986	3.002568565	1.047623196
8	-0.418468150	1.738204337	0.308030029
8	-0.985952149	3.236750660	2.164483356
8	-0.035258228	4.145994137	0.098589160
8	1.360461678	2.808254404	1.598841350
17	0.157400920	-2.776840601	1.390699946
8	0.509250425	-1.490901145	0.665881682
8	1.155289769	-3.035165058	2.462079221
8	0.139738056	-3.890484887	0.404980752
8	-1.211669567	-2.591782115	1.989280289
1	-3.259636364	4.553368368	-3.202955559
1	-2.794341652	3.694468802	-4.655916039
1	3.112645540	-5.402813933	-1.547052185
1	2.589374237	-5.093318364	-3.188403439

¹³*trans*-2{UB3LYP} (U form)

26	4.098704000	0.136784000	0.257344000
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8	2.384885000	0.166072000	1.470248000
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8	5.238713000	0.654022000	-3.198866000
8	6.291946000	-1.460210000	-2.560917000
8	7.617893000	0.598916000	-2.624346000
7	3.274992000	-1.174508000	-1.076548000
7	4.883531000	-1.436946000	1.301916000
7	5.028524000	1.437829000	1.516908000
7	3.770702000	1.695863000	-0.876638000
6	2.487987000	-0.859672000	-2.128240000
6	2.419080000	-1.970525000	-3.066447000
6	3.110960000	-3.010466000	-2.479211000
6	3.621066000	-2.507849000	-1.214407000
6	4.274137000	-3.249182000	-0.233293000
1	4.359813000	-4.315261000	-0.406721000
6	4.811625000	-2.762714000	0.906380400
6	5.415240000	-3.580672000	2.017266000
6	5.853967000	-2.712513000	2.980917000
6	5.529456000	-1.361838000	2.506104000
6	5.878194000	-0.174809000	3.155728000
1	6.406509000	-0.271452000	4.095830000
6	5.684928000	1.125840000	2.671947000
6	6.220425000	2.347299000	3.286236000
6	5.900064000	3.380154000	2.444552000
6	5.143924000	2.794608000	1.334561000
6	4.603669000	3.502392000	0.261358000
1	4.798970000	4.567379000	0.240621000
6	3.779441000	3.006632000	-0.754343000
6	3.134658000	3.810853000	-1.782886000
6	2.292321000	2.971119000	-2.472689000
6	2.459531000	1.645016000	-1.870344000
6	1.771310000	0.411703000	-2.211854000
6	1.875348000	-1.917384000	-4.468396000
1	1.429198000	-2.883327000	-4.729476000
1	1.073697000	-1.178528000	-4.536552000
6	2.966758000	-1.568298000	-5.502081000
1	2.527415000	-1.476582000	-6.500284000
1	3.736432000	-2.343993000	-5.338515000
1	3.460493000	-0.625398000	-5.250226000

6	3.355392000	-4.388135000	-3.019020000
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1	6.285936000	-5.419597000	2.649310000
1	5.661822000	-5.451470000	1.015833000
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6	6.957340000	2.397137000	4.591656000
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1	7.558307000	3.311074000	4.630836000
6	6.023595000	2.349272000	5.819004000
1	6.609688000	2.378149000	6.742405000
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1	5.337791000	3.201466000	5.821846000
6	6.201413000	4.841924000	2.598530000
1	7.082939000	4.961461000	3.236223000
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6	5.029604000	5.648887000	3.195297000
1	5.299961000	6.706169000	3.273394000
1	4.773739000	5.286606000	4.195198000
1	4.132312000	5.570775000	2.574277000
6	3.348948000	5.283164000	-1.984094000
1	3.189298000	5.530264000	-3.038393000
1	4.394992000	5.533684000	-1.774201000
6	2.422507000	6.154065000	-1.110303000
1	2.615231000	7.215097000	-1.296147000
1	2.577580000	5.957184000	-0.045631000
1	1.371312000	5.947316000	-1.327810000
6	1.480736000	3.335626000	-3.684805000
1	1.463570000	4.425859000	-3.769646000
1	0.435881000	3.038489000	-3.559715000
6	2.032006000	2.736733000	-4.993392000
1	1.425072000	3.061876000	-5.844015000
1	2.022263000	1.643628000	-4.968925000
1	3.063354000	3.058335000	-5.164962000
6	0.396256000	0.463774000	-2.443109000
1	-0.055965000	1.446121000	-2.413567000
6	4.798982000	-4.619550000	-3.513020000
1	4.903804000	-5.638438000	-3.897766000
1	5.524515000	-4.480688000	-2.707071000
1	5.059774000	-3.920851000	-4.312273000
1	1.763330000	-0.472967000	1.211265000
1	1.960418000	1.049215000	1.586730000
7	-3.291954000	1.101605000	-1.155977000
7	-4.864585000	1.533751000	1.234264000
7	-5.046288000	-1.338415000	1.629402000
7	-3.425030000	-1.764915000	-0.768312000
6	-2.546462000	0.715518000	-2.202874000
6	-2.461187000	1.767335000	-3.195481000
6	-3.124033000	2.856818000	-2.656781000
6	-3.620372000	2.441616000	-1.362738000
6	-4.241404000	3.233169000	-0.4211105000
1	-4.329464000	4.288074000	-0.658071000
6	-4.767373000	2.831466000	0.830372000
6	-5.310615000	3.713610000	

6	-3.837294000	-3.075147000	-0.543701000
6	-3.207951000	-3.942475000	-1.519846000
6	-2.370377000	-3.150720000	-2.277271000
6	-2.538529000	-1.793263000	-1.775509000
6	-1.860108000	-0.579158000	-2.221954000
6	-1.936998000	1.620490000	-4.598730000
1	-1.534610000	2.578561000	-4.946256000
1	-1.106058000	0.910270000	-4.621372000
6	-3.024851000	1.142726000	-5.582722000
1	-2.598472000	0.990338000	-6.579468000
1	-3.830662000	1.877555000	-5.664858000
1	-3.472199000	0.202737000	-5.247262000
6	-3.349836000	4.203799000	-3.278373000
6	-5.312988000	5.214692000	1.769958000
1	-6.120250000	5.604611000	2.398594000
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1	-4.002650000	6.924294000	2.120220000
1	-3.140167000	5.458185000	1.611773000
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6	-7.969035000	3.310185000	4.041703000
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1	-7.574073000	-1.219571000	4.855230000
1	-7.517128000	-2.967241000	4.903550000
6	-5.928505000	-2.011553000	6.021407000
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6	-6.168576000	-4.644574000	2.985047000
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1	-6.435804000	-5.153215000	2.051162000
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1	-5.254503000	-6.440540000	3.819922000
1	-4.745346000	-4.942957000	4.619415000
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1	-3.282110000	-5.739824000	-2.661250000
1	-4.455689000	-5.668705000	-1.369358000
6	-2.464650000	-6.236120000	-0.717346000
1	-2.644579000	-7.308759000	-0.840452000
1	-2.607577000	-5.981795000	0.336821000
1	-1.419724000	-6.026978000	-0.961358000
6	-1.562350000	-3.601505000	-3.463874000
1	-1.535427000	-4.695228000	-3.465836000
1	-0.518451000	-3.288301000	-3.366933000
6	-2.120307000	-3.109840000	-4.812805000
1	-1.509846000	-3.486701000	-5.639770000
1	-2.127999000	-2.017652000	-4.867871000
1	-3.147221000	-3.457366000	-4.959519000
6	-0.482427000	-0.649375000	-2.410051000
1	-0.032310000	-1.627166000	-2.296197000
6	-4.777225000	4.404843000	-3.828573000
1	-4.874638000	5.402528000	-4.267774000
1	-5.525793000	4.301693000	-3.038415000
1	-5.010533000	3.665804000	-4.599831000
26	-4.135218000	-0.120887000	0.268360000
17	-6.354425000	-0.140454000	-2.327296000
8	-2.385040000	-0.097726000	1.462178000
8	-6.017837000	-0.319500000	-0.824628000
8	-5.313182000	-0.821993000	-3.140472000
8	-6.392425000	1.312953000	-2.625312000
8	-7.681891000	-0.767108000	-2.528270000
1	-1.688679000	0.540156000	1.179326000
1	-1.950048000	-0.969941000	1.593179000
17	-0.092436000	2.868584000	1.339944000
8	-0.447850000	1.628930000	0.539121000
8	-1.041491000	3.029539000	2.464387000

8	-0.125425000	4.053640000	0.439174000
8	1.311352000	2.678577000	1.867322000
17	0.128919000	-2.799025000	1.342431000
8	0.461979000	-1.533005000	0.574791000
8	1.135664000	-3.011039000	2.415118000
8	0.109904000	-3.946449000	0.399399000
8	-1.238784000	-2.611114000	1.951767000
1	-3.138228000	4.983471000	-2.536017000
1	-2.626808000	4.352372000	-4.086891000
1	3.119050000	-5.125065000	-2.240991000
1	2.656753000	-4.579987000	-3.839067000

⁹*trans*-2{UB97D} (U form)

26	-4.062918000	-0.057189000	0.320412000
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1	-1.870777000	-1.075135000	1.471097000
8	-6.034620000	-0.137685000	-0.782618000
8	-7.604970000	-0.505045000	-2.620268000
8	-5.191261000	-0.793124000	-3.037811000
8	-6.112674000	1.462164000	-2.676865000
7	-3.459180000	-1.631650000	-0.747796000
7	-4.901494000	-1.264819000	1.650203000
7	-4.655119000	1.518997000	1.367202000
7	-3.303402000	1.150812000	-1.050601000
6	-2.530410000	-1.664691000	-1.730523000
6	-2.361263000	-3.003188000	-2.263419000
6	-3.271272000	-3.793561000	-1.582764000
6	-3.909159000	-2.944334000	-0.604502000
6	-4.718421000	-3.385361000	0.420120000
1	-4.983029000	-4.440389000	0.431987000
6	-5.121252000	-2.612335000	1.525788000
6	-5.720204000	-3.152199000	2.722503000
6	-5.833426000	-2.093198000	3.611954000
6	-5.341321000	-0.926461000	2.917874000
6	-5.374312000	0.374875000	3.417270000
1	-5.725604000	0.510606000	4.438200000
6	-5.086182000	1.523611000	2.682476000
6	-5.309955000	2.874813000	3.138523000
6	-5.063904000	3.698183000	2.049717000
6	-4.644279000	2.833780000	0.975714000
6	-4.250693000	3.279427000	-0.300758000
1	-4.380404000	4.336392000	-0.523421000
6	-3.642529000	2.494336000	-1.252675000
6	-3.134143000	2.941632000	-2.524655000
6	-2.406223000	1.886054000	-3.052257000
6	-2.513519000	0.813650000	-2.092869000
6	-1.835263000	-0.467806000	-2.153794000
6	-1.471752000	-3.447275000	-3.393084000
1	-0.412878000	-3.324085000	-3.122620000
1	-1.613811000	-4.528436000	-3.529071000
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1	-1.117231000	-3.117789000	-5.523860000
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1	-2.815695000	-2.882258000	-5.021909000
6	-3.483097000	-5.273106000	-1.708611000
1	-3.317005000	-5.578437000	-2.752154000
1	-4.526956000	-5.524544000	-1.468448000
6	-2.524649000	-6.060730000	-0.779801000
1	-2.682990000	-7.142932000	-0.896422000
1	-2.699132000	-5.789010000	0.271158000
1	-1.478992000	-5.820114000	-1.013429000
6	-6.032478000	-4.601107000	2.957741000
1	-6.453544000	-5.047276000	2.043248000
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1	-5.023021000	-6.456081000	3.543586000
1	-4.366683000	-4.990480000	4.326370000
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1	-6.949327000	-3.002649000	5.184771000

1	-6.931074000	-1.235440000	5.239359000
6	-5.128012000	-2.161555000	6.036255000
1	-5.502028000	-2.182972000	7.070251000
1	-4.485924000	-1.276901000	5.913517000
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6	3.777847000	3.013662000	-0.672837000
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6	5.781247000	3.249180000	2.599043000
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6	5.369285000	-1.511918000	2.532472000
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6	5.177214000	-3.712023000	1.994668000
6	4.658435000	-2.865895000	0.943690000
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6	3.471035000	-2.565220000	-1.244784000
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1	1.613328000	-2.807648000	-4.892482000	1	-2.943911000	-5.742975000	-2.636318000	6	3.051451000	-2.947150000	-2.559336000
6	2.839834000	-1.080280000	-5.420874000	1	-4.204326000	-5.682776000	-1.402524000	6	2.381702000	-1.872458000	-3.126779000
1	2.439347000	-0.986032000	-6.441015000	6	-2.216291000	-6.119083000	-0.617951000	6	2.479195000	-0.785644000	-2.165411000
1	3.783662000	-1.642648000	-5.458412000	1	-2.343940000	-7.209002000	-0.693982000	6	1.804206000	0.507198000	-2.239753000
1	3.065950000	-0.077258000	-5.033334000	1	-2.434228000	-5.809115000	0.414057000	6	1.273714000	3.528098000	-3.395278000
6	0.437497000	0.563005000	-2.461003000	1	-1.170186000	-5.859805000	-0.825638000	1	0.219053000	3.358586000	-3.130942000
1	-0.021091000	1.542443000	-2.389818000	6	-5.910542000	-4.744904000	2.969937000	1	1.374434000	4.616596000	-3.507729000
26	4.084176000	0.108303000	0.256563000	1	-6.179654000	-5.276965000	2.044209000	6	1.597563000	2.847434000	-4.744797000
17	6.088816000	0.011979000	-2.456605000	1	-6.748307000	-4.872941000	3.670941000	1	0.932186000	3.228857000	-5.532414000
8	2.280438000	0.199559000	1.476689000	6	-4.629683000	-5.375640000	3.573746000	1	1.470335000	1.759057000	-4.682606000
1	1.589860000	-0.395280000	1.088598000	1	-4.780520000	-6.449236000	3.758253000	1	2.638610000	3.050283000	-5.034979000
1	1.904790000	1.107192000	1.419941000	1	-4.374612000	-4.887324000	4.525209000	6	3.160621000	5.400644000	-1.614431000
8	5.936214000	0.215520000	-0.910349000	1	-3.776657000	-5.252087000	2.890606000	1	2.943508000	5.742768000	-2.636976000
8	7.472743000	0.464866000	-2.791940000	6	-6.616222000	-2.211155000	5.683781000	1	4.203272000	5.683289000	-1.402410000
8	5.062719000	0.842015000	-3.164585000	1	-7.159685000	-3.153993000	5.025830000	6	2.214513000	6.118812000	-0.619021000
8	5.900764000	-1.440165000	-2.763553000	1	-7.352517000	-1.396099000	4.953681000	1	2.341358000	7.208808000	-0.695350000
17	0.188206000	-2.806866000	0.804205000	6	-5.537433000	-2.043315000	5.968845000	1	2.432350000	5.809288000	0.413172000
8	0.367525000	-1.381925000	0.289986000	1	-6.003356000	-2.036873000	6.964937000	1	1.168648000	5.858626000	-0.826960000
8	1.220061000	-3.100411000	1.851839000	1	-4.987656000	-1.100654000	5.832409000	6	5.907648000	4.746378000	2.971072000
8	0.314743000	-3.760219000	-0.345622000	1	-4.812036000	-2.868420000	5.924817000	1	6.176965000	5.278778000	2.045551000
8	-1.206446000	-2.895075000	1.404559000	6	-6.223599000	3.205683000	4.322948000	1	6.744735000	4.875122000	3.672800000
17	-0.188012000	2.807055000	0.804201000	1	-5.958840000	4.242591000	4.574851000	6	4.625540000	5.375595000	3.573877000
8	-0.367135000	1.382290000	0.289462000	1	-5.821952000	2.567407000	5.125517000	1	4.774998000	6.449340000	3.758662000
8	-1.219680000	3.099965000	1.852204000	6	-7.765731000	3.061773000	4.271813000	1	4.370188000	4.886765000	4.520340000
8	-0.315007000	3.760857000	-0.345199000	1	-8.208461000	3.331189000	5.241778000	1	3.773280000	5.251101000	2.889878000
8	1.206777000	2.895320000	1.404271000	1	-8.051845000	2.027465000	4.030999000	6	6.613149000	2.212646000	4.870803000
				1	-8.186285000	3.719736000	3.497611000	1	7.155566000	3.155983000	5.028715000
				6	-5.161677000	5.175016000	1.966489000	1	7.350139000	1.398208000	4.956194000
				1	-5.884084000	5.566349000	2.697051000	6	5.533256000	2.043345000	5.969566000
				1	-5.483127000	5.533380000	0.975392000	1	5.998080000	2.036766000	6.966174000
				6	-3.746713000	5.725332000	2.279463000	1	4.984431000	1.100246000	5.831935000
				1	-3.738108000	6.822859000	2.206999000	1	4.807187000	2.867867000	5.925106000
				1	-3.003943000	5.314917000	1.581241000	6	6.223646000	-3.204479000	4.324564000
				1	-3.442108000	5.437035000	3.296039000	1	5.959288000	-4.241479000	4.576532000
				6	-3.260809000	4.316128000	-3.132583000	1	5.821248000	-2.566211000	5.126814000
				1	-4.285026000	4.648070000	-2.903327000	6	7.765720000	-3.059698000	4.274157000
				1	-3.177827000	4.266942000	-4.227632000	1	8.208127000	-3.328736000	5.244384000
				6	-2.250281000	5.354585000	-2.582009000	1	8.051297000	-2.025213000	4.033370000
				1	-2.478689000	6.351564000	-2.986290000	1	8.187065000	-3.717483000	3.500210000
				1	-1.224698000	5.084559000	-2.866687000	6	5.161960000	-5.174642000	1.968151000
				1	-2.287866000	5.395469000	-1.485466000	1	5.883524000	-5.565926000	2.699546000
				6	-1.869467000	1.765865000	-4.535969000	1	5.484427000	-5.533110000	0.977425000
				1	-0.924240000	1.209168000	-4.572097000	6	3.746652000	-5.724873000	2.279946000
				1	-1.660801000	2.772701000	-4.924383000	1	3.737966000	-6.822387000	2.207285000
				6	-2.909690000	1.057858000	-5.439448000	1	3.004315000	-5.314170000	1.581404000
				1	-2.527655000	0.970728000	-6.467315000	1	3.441452000	-5.436717000	3.296391000
				1	-3.851865000	1.624146000	-5.455831000	6	3.261497000	-4.317132000	-3.131201000
				1	-3.131596000	0.052601000	-5.055500000	1	4.285496000	-4.649382000	-2.901346000
				6	-0.423272000	-0.560007000	-2.507025000	1	3.179057000	-4.268271000	-4.226315000
				1	0.042829000	-1.535186000	-2.431582000	6	2.250241000	-5.355093000	-2.580995000
				7	3.387720000	1.734646000	-0.833043000	1	2.478496000	-6.352213000	-2.985011000

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26	-4.091024000	-0.126371000	0.241851000
17	-6.148680000	-0.017052000	-2.426265000
8	-2.275263000	-0.212831000	1.451026000
1	-1.590149000	0.385489000	1.059192000
1	-1.894535000	-1.117941000	1.392348000
8	-5.970315000	-0.229038000	-0.884664000
8	-7.529389000	-0.490697000	-2.747292000
8	-5.118140000	-0.822379000	-3.154886000
8	-5.991226000	1.441492000	-2.722435000
7	-3.386812000	-1.734884000	-0.832321000
7	-4.975691000	-1.375193000	1.595512000
7	-4.772386000	1.501180000	1.297721000
7	-3.218337000	1.151139000	-1.099156000
6	-2.434949000	-1.728074000	-1.806006000
6	-2.174319000	-3.089723000	-2.272932000
6	-3.023103000	-3.908070000	-1.545666000
6	-3.727739000	-3.052933000	-0.608630000
6	-4.524879000	-3.506420000	0.450566000
1	-4.677475000	-4.582526000	0.509914000
6	-5.060700000	-2.745811000	1.501929000
6	-5.719073000	-3.286134000	2.681843000
6	-6.012846000	-2.205860000	3.496465000

1	1.224934000	-5.084637000	-2.866293000
1	2.287160000	-5.395838000	-1.484415000
6	1.870228000	-1.767081000	-4.535434000
1	0.924418000	-1.211351000	-4.571747000
1	1.662771000	-2.774016000	-4.924207000
6	2.910650000	-1.057624000	-5.438271000
1	2.528068000	-0.969862000	-6.466099000
1	3.852647000	-1.623230000	-5.455048000
1	3.131256000	-0.052505000	-5.053430000
6	0.423572000	0.559056000	-2.507303000
1	-0.042354000	1.534371000	-2.432382000
26	4.092350000	0.126410000	0.241482000
17	6.149837000	0.016812000	-2.426590000
8	2.276025000	0.212825000	1.450938000
1	1.590680000	-0.384981000	1.058548000
1	1.895888000	1.118328000	1.392365000
8	5.972212000	0.229464000	-0.884891000
8	7.531129000	0.488856000	-2.747872000
8	5.120080000	0.823160000	-3.155136000
8	5.990659000	-1.441679000	-2.722463000
17	0.212127000	-2.805636000	0.801047000
8	0.381497000	-1.389606000	0.261182000
1	1.219714000	-3.059914000	1.882050000
8	0.384993000	-3.781825000	-0.323680000
8	-1.197011000	-2.905437000	1.366178000
17	-0.212542000	2.804922000	0.800431000
8	-0.380832000	1.388624000	0.260903000
8	-1.220311000	3.058505000	1.881588000
8	-0.386477000	3.780849000	-0.324477000
8	1.196609000	2.905948000	1.365390000

⁹*trans*-2 (without counteranion)

{UB3LYP}(U form)

26	-4.545474000	-0.125817000	0.4411762000
17	-6.252310000	-0.805976000	-2.355448000
8	-2.919449000	0.331809000	2.004200000
8	-6.209063000	-0.636089000	-0.804516000
8	-5.014084000	-1.507855000	-2.783904000
8	-6.328548000	0.548399000	-2.954600000
8	-7.458293000	-1.606720000	-2.646396000
7	-3.565656000	0.864060000	-0.948641000
7	-5.423373000	1.549032000	1.024107000
7	-5.479592000	-1.111844000	1.873395000
7	-3.574553000	-1.782962000	-0.099937000
6	-2.569514000	0.401401000	-1.752958000
6	-2.417832000	1.243523000	-2.929689000
6	-3.291726000	2.295515000	-2.761854000
6	-3.975007000	2.069907000	-1.502891000
6	-4.815825000	2.969076000	-0.874775000
1	-4.974634000	3.927408000	-1.352720000
6	-5.428046000	2.748192000	0.357403000
6	-6.171059000	3.755951000	1.107915000
6	-6.604589000	3.142584000	2.251043000
6	-6.157150000	1.751581000	2.168085000
6	-6.510647000	0.759779000	3.070406000
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6	-6.255799000	-0.594709000	2.877934000
6	-6.867756000	-1.668202000	3.661762000
6	-6.496430000	-2.841842000	3.063272000
6	-5.612399000	-2.478721000	1.958597000
6	-4.959317000	-3.389962000	1.138550000
1	-5.174315000	-4.439883000	1.288576000
6	-3.988607000	-3.064629000	0.202417000
6	-3.183509000	-4.034983000	-0.518011000
6	-2.222680000	-3.326422000	-1.195987000
6	-2.492432000	-1.914993000	-0.918772000
6	-1.784640000	-0.772209000	-1.434935000
6	-1.636848000	0.923777000	-4.175512000
1	-1.209293000	1.845109000	-4.584366000
1	-0.794159000	0.271636000	-3.944201000
6	-2.510984000	0.246271000	-5.251888000

1	-1.897482000	-0.018742000	-6.117940000
1	-3.309257000	0.910595000	-5.592426000
1	-2.979370000	-0.663000000	-4.865357000
6	-3.552154000	3.452156000	-3.680409000
6	-6.356392000	5.183871000	0.684513000
1	-7.226369000	5.597730000	1.202196000
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6	-5.125646000	6.068873000	0.970729000
1	-5.315118000	7.094417000	0.641995000
1	-4.237214000	5.704102000	0.445761000
1	-4.899358000	6.090157000	2.040827000
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1	-7.262411000	4.793574000	3.414266000
1	-7.104280000	3.305719000	4.320818000
6	-8.947821000	3.452318000	3.180995000
1	-9.505472000	3.885372000	4.016021000
1	-9.167495000	2.381271000	3.142670000
1	-9.315322000	3.901257000	2.253910000
6	-7.734650000	-1.461402000	4.867928000
1	-8.445453000	-0.649456000	4.675401000
1	-8.338079000	-2.359048000	5.030309000
6	-6.933506000	-1.149468000	6.149011000
1	-7.615255000	-1.001237000	6.990922000
1	-6.331408000	-0.242250000	6.037356000
1	-6.257624000	-1.972465000	6.398972000
6	-6.868050000	-4.245995000	3.438924000
1	-7.828235000	-4.229428000	3.963126000
1	-7.031473000	-4.835133000	2.529388000
6	-5.818674000	-4.945929000	4.326841000
1	-6.144792000	-5.962674000	4.562525000
1	-5.678098000	-4.406715000	5.268032000
1	-4.847380000	-5.009370000	3.826449000
6	-3.383566000	-5.522442000	-0.472992000
1	-3.078965000	-5.953812000	-1.431066000
1	-4.450104000	-5.748256000	-0.370879000
6	-2.597878000	-6.203886000	0.666665000
1	-2.778348000	-7.282212000	0.656357000
1	-2.899736000	-5.818535000	1.645757000
1	-1.522084000	-6.036879000	0.556154000
6	-1.245415000	-3.918076000	-2.176927000
1	-1.146509000	-4.983835000	-1.952753000
1	-0.241740000	-3.503269000	-2.054408000
6	-1.699008000	-3.752486000	-3.641945000
1	-0.985963000	-4.238206000	-4.314353000
1	-1.770469000	-2.698631000	-3.924538000
1	-2.680579000	-4.208023000	-3.798326000
6	-0.384595000	-0.790346000	-1.545674000
1	0.115132000	-1.733637000	-1.363980000
6	-4.909343000	3.382219000	-4.412731000
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1	-2.207081000	0.905610000	1.689061000
1	-2.492913000	-0.462745000	2.354733000
7	3.649586000	-1.072977000	-0.796515000
7	5.504027000	-1.315503000	1.303503000
7	5.404228000	1.458716000	1.703874000
7	3.511690000	1.691979000	-0.383833000
6	2.638284000	-0.821605000	-1.664884000
6	2.513861000	-1.875142000	-2.643650000
6	3.459961000	-2.828487000	-2.301509000
6	4.130751000	-2.339710000	-1.126758000
6	5.026565000	-3.048514000	-0.359793000
1	5.261695000	-4.058277000	-0.675031000
6	5.619243000	-2.595664000	0.827503000
6	6.413495000	-3.405075000	1.712049000
6	6.769449000	-2.587839000	2.770264000
6	6.220598000	-1.288307000	2.479424000
6	6.474276000	-0.136061000	3.218436000
1	7.057592000	-0.248449000	4.124330000
6	6.140313000	1.152966000	2.831230000
6	6.614488000	2.358249000	3.467753000
6	6.195749000	3.407894000	2.670102000

6	5.437497000	2.819408000	1.596676000
6	4.776758000	3.549941000	0.592564000
1	4.947447000	4.619636000	0.570805000
6	3.875421000	3.036034000	-0.305663000
6	3.072208000	3.813627000	-1.217259000
6	2.166713000	2.945244000	-1.792008000
6	2.480156000	1.634172000	-1.255421000
6	1.828134000	0.377722000	-1.576892000
6	1.699595000	-1.846407000	-3.910891000
1	1.307050000	-2.847897000	-4.118922000
1	0.831207000	-1.197378000	-3.792568000
6	2.516919000	-1.359084000	-5.124708000
1	1.874174000	-1.281718000	-6.006929000
1	3.330505000	-2.049733000	-5.359372000
1	2.961778000	-0.378980000	-4.930564000
6	3.782566000	-4.112428000	-3.009633000
6	6.742144000	-4.859744000	1.525508000
1	7.698987000	-5.072303000	2.012552000
1	6.896592000	-5.073536000	0.462111000
6	5.664335000	-5.806612000	2.089724000
1	5.957210000	-6.849947000	1.940312000
1	4.700349000	-5.650303000	1.594842000
1	5.520414000	-5.644177000	3.162411000
6	7.626222000	-2.941558000	3.952897000
1	7.472453000	-3.997592000	4.198120000
1	7.298467000	-2.378979000	4.834171000
6	9.128987000	-2.690545000	3.711697000
1	9.707280000	-2.968037000	4.597858000
1	9.325356000	-1.637013000	3.490962000
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6	7.402765000	2.422000000	4.743948000
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6	6.522330000	2.344402000	6.007960000
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1	5.806599000	3.171361000	6.039212000
6	6.433210000	4.878277000	2.867921000
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1	6.622741000	5.354570000	1.899438000
6	5.271594000	5.603447000	3.575839000
1	5.503001000	6.665797000	3.695842000
1	5.089276000	5.181255000	4.568775000
1	4.343195000	5.521910000	3.000919000
6	3.203961000	5.292657000	-1.444632000
1	2.968468000	5.517022000	-2.489533000
1	4.245674000	5.597274000	-1.303766000
6	2.292730000	6.132195000	-0.525970000
1	2.421681000	7.197689000	-0.736108000
1	2.529112000	5.963469000	0.529516000
1	1.238820000	5.880095000	-0.679276000
6	1.216672000	3.305105000	-2.906219000
1	1.089874000	4.391716000	-2.905439000
1	0.214249000	2.900379000	-2.738747000
6	1.723864000	2.861351000	-4.292411000
1	1.037804000	3.197646000	-5.075828000
1	1.808104000	1.773229000	-4.357361000
1	2.710757000	3.284510000	-4.498514000
6	0.431763000	0.355698000	-1.650706000
1	-0.071040000	1.315344000	-1.611405000
6	5.109440000	-4.077389000	-3.797497000
1	5.271339000	-5.037414000	-4.296026000
1	5.960265000	-3.882254000	-3.139784000
1	5.099048000	-3.292172000	

1	3.825438000	-4.928708000	-2.277364000
1	2.962754000	-4.361398000	-3.690206000
1	-3.504620000	4.385153000	-3.103962000
1	-2.745072000	3.510509000	-4.416270000

⁹*trans*-2 (without counteranion)

{UB97D} (U form)

26	-4.658322000	-0.116302000	0.444423000
17	-6.085479000	-0.659260000	-2.531608000
8	-2.972774000	0.218873000	2.021094000
1	-2.285419000	0.720580000	1.553996000
1	-2.594238000	-0.666322000	2.149399000
8	-6.239212000	-0.557347000	-0.967336000
8	-7.292230000	-1.393532000	-3.009732000
8	-4.830210000	-1.411324000	-2.851945000
8	-6.027330000	0.729359000	-3.081395000
7	-3.655266000	-1.747063000	-0.148866000
7	-5.610161000	-1.193491000	1.803171000
7	-5.555975000	1.516937000	1.103424000
7	-3.640722000	0.973737000	-0.865189000
6	-2.580830000	-1.830582000	-0.967750000
6	-2.295858000	-3.201795000	-1.341765000
6	-3.279567000	-3.968172000	-0.734961000
6	-4.087394000	-3.064057000	0.046979000
6	-5.053583000	-3.435294000	0.956449000
1	-5.276844000	-4.495855000	1.051230000
6	-5.705132000	-2.561451000	1.850224000
6	-6.498925000	-2.991282000	2.974723000
6	-6.877563000	-1.836492000	3.647549000
6	-6.343397000	-0.731414000	2.885517000
6	-6.617221000	0.611729000	3.126999000
1	-7.211784000	0.852676000	4.005890000
6	-6.290709000	1.661270000	2.266267000
6	-6.782656000	3.011469000	2.396133000
6	-6.385884000	3.682232000	1.246537000
6	-5.610482000	2.741558000	0.477807000
6	-4.958608000	3.040745000	-0.730812000
1	-5.151051000	4.015512000	-1.174683000
6	-4.040209000	2.221918000	-1.357084000
6	-3.280760000	2.552936000	-2.531908000
6	-2.359010000	1.527035000	-2.713449000
6	-2.601931000	0.584531000	-1.649796000
6	-1.862331000	-0.639592000	-1.393239000
6	-1.306248000	-3.709917000	-2.356668000
1	-0.280707000	-3.376722000	-2.146602000
1	-1.283722000	-4.806324000	-2.289636000
6	-1.701756000	-3.294771000	-3.792891000
1	-1.005015000	-3.729676000	-4.523285000
1	-1.681491000	-2.203109000	-3.903246000
1	-2.718503000	-3.641302000	-4.023030000
6	-3.452116000	-5.456672000	-0.806865000
1	-3.220515000	-5.795425000	-1.827334000
1	-4.501201000	-5.723801000	-0.616286000
6	-2.531767000	-6.190438000	0.199929000
1	-2.666993000	-7.277953000	0.115507000
1	-2.765008000	-5.887971000	1.231188000
1	-1.476452000	-5.951997000	0.002401000
6	-6.750041000	-4.419566000	3.359701000
1	-6.985353000	-5.012721000	2.462402000
1	-7.631120000	-4.467040000	4.014882000
6	-5.530656000	-5.042939000	4.084143000
1	-5.741780000	-6.086110000	4.358879000
1	-5.294927000	-4.479823000	4.998762000
1	-4.643095000	-5.025781000	3.434145000
6	-7.643915000	-1.720075000	4.931109000
1	-8.244974000	-2.62896000	5.075535000
1	-8.348011000	-0.876167000	4.873315000
6	-6.703485000	-1.523923000	6.147123000
1	-7.291485000	-1.438595000	7.071958000
1	-6.101069000	-0.611069000	6.029425000
1	-6.017989000	-2.377915000	6.245644000

6	-7.645543000	3.524526000	3.511095000
1	-7.509326000	4.611794000	3.599522000
1	-7.325012000	3.083013000	4.466902000
6	-9.143098000	3.208440000	3.267521000
1	-9.752941000	3.589264000	4.099145000
1	-9.301730000	2.123478000	3.182645000
1	-9.487910000	3.677288000	2.334768000
6	-6.621697000	5.119817000	0.887347000
1	-7.503982000	5.484700000	1.431500000
1	-6.851007000	5.203799000	-0.185948000
6	-5.396906000	6.005898000	1.226020000
1	-5.591293000	7.050694000	0.945050000
1	-4.505126000	5.657865000	0.683786000
1	-5.178306000	5.966560000	2.303010000
6	-3.440578000	3.792101000	-3.359671000
1	-4.495683000	4.100713000	-3.368979000
1	-3.162388000	3.567368000	-4.398989000
6	-2.561376000	4.953497000	-2.829713000
1	-2.702683000	5.849050000	-3.450899000
1	-1.498413000	4.676171000	-2.852827000
1	-2.827708000	5.201823000	-1.791892000
6	-1.512773000	1.332547000	-3.941735000
1	-0.593029000	0.778544000	-3.722233000
1	-1.199980000	2.313962000	-4.322966000
6	-2.317752000	0.584314000	-5.032084000
1	-1.689593000	0.408983000	-5.917271000
1	-3.196384000	1.173786000	-5.330313000
1	-2.679959000	-0.380642000	-4.652218000
6	-0.475453000	-0.681233000	-1.424497000
1	0.005485000	-1.638377000	-1.241186000
7	3.477286000	1.749532000	-0.255567000
7	5.741782000	1.455768000	1.570395000
7	5.746567000	-1.413240000	1.126187000
7	3.507719000	-1.137991000	-0.703735000
6	2.428706000	1.709303000	-1.102790000
6	2.084449000	3.038837000	-1.585493000
6	2.991895000	3.902871000	-0.988534000
6	3.840255000	3.097070000	-1.135801000
6	4.829417000	3.572586000	0.709250000
1	4.961636000	4.653158000	0.739451000
6	5.670235000	2.821689000	1.570668000
6	6.554245000	3.381339000	2.568773000
6	7.165663000	2.299958000	3.198638000
6	6.653752000	1.109300000	2.552856000
6	7.058703000	-0.203420000	2.823022000
1	7.793939000	-0.326813000	3.617166000
6	6.665064000	-1.375517000	2.155500000
6	7.202753000	-2.697567000	2.395661000
6	6.606708000	-3.538670000	1.460086000
6	5.696153000	-2.715672000	0.696661000
6	4.866720000	-3.166146000	-0.356675000
1	5.008722000	-4.199084000	-0.672461000
6	3.888890000	-2.445266000	-1.029776000
6	3.109046000	-2.911940000	-2.150407000
6	2.233409000	-1.881665000	-2.484368000
6	2.492083000	-0.816232000	-1.539766000
6	1.758811000	0.445383000	-1.424984000
6	1.121456000	3.409892000	-2.681548000
1	0.100746000	3.057256000	-2.477807000
1	1.054279000	4.505604000	-2.725656000
6	1.589408000	2.870903000	-4.053979000
1	0.898426000	3.190525000	-4.846802000
1	1.631368000	1.773938000	-4.050646000
1	2.594763000	3.247381000	-4.286247000
6	3.077417000	5.392230000	-1.146842000
1	2.814717000	5.663423000	-2.179448000
1	4.112352000	5.726500000	-0.986682000
6	2.132752000	6.127399000	-0.163094000
1	2.216407000	7.215196000	-0.297118000
1	2.390243000	5.882218000	0.877946000
1	1.080666000	5.831623000	-0.338792000
6	6.691238000	4.842132000	2.879257000
1	6.785238000	5.412300000	1.941552000

1	7.616063000	5.009064000	3.448920000
6	5.481259000	5.378268000	3.686038000
1	5.605848000	6.450927000	3.891520000
1	5.389606000	4.845838000	4.643659000
1	4.545047000	5.236682000	3.125079000
6	8.122082000	2.318964000	4.352543000
1	8.620838000	3.297245000	4.397196000
1	8.908250000	1.563998000	4.197598000
6	7.402362000	2.042890000	5.697459000
1	8.125874000	2.057412000	6.524919000
1	6.910090000	1.059331000	5.678864000
1	6.635278000	2.806988000	5.888455000
6	8.263924000	-3.041874000	3.397951000
1	8.203443000	-4.113660000	3.634512000
1	8.082017000	-2.495000000	4.336005000
6	9.682640000	-2.706216000	2.871304000
1	10.439441000	-2.967971000	3.624490000
1	9.769067000	-1.633474000	2.644773000
1	9.894148000	-3.267384000	1.949767000
6	6.786741000	-5.019182000	1.302447000
1	7.751322000	-5.316113000	1.737161000
1	6.824560000	-5.277903000	0.232985000
6	5.642067000	-5.810577000	1.984006000
1	5.787818000	-6.891106000	1.843738000
1	4.668238000	-5.529993000	1.555144000
1	5.614926000	-5.596481000	3.062266000
6	3.227366000	-4.257946000	-2.800119000
1	4.287900000	-4.537421000	-2.886040000
1	2.825662000	-4.205315000	-3.821257000
6	2.466720000	-5.348298000	-2.001574000
1	2.568200000	-6.322491000	-2.500068000
1	1.397723000	-5.100400000	-1.931792000
1	2.865476000	-5.435677000	-0.980294000
6	1.416484000	-1.799374000	-3.743602000
1	0.5172228000	-1.189297000	-3.600939000
1	1.071743000	-2.803393000	-4.023681000
6	2.259509000	-1.198144000	-4.894917000
1	1.652585000	-1.120910000	-5.808567000
1	3.134176000	-1.831456000	-5.098934000
1	2.629350000	-0.199913000	-4.623712000
6	0.371088000	0.467601000	-1.478036000
1	-0.123707000	1.431734000	-1.396078000
26	4.712365000	0.178670000	0.350146000
17	5.778474000	0.408008000	-2.762616000
8	3.236823000	-0.086549000	2.118358000
1	2.673117000	-0.824405000	1.832587000
1	2.668511000	0.699729000	2.062146000
8	6.059823000	0.525848000	-1.199174000
8	6.974241000	1.001988000	-3.417722000
8	4.535328000	1.179551000	-3.072009000
8	5.616131000	-1.038238000	-3.088420000

⁹*trans*-2{UB3LYP} (P form)

26	5.068510000	0.045208000	-0.769529000
17	5.237042000	-0.618021000	-3.894566000
8	4.493933000	0.143461000	1.103224000
8	5.745935000	0.164711000	-2.613180000
8	3.779318000	-0.403252000	-4.027869000
8	5.567195000	-2.052123000	-3.738091000
8	5.990840000	0.002471000	-5.001636000
7	3.764382000	-1.438865000	-1.030808000
7	6.469572000	-1.277951000	-0.274732000
7	6.361551000	1.542576000	-0.467842000
7	3.664677000	1.354217000	-1.244305000
6	2.418930000	1.338920000	-1.171067000
6	1.829851000	-2.665884000	-1.440276000
6	2.867041000	-3.555006000	-1.420570000
6	4.065366000	-2.789929000	-1.108884000
6	5.283252000	-3.347053000	-0.810083000
1	5.373346000	-4.423832000	-0.868857000
6	6.403413000	-2.631812000	-0.359991000
6	7.630574000	-3.255031000	0.121928000

6	8.441101000	-2.235074000	0.531574000	7	-3.532188000	-1.370973000	0.827983000	6	0.329270000	2.694220000	3.006680000
6	7.716373000	-0.994442000	0.255897000	7	-6.397890000	-1.429746000	0.320504000	1	1.378499000	2.983552000	3.118807000
6	8.231509000	0.263251000	0.451946000	7	-6.496425000	1.447905000	0.589032000	1	0.246643000	1.026105000	3.229302000
1	9.218280000	0.338791000	0.888008000	7	-3.603666000	1.490260000	1.126884000	1	-0.256592000	3.229672000	3.759451000
6	7.607135000	1.457163000	0.056486000	6	-2.211795000	-1.160533000	1.038900000	6	-0.124869000	0.130990000	0.553747000
6	8.268381000	2.763504000	0.064301000	6	-1.551261000	-2.419013000	1.390823000	1	0.630424000	0.378272000	1.295410000
6	7.404672000	3.632544000	-0.538461000	6	-2.516681000	-3.399428000	1.308419000	6	-2.770984000	-5.219726000	3.062200000
6	6.204671000	2.860890000	-0.858936000	6	-3.752990000	-2.741524000	0.931608000	1	-2.697482000	-6.300234000	3.218152000
6	5.061695000	3.368620000	-1.424682000	6	-4.948187000	-3.371240000	0.659474000	1	-3.793596000	-4.905033000	3.287237000
1	5.060149000	4.412052000	-1.711986000	1	-4.948419000	-4.453764000	0.709120000	1	-2.107553000	-4.725410000	3.772960000
6	3.853475000	2.663496000	-1.555584000	6	-6.183920000	-2.764984000	0.314590000	26	-5.015433000	0.038143000	0.754460000
6	2.601651000	3.291963000	-1.938083000	6	-7.389755000	-3.480973000	-0.072526000	17	-4.781451000	-0.651260000	4.009975000
6	1.620414000	2.356464000	-1.756759000	6	-8.347130000	-2.524012000	-0.313444000	8	-4.619884000	0.256651000	-1.373427000
6	2.300930000	1.121845000	-1.319024000	6	-7.722291000	-1.235655000	-0.041986000	8	-5.548637000	-0.017721000	2.806513000
6	1.693752000	-0.110487000	-1.096615000	6	-8.351214000	-0.009315000	-0.086792000	8	-3.359553000	-0.236601000	3.932878000
6	0.410536000	-2.992444000	-1.817905000	1	-9.391631000	-0.006967000	-0.386347000	8	-4.916939000	-2.124119000	3.907898000
1	0.273968000	-4.074248000	-1.725937000	6	-7.791391000	1.251229000	0.242873000	8	-5.474711000	-0.124782000	5.225805000
1	-0.296778000	-2.547646000	-1.114435000	6	-8.534125000	2.501078000	0.301831000	1	-4.981343000	-0.503520000	-1.879317000
6	0.049746000	-2.575050000	-3.257734000	6	-7.644627000	3.462984000	0.722930000	1	-5.153326000	0.978571000	-1.768268000
1	-0.989691000	-2.834291000	-3.480635000	6	-6.360464000	2.793384000	0.890632000	17	-7.042029000	0.090552000	-3.702154000
1	0.690302000	-3.082263000	-3.982399000	6	-5.171364000	3.393067000	1.247403000	17	6.385749000	0.053050000	3.820061000
1	0.171565000	-1.499014000	-3.413925000	1	-5.211104000	4.455726000	1.455589000	8	5.813871000	0.110436000	5.186914000
6	2.853360000	-5.030348000	-1.697745000	6	-3.880838000	2.802284000	1.312049000	8	5.816429000	-1.144045000	3.083118000
6	7.881743000	-4.734666000	0.193938000	6	-2.659961000	3.557145000	1.511585000	8	7.867371000	-0.058584000	3.867065000
1	8.961814000	-4.910710000	0.210847000	6	-1.616367000	2.672072000	1.369821000	8	5.999275000	1.303409000	3.056617000
1	7.514791000	-5.217816000	-0.719527000	6	-2.218602000	1.353400000	1.131429000	8	-6.568372000	1.348349000	-3.009681000
6	7.239437000	-5.403295000	1.426021000	6	-1.567119000	0.132490000	0.947279000	8	-8.493283000	-0.106673000	-3.430171000
1	7.454003000	-6.476308000	1.433164000	1	-0.160472000	-2.611592000	1.933169000	8	-6.260664000	-1.082784000	-3.144830000
1	6.152619000	-5.274273000	1.430519000	1	0.070608000	-3.681136000	1.923040000	8	-6.792773000	0.202673000	-5.161022000
1	7.627782000	-4.969173000	2.352013000	1	0.583244000	-2.135570000	1.291248000	1	3.499842000	-5.544288000	-0.976818000
6	9.821221000	-2.312823000	1.114824000	6	-0.003046000	-2.082584000	3.373705000	1	1.846911000	-5.425020900	-1.522095000
1	9.952960000	-3.292928000	1.583467000	1	1.017415000	-2.253335000	3.729591000	1	-3.009621000	-5.437966000	0.918804000
1	9.914971000	-1.577574000	1.922012000	1	-0.694601000	-2.585644000	4.055320000	1	-1.355052000	-5.184147000	1.421905000
6	10.938803000	-2.094442000	0.074115000	1	-0.209784000	-1.009952000	3.435000000				
1	11.920689000	-2.159436000	0.552383000	6	-2.384157000	-4.863264000	1.611516000				
1	10.856488000	-1.112887000	-0.402332000	6	-7.507754000	-4.971270000	-0.218461000				
1	10.891304000	-2.851449000	-0.714436000	1	-8.562007000	-5.255277000	-0.145659000				
6	9.620318000	3.033779000	0.656835000	1	-7.006384000	-5.465116000	0.622845000				
1	10.319871000	2.243587000	0.358251000	6	-6.928178000	-5.501702000	-1.545208000				
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1	-1.050406674	1.090193797	-4.525935221	1	-6.308491481	5.250212391	-1.912749056	6	7.280628982	1.635791283	0.987086547
1	0.461404829	0.210229637	-4.229360377	6	-3.149808118	5.481201858	1.409020803	6	7.787512734	3.005304311	1.077994938
1	0.513279267	1.882405524	-4.789811335	1	-2.440545253	5.813533532	2.174049775	6	6.923797090	3.784942951	0.355803112
6	0.318861472	-0.467580420	-0.044316774	1	-4.141231442	5.753804766	1.785290624	6	5.871618937	2.896066707	-0.125943834
1	-0.046311356	-1.439643428	0.257567856	6	-2.871912268	6.236773041	0.093797064	6	4.778627999	3.302949500	-0.889737544
6	3.186911148	-5.563159137	-3.038029272	1	-2.954302483	7.316720775	0.248934394	1	4.755375792	4.332030305	-1.224920663
1	3.280138955	-6.640235132	-3.205154232	1	-3.584182173	5.948925594	-0.685732333	6	3.688511642	2.504830276	-1.183803897
1	4.103954937	-5.077323235	-3.382826769	1	-1.865481637	6.021817326	-0.278703138	6	2.495231684	2.935848395	-1.886664433
1	2.363495796	-5.190972739	-3.654170690	6	-0.549774775	3.670784199	1.713559950	6	1.603512884	1.890036689	-1.827909682
1	4.771994583	-0.548166902	1.943725615	1	-0.556493844	4.764729931	1.698270918	6	2.266435486	0.838634797	-1.065134269
1	4.577536655	0.928428270	1.768794010	1	0.194821085	3.381903566	0.963125555	6	1.694694246	-0.437962249	-0.696630452
7	-3.452214797	-0.929189131	1.516484002	6	-0.084390132	3.197676836	3.103614194	6	0.753695313	-3.434911415	-1.647136870
7	-6.065842492	-1.405581712	0.630954730	1	0.898330864	3.618190082	3.338126510	1	0.808065164	-4.519505654	-1.770557176
7	-6.357652153	1.318777360	0.040974737	1	-0.005051438	2.108555666	3.153895759	1	-0.014570962	-3.275604727	-0.883374579
7	-3.726548215	1.793350105	0.938185404	1	-0.788146138	3.516736098	3.877753809	6	0.298611894	-2.813996829	-2.982222547
6	-2.153451714	-0.592797367	1.674456349	6	-0.388523110	0.656164845	0.416957356	1	-0.651519023	-3.257485369	-3.294068239
1	-1.453637282	-1.571860126	2.477201324	1	-0.028159288	1.629927232	0.112872530	1	1.036348223	-3.000280456	-3.767507106
6	-2.379157114	-2.561939085	2.760196050	6	-2.903403331	-3.741670810	4.959734589	1	0.158343844	-1.732975479	-2.904015446
6	-3.606369501	-2.177559511	2.17256359	1	-2.722712156	-4.666263005	5.165295941	6	3.426284847	-5.169671386	-1.521070053
6	-4.717888352	-2.971841269	1.948250589	1	-3.982951595	-3.615751962	4.841832930	6	8.250879331	-4.459361765	0.767624861
1	-4.695576048	-3.960904594	2.391310210	1	-2.541445939	-2.902775748	5.559945497	1	9.342671216	-4.497896653	0.823426576
6	-5.844606873	-2.640837841	1.180979440	26	-4.904376680	0.189532413	0.770287491	1	7.983065053	-4.897507245	-0.200131554
6	-6.898083944	-3.554633016	0.827959783	17	-5.096837472	0.738459781	4.147477786	6	7.651631817	-5.311485136	1.905692234
6	-7.766844288	-2.850397810	0.014609217	8	-4.088686676	-0.156802000	-1.247770425	1	7.994902801	-6.346231026	1.821325267
6	-7.249136321	-1.509687641	-0.064860636	8	-5.772687451	0.666511149	2.760101899	1	6.557720841	-5.312567939	1.872405535
6	-7.898846812	-0.439895159	-0.673941925	8	-3.772379992	1.401141428	4.009444340	1	7.957245913	-4.929670590	2.884277706
1	-8.816830641	-0.656227171	-1.204438169	8	-4.939561771	-0.646272501	4.661887863	6	9.789533780	-1.919096643	2.048426895
6	-7.512999708	0.889378603	-0.579472356	8	-6.000192022	1.533302440	5.014359488	1	9.995373358	-2.902331070	2.481897481
6	-8.307267241	2.016780874	-1.00592780	1	-4.279395261	-1.065869212	-1.562678879	1	9.759452170	-1.218460610	2.890748734
6	-7.637449602	3.146462379	-0.566785522	1	-4.559240240	0.357127127	-1.934169934	6	10.938082889	-1.530841777	1.093572747
6	-6.426656866	2.682364497	0.060215043	1	3.718466128	-5.742111378	-0.942655973	1	11.887982562	-1.516861443	1.635244548
6	-5.419599329	3.519366443	0.574831900	1	1.997147583	-5.758614776	-1.234424924	1	10.780035901	-0.540049460	0.656908476
1	-5.627877356	4.582491341	0.593983396	1	-2.560611855	-4.668917347	3.034427279	1	11.023302757	-2.247476198	0.942112446
6	-4.164112886	3.113363427	0.955817690	1	-1.121926080	-3.968349229	3.744418653	6	9.021133965	3.413498761	1.826209626
6	-3.056599113	3.988599297	1.263992311	17	6.591158493	0.280978820	3.832523759	1	9.819921201	2.685053871	1.645143920
6	-1.930840049	3.195843613	1.337189262	17	-5.938184302	-1.325064684	-3.824526055	1	9.383137771	4.364614595	1.425056202
6	-2.394477436	1.832549682	1.136564789	8	5.984670406	1.473232354	3.136428417	6	8.791439923	3.557556519	3.344944472
6	-1.597834309	0.622653738	1.115162390	8	6.034589284	-0.978280048	3.194950245	1	9.722335837	3.847984911	3.839590673
6	-0.070839198	-1.453206114	3.067121495	8	6.235977952	0.303558211	5.273048717	1	8.449854421	2.618316274	3.791004629
1	0.424692219	-2.430825701	3.031822362	8	8.071041829	0.298887284	3.655095560	1	8.040217996	4.324254468	3.555928272
1	0.547477130	-0.779561290	2.471787999	8	-5.173501782	-2.166690756	-2.826549845	6	6.981296696	5.263265548	0.104232060
6	-0.089271099	-0.944878141	4.522810361	8	-7.400360732	-1.565876713	-3.653662288	1	8.015694334	5.601012350	0.216317530
1	0.932808508	-0.826590114	4.895846459	8	-5.509866966	-1.678694847	-5.201521136	1	6.708577210	5.467611793	-0.937460743
1	-0.613038703	-1.641559247	5.182754595	8	-5.634082065	0.129388641	-3.557835872	6	6.075918768	6.085128992	1.044782133
1	-0.596684026	0.021798824	4.593702094					1	6.160807636	7.149916592	0.810898209
6	-2.192267231	-3.798123291	3.591974509					1	6.362749347	5.942488735	2.090754561
6	-6.977046238	-5.003196144	1.221338900					1	5.024333458	5.799063444	0.942113857
1	-8.025576878	-5.317726835	1.209810747					6	2.300319298	4.283449097	-2.517401914
1	-6.639713311	-5.127162852	2.257019793					1	1.597056371	4.191128909	-3.349492873
6	-6.159547083	-5.930558064	0.299956907					1	3.243251009	4.628923057	-2.954053029
1	-6.253126787	-6.971796959	0.623783573	26	5.007545415	0.018445647	-0.179421220	6	1.772256444	5.340496856	-1.523724549
1	-5.097896916	-5.664278136	0.310656182	17	5.361779571	-0.429876767	-3.474335242	1	1.647412905	6.301903912	-2.029412615
1	-6.507739521	-5.861164564	-0.734907917	8	4.078303482	0.039712408	1.925134671	1	2.462342487	5.484786240	-0.686928374
6	-9.026126541	-3.342896250	-0.639133397	8	5.918190345	0.099802132	-2.116056065	1	0.802726945	5.043421066	-1.111454556
1	-8.942806366	-4.423258875	-0.795931748	8	3.933193063	-0.035830939	-3.580037837	6	0.312386339	1.795901210	-2.599765453
1	-9.110732246	-2.900920474	-1.638008208	8	5.507523875	-1.905910562	-3.481410972	1	-0.209110926	2.757888054	-2.546011982

⁹*trans*-2 (without counteranion)

{UB3LYP} (P form)

1	-0.359451477	1.059497897	-2.157796297	1	-7.701531538	6.526605854	-1.690357623
6	0.555617458	1.420191872	-4.077001892	1	-7.645089599	5.144666909	-2.796245986
1	-0.398621117	1.346765412	-4.607359169	1	-6.290233437	5.456368787	-1.703481938
1	1.071716610	0.459458500	-4.155938579	6	-3.286819135	5.112809899	1.746974159
1	1.171110390	2.167518177	-4.584995048	1	-2.605432671	5.321530667	2.577437570
6	0.397264077	-0.570593709	-0.174458357	1	-4.291550902	5.318359943	2.129705849
1	0.028770413	-1.576279216	-0.034667830	6	-2.975324721	6.070110783	0.578063305
6	4.005229782	-5.365001572	-2.938329416	1	-3.070961830	7.109773470	0.904130207
1	4.150997334	-6.430294484	-3.138121969	1	-3.663016518	5.912230592	-0.258781135
1	4.967357599	-4.857875187	-3.050795896	1	-1.956655479	5.922406670	0.205731705
1	3.327186014	-4.963646887	-3.696553671	6	-0.717720769	3.260953687	1.972262319
1	4.502066311	-0.602067700	2.513684073	1	-0.708467507	4.350192843	2.070284641
1	4.204817301	0.902041465	2.346694493	1	0.105441869	3.031699556	1.287541736
7	-3.562529886	-1.236820065	0.774874124	6	-0.428045628	2.637009794	3.350783012
7	-6.107369306	-1.542724717	-0.370920988	1	0.529957759	2.998828303	3.737381225
7	-6.393692140	1.251115503	-0.460299888	1	-0.384160511	1.545714721	3.298889478
7	-3.813546040	1.550321246	0.653107862	1	-1.208559317	2.904148566	4.068539003
6	-2.295934895	-0.932828220	1.137341457	6	-0.407435429	0.477933653	0.300497642
6	-1.673806588	-2.030606333	1.843247942	1	-0.043465621	1.486583366	0.159783505
6	-2.597032416	-3.062216229	1.831634036	6	-3.352295215	-4.628132551	3.702465274
6	-3.751373804	-2.574103076	1.122812960	1	-3.204651202	-5.635909632	4.101347575
6	-4.827656785	-3.327294215	0.720997419	1	-4.413140609	-4.500781220	3.472509221
1	-4.826409667	-4.379614494	0.979720415	1	-3.100691849	-3.907525046	4.484510596
6	-5.907792859	-2.859261799	-0.042880108	26	-4.992627268	0.003823044	0.188936461
6	-6.950312045	-3.689835369	-0.580289834	17	-5.356356721	-0.099405104	3.532645595
6	-7.804461593	-2.845347094	-1.267501862	8	-4.048373217	0.032979452	-1.918548510
6	-7.280085305	-1.514981255	-1.097616846	8	-5.961924040	0.091766377	2.111329465
6	-7.917965986	-0.350627596	-1.512421799	8	-4.024064952	0.558648331	3.576413708
1	-8.837282495	-0.463941141	-2.074331466	8	-5.235486869	-1.555963022	3.784094151
6	-7.534101974	0.939712086	-1.175659399	8	-6.303081808	0.540866759	4.471285880
6	-8.321059717	2.124502586	-1.415436860	1	-4.282527075	-0.783469587	-2.383835332
6	-7.661866423	3.162704242	-0.781839716	1	-4.449600091	0.746843711	-2.435545247
6	-6.469868210	2.593436101	-0.209074328	1	4.084983213	-5.651463156	-0.789510548
6	-5.489272552	3.327140108	0.480240075	1	2.467590861	-5.689633558	-1.444884013
1	-5.701669165	4.372456674	0.669520707	1	-2.740354205	-5.184389795	1.702314891
6	-4.254479908	2.854723273	0.852882397	1	-1.426892188	-4.607821045	2.705690910
6	-3.175850613	3.662746590	1.370825726				
6	-2.055172376	2.859371656	1.400577431				
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6	-1.694420614	0.350525440	0.833756872				
6	-0.391264708	-1.999714024	2.636980007				
1	0.149634225	-2.943243123	2.496488024				
1	0.269940582	-1.211685828	2.273377191				
6	-0.642182389	-1.771737077	4.141508731				
1	0.308933691	-1.688162818	4.676739217				
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1	-1.216308419	-0.855408017	4.306435546				
6	-2.474890803	-4.425116414	2.449114548				
1	-7.045263430	-5.183279025	-0.441441318				
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1	-6.752889931	-5.480940762	0.571941714				
6	-6.187868967	-5.948288095	-1.469325969				
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1	-11.209475780	-3.466665331	-1.622802231				
1	-10.472486974	-2.191995207	-0.635259475				
1	-10.198148047	-3.890406839	-0.230731749				
6	-9.600575432	2.176364740	-2.199879117				
1	-10.231514154	1.319774944	-1.936129948				
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6	-9.384562792	2.199376209	-3.726694099				
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1	-8.847274526	1.308275504	-4.066592393				
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6	-8.055259753	4.611333004	-0.713882181				
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1	-7.820239489	5.009861661	0.279535434				
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