

Dependence between luminescent properties of Cu(I) complexes and electronic/structural parameters derived from steric effects

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S1. Benchmark study with other DFT functionals

A benchmark study was performed to test the reliability of the selected methodology. The absorption spectra and emission energies were determined for complex **B1** ([Cu(bathocuproine)(POP)]⁺) and was compared against the experimental data. The absorption spectra were obtained from the optimized geometry in the ground state using the TD-DFT methodology and the T₁ state was fully optimized through TD-DFT optimization with eight different DFT functionals: B3LYP [1], B3PW91 [2-5], BLYP [6], M06 [7], TPSSH [8], wB97XD [9], M06-2X [7] and PBE0 [10].

The benchmark study was carried out mainly to find the methodology that best reproduced the experimental luminescent properties for the **B1** complex. The emission energy was calculated as the vertical energy difference between the relaxed triplet state and ground state at the optimized triplet geometry. The implicit solvent effects by the IEF-PCM method were also included using dichloromethane as solvent. The basis set and pseudo-potential used are the same for all the methodologies as described in the manuscript.

Table S1. Emission wavelengths from the triplet excited states for the complex **B1**.

Functional	λ_{emi} (nm)
B3LYP	634
B3Pw91	643
BLYP	916
M06	692
TPSSH	768
wB97XD	726
M06-2X	555
PBE0	672
<i>Experimental</i>	<i>558 [11]</i>

According to the results obtained, it is observed that the functional M06-2X presents the smallest deviation (3 nm) with respect to the experimental emission energy of the **B1** complex, then, this functional was selected to describe the emission of the Cu(I) complexes studied. However, it overestimates the values of the MLCT band (270 to 310 nm) of the absorption spectrum, therefore, PBE0 functional was chosen to reproduce the absorption properties due to the MLCT band was determined in a range between 340 and 390 nm which is close to the experimental data (350-450 nm) [11]. The choice of two different functionals that allow describing the ground and the excited state is a strategy that has already been used previously in compounds with transition metals [12, 13].

S2. Energies of the molecular orbitals from HOMO-3 to LUMO+2, in the ground state.

Table S2. Energy of frontier molecular orbitals (eV) and H-L gaps of the ground state (S_0) obtained at the PBE0/6-31G(d,p)/LANL2DZ level of theory.

Orbital	A1	A2	A3	A4	B1	B2	B3	B4	B4-1	B4-2
L+2	-1.26	-1.23	-1.35	-1.27	-1.22	-1.23	-1.34	-1.27	-1.85	-1.27
L+1	-1.91	-1.91	-1.93	-1.99	-2.08	-2.02	-2.04	-2.10	-2.24	-2.05
L	-2.10	-2.09	-2.12	-2.17	-2.22	-2.17	-2.18	-2.24	-2.58	-2.19
H	-6.24	-6.23	-6.35	-6.36	-6.24	-6.20	-6.32	-6.32	-6.19	-5.47
H-1	-6.88	-6.90	-6.75	-6.78	-6.86	-6.85	-6.74	-6.77	-6.52	-5.52
H-2	-6.90	-6.98	-6.85	-6.88	-6.90	-6.88	-6.80	-6.80	-6.61	-6.30
H-3	-7.07	-7.02	-7.06	-7.05	-6.93	-6.98	-6.87	-6.94	-6.78	-6.70
Δ H-L	4.14	4.14	4.19	4.19	4.02	4.03	4.08	4.08	3.61	3.28

S3. Contribution to molecular orbitals from HOMO-3 to LUMO+2

Table S3. Contribution to molecular orbitals (%) of all complexes calculated from HOMO-3 to LUMO+2 in the ground state (S_0), obtained at the PBE0/6-31G(d,p)/LANL2DZ level of theory.

Orbital	A1			A2			A3			A4		
	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>
L+2	1	99	0	1	98	1	0	99	1	0	99	1
L+1	0	1	99	0	1	99	0	1	99	0	1	99
L	2	1	97	2	1	97	2	2	96	2	1	97
H	33	61	6	35	59	6	34	58	8	34	59	7
H-1	40	51	9	58	16	26	42	47	11	37	53	10
H-2	61	13	26	45	45	10	61	13	26	57	11	32
H-3	8	55	37	9	74	17	1	13	86	4	15	81

Orbital	B1			B2			B3			B4		
	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>
L+2	1	99	1	1	98	1	0	99	1	0	99	1
L+1	0	1	99	0	0	100	0	1	99	0	1	99
L	2	2	96	2	1	97	2	2	96	2	2	96
H	34	54	12	34	57	9	33	52	15	33	54	13
H-1	31	12	57	34	8	58	44	42	14	38	51	11
H-2	34	15	51	29	13	58	56	17	27	43	11	46
H-3	41	50	9	46	44	10	4	14	82	18	11	71

Orbital	B4-1			B4-2		
	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>	<i>Cu</i>	<i>P^P</i>	<i>N^N</i>
L+2	0	2	98	0	99	1
L+1	2	1	96	0	1	99
L	0	1	99	2	2	96
H	18	26	56	0	0	100
H-1	18	36	46	0	0	100
H-2	0	4	96	33	53	14
H-3	40	48	12	38	52	10

S4. Simulated electronic absorption spectra

The results show a good agreement with the experimental absorption spectra of the complexes **A1**, **A2**, **A4** and **B1** [11, 14]. The analysis of the absorptions was focused on MLCT bands, since these allowed electronic transitions are responsible of the optical properties of Cu(I) complexes, therefore, for the emission processes. Table S4 shows the properties of the first allowed singlet transitions between 350-500 nm for all complexes, namely, the calculated absorption energies, oscillator strength, main contributions of the electronic transitions and their assignments.

According to the compositions of the molecular orbitals, **A1** and **A4** have ¹MLCT, ¹LLCT (singlet ligand-to-ligand charge transfer) and ¹ILCT (singlet intraligand charge transfer) mixed characters, where the electron is promoted from both the metal center and POP ligand to phenanthroline-based skeleton, and from π to π^* orbitals of the N[^]N ligand, these absorption bands are located at higher energy than the other complexes (between 320 and 370 nm). For **A2** and **A3** are characterized by a ¹MLCT and ¹LLCT, due to the contributions of the S₁, S₂ and S₃ excited states. In agreement with the largest Δ_{H-L} observed for the series **A**.

In series **B**, different allowed singlet–singlet transitions are observed, such as ¹MLCT and ¹LLCT for the complexes **B1** and **B2**, mainly due to the HOMO→LUMO and HOMO→LUMO+1 transitions associated to electron promotions from metal/P[^]P ligand moieties toward the N[^]N ligand. For the **B4** complex, transitions with mixed character ¹MLCT/¹LLCT/¹ILCT were observed, these transitions involve the orbitals from HOMO-1 to LUMO+1. The **B4-2** complex have a mixed contribution of ¹MLCT, ¹ILCT and ¹LLCT

transitions. The presence of electron-withdrawing groups (phenyl substituents) on N[^]N ligand produces a slight redshift of the MLCT band (between 340 to 380 nm) with respect to the series **A**, caused by the energy stabilization of the LUMO orbital. On the other hand, the destabilization of the HOMO orbital due to the presence of an electron-donor amino group in the **B4** complex considerably reduces the H-L energy gap, shifting the MLCT band even more red-shifted.

Finally, the absorptions for **B4-1** are more displaced at lower energy compared to the other complexes due to the presence of double bond chains in the N[^]N ligand, which stabilizes the LUMO energy and significantly reduces the H-L gap. The use of ligands with extended π systems to lower the energy of the π^* level is a strategy commonly used in solar cell design to improve the redshift in the ¹MLCT band [15]. Singlet-singlet transitions with mixed character ¹MLCT, ¹LLCT and ¹ILCT are observed.

Table S4. Properties of the computed low-lying singlet-singlet transitions of all complexes: absorption energies (E_{abs} , in eV) and absorption wavelengths (λ_{abs} , in nm); oscillator strength (f); monoexcitations with weighting coefficients and percentage of contribution to the excited state wavefunction; and character of the excited state based on monoexcitations. Values are in dichloromethane as solvent. Determined at the PBE0/6-31G(d)/LANL2DZ level of theory.

<i>system</i>	<i>state</i>	E_{abs} (λ_{abs})	f	<i>monoexcitations</i>	<i>Description</i>
A1	S ₁	3.33 (372)	0.071	H→L (0.97, 95%)	Cu(d)+ P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
	S ₂	3.58 (346)	0.016	H→L+1 (0.98, 96%)	Cu(d)+ P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
	S ₄	3.85 (322)	0.010	H-1→L (0.87, 76%)	Cu(d)+P [^] P(π)+N [^] N→N [^] N (π^*); ¹ MLCT/ ¹ LLCT/ ¹ ILCT
A2	S ₁	3.32 (374)	0.063	H→L (0.98, 95%)	Cu(d)+P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
	S ₂	3.57 (347)	0.016	H→L+1 (0.98, 96%)	Cu(d)+ P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
A3	S ₁	3.40 (365)	0.070	H→L (0.98, 95%)	Cu(d)+P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
	S ₃	3.65 (339)	0.021	H→L+1 (0.98, 96%)	Cu(d)+P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
A4	S ₁	3.35 (370)	0.061	H→L (0.97, 95%)	Cu(d)+P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
	S ₃	3.60 (344)	0.021	H→L+1 (0.97, 95%)	Cu(d)+P [^] P(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT
	S ₄	3.68 (337)	0.016	H-1→L (0.88, 77%)	Cu(d)+P [^] P(π)+N [^] N(π)→N [^] N (π^*); ¹ MLCT/ ¹ LLCT/ ¹ ILCT

B1	S ₁	3.21 (386)	0.134	H→L (0.97, 93%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₂	3.43 (361)	0.071	H→L+1 (0.98, 96%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLC
B2	S ₁	3.24 (383)	0.113	H→L (0.98, 96%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₂	3.46 (358)	0.054	H→L+1 (0.98, 97%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
B3	S ₁	3.32 (373)	0.132	H→L (0.97, 95%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₃	3.54 (350)	0.082	H→L+1 (0.97, 95%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₄	3.66 (339)	0.015	H-1→L (0.73, 54%) H-2→L (0.58, 33%)	Cu(d)+N ^Λ N(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT/ ¹ ILCT
B4	S ₁	3.28 (378)	0.121	H→L (0.98, 96%)	Cu(d)+P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₃	3.49 (355)	0.074	H→L+1 (0.98, 96%)	Cu(d)+ P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₄	3.63 (342)	0.027	H-1→L (0.86, 73%)	Cu(d)+ P ^Λ P(π)+N ^Λ N(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT/ ¹ ILCT
B4-1	S ₁	2.93 (422)	0.375	H→L (0.97, 95%)	Cu(d)+P ^Λ P(π)+N ^Λ N(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT/ ¹ ILCT
	S ₃	3.23 (384)	0.437	H-1→L (0.94, 88%)	Cu(d) +P ^Λ P(π)+N ^Λ N(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT/ ¹ ILCT
	S ₆	3.44 (360)	0.304	H-2→L (0.74, 54%) H-1→L+1(0.42,17%)	N ^Λ N(π)→N ^Λ N (π*); ¹ ILCT Cu(d)+N ^Λ N(π)→N ^Λ N (π*); ¹ MLCT/ ¹ ILCT
B4-2	S ₄	3.07 (403)	0.257	H-1→L+1(0.97,95%)	N ^Λ N (π)→N ^Λ N (π*); ¹ ILCT
	S ₅	3.31 (374)	0.085	H-2→L (0.98, 96%)	Cu(d)+ P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT
	S ₇	3.51 (353)	0.072	H-2→L+2(0.98,96%)	Cu(d)+ P ^Λ P(π)→N ^Λ N (π*); ¹ MLCT/ ¹ LLCT

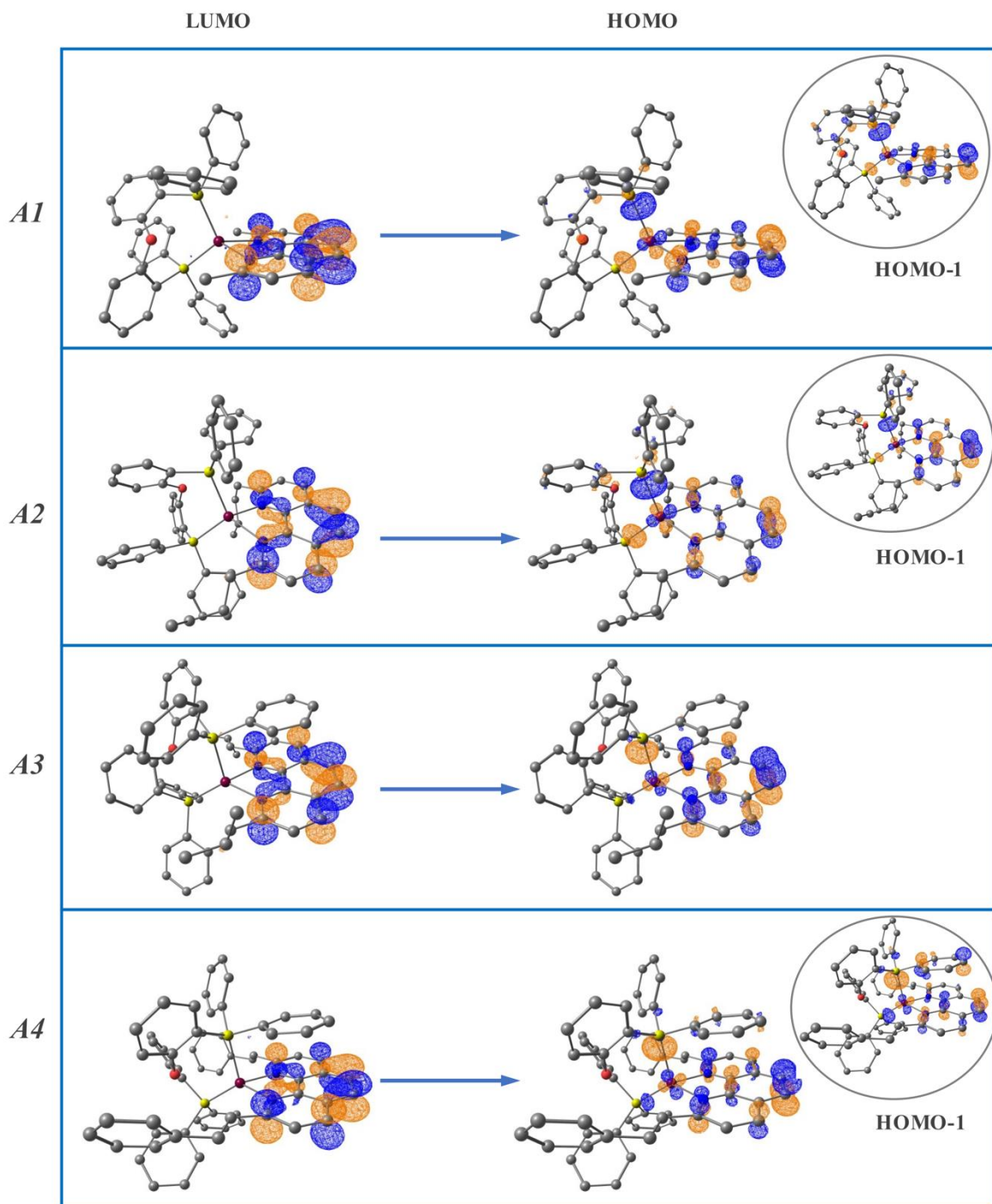
S5. Molecular orbitals from HOMO-2 to LUMO+1, in the triplet excited state

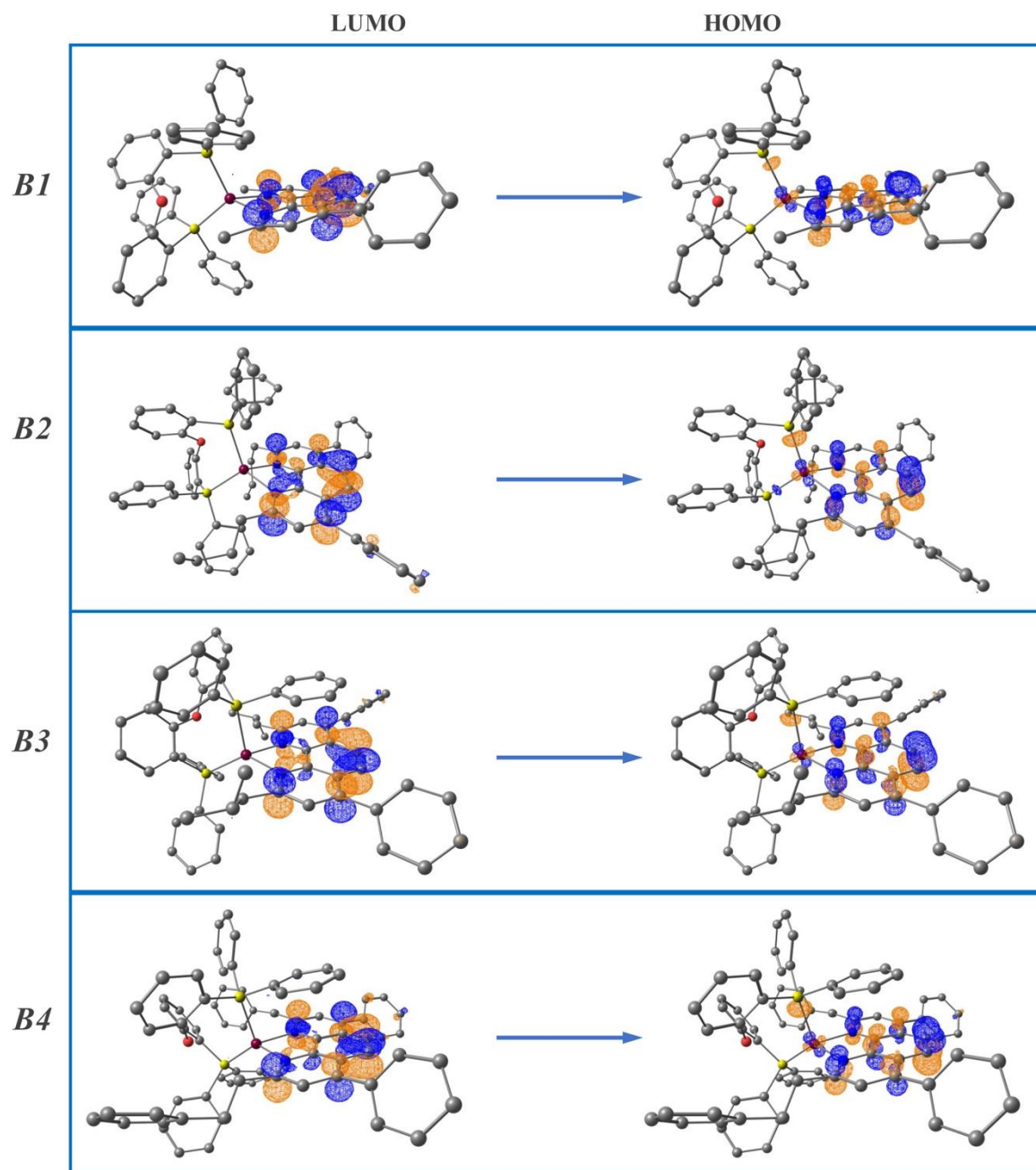
Table S5. Contribution to molecular orbitals (%) involved in deactivating the triplet excited state (T_1) (from HOMO-2 to LUMO+1) of all complexes under study, obtained at the M06-2X/6-31G(d,p)/LANL2DZ level of theory. Contribution to the molecular orbitals (%) involved in the deactivation of the excited triplet state (T_1) (from HOMO-2 to LUMO + 2) of all the complexes under study, obtained in the M06-2X / 6-31G (d, p) / Theoretical level LANL2DZ.

Orbital	A1			A2			A3			A4		
	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N
L	0	1	99	0	1	99	0	1	99	0	1	99
H	10	40	50	12	46	42	7	25	68	8	32	60
H-1	7	43	50	6	36	58	11	57	32	10	50	40

Orbital	B1			B2			B3			B4		
	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N
L	0	1	99	0	0	100	0	0	100	0	0	100
H	4	12	84	6	18	76	3	10	87	4	12	84

Orbital	B4-1			B4-2		
	Cu	P [^] P	N [^] N	Cu	P [^] P	N [^] N
L+1	2	1	97	2	2	96
L	0	1	99	0	0	100
H	2	7	91	0	0	100
H-1	0	4	96	0	1	99
H-2	15	71	14	4	13	83





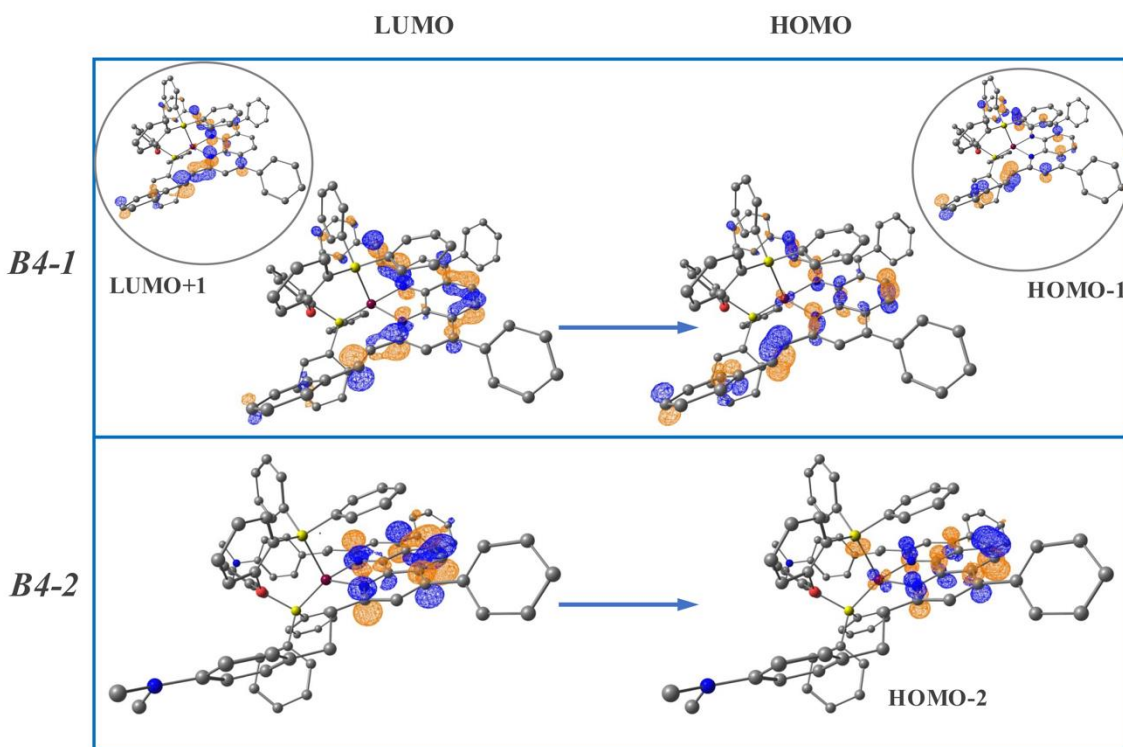


Figure S1. Frontier molecular orbitals involved in the radiative deactivation of the lowest-lying triplet excited state of all complexes.

S6. Geometries of the ground states and the triplet states

Table S6. Geometrical parameters of the ground states (S_0) and lowest triplet states (T_1 or T_2) for all complexes determined at the level PBE0/6-31G(d,p)/LANL2DZ and M06-2X/6-31G(d,p)/LANL2DZ, respectively. Using dichloromethane as solvent.

Parameter	A1		A2		A3		A4	
	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1
<i>Bond length</i> (Å)								
Cu-P1	2.366	2.420	2.362	2.426	2.405	2.499	2.342	2.358
Cu-P2	2.368	2.434	2.387	2.433	2.341	2.389	2.386	2.480
Cu-N1	2.158	2.199	2.172	2.196	2.142	2.168	2.150	2.146
Cu-N2	2.173	2.174	2.191	2.197	2.163	2.191	2.158	2.178
<i>Bond angle</i> (deg)								
P1-Cu-P2	114.19	110.17	111.51	108.40	117.44	113.02	117.28	114.03

P1-Cu-N1	116.11	121.46	123.17	125.76	102.87	98.63	117.67	131.13
P1-Cu-N2	112.30	118.88	117.45	115.23	105.97	98.89	121.16	125.86
P2-Cu-N1	109.97	106.88	105.39	105.14	121.79	128.26	107.97	100.47
P2-Cu-N2	121.14	118.81	117.75	123.47	122.34	132.09	107.07	99.57
N1-Cu-N2	78.36	76.91	77.70	76.75	79.37	77.27	79.21	77.48
<i>Dihedral angle</i> (deg)								
P1-P2-N2-N1	-80.39	-82.42	83.17	87.96	-72.41	-74.13	-74.96	-79.86
τ_4	0.870	0.849	0.844	0.786	0.822	0.707	0.859	0.730

Parameter	B1		B2		B3		B4	
	S ₀	T ₁	S ₀	T ₁	S ₀	T ₁	S ₀	T ₁
<i>Bond length</i> (Å)								
Cu-P1	2.358	2.419	2.360	2.429	2.411	2.499	2.343	2.355
Cu-P2	2.381	2.433	2.392	2.434	2.339	2.389	2.388	2.468
Cu-N1	2.149	2.200	2.163	2.190	2.134	2.162	2.143	2.158
Cu-N2	2.171	2.169	2.182	2.190	2.153	2.187	2.147	2.148
<i>Bond angle</i> (deg)								
P1-Cu-P2	112.40	110.22	111.39	107.91	117.33	113.14	117.24	115.69
P1-Cu-N1	120.24	121.88	123.62	125.54	102.05	98.16	118.56	131.26
P1-Cu-N2	115.41	119.15	118.83	115.83	105.36	98.23	120.91	124.97
P2-Cu-N1	107.15	106.16	105.07	105.85	123.11	128.67	107.39	98.12
P2-Cu-N2	119.88	119.04	116.69	123.42	122.88	132.81	107.58	100.51
N1-Cu-N2	77.56	76.43	77.07	76.26	78.75	76.72	78.63	77.49
<i>Dihedral angle</i> (deg)								
P1-P2-N2-N1	-82.22	-82.96	82.84	87.62	-72.18	-74.24	-75.85	-81.31
τ_4	0.850	0.844	0.834	0.788	0.808	0.699	0.854	0.736

Parameter	B4-1		B4-2	
	S ₀	T ₁	S ₀	T ₁
<i>Bond length</i> (Å)				
Cu-P1	2.335	2.366	2.325	2.357
Cu-P2	2.405	2.489	2.399	2.468
Cu-N1	2.138	2.147	2.133	2.157
Cu-N2	2.148	2.159	2.138	2.154
<i>Bond angle</i> (deg)				
P1-Cu-P2	118.70	113.09	117.55	115.45
P1-Cu-N1	122.41	129.99	122.81	130.85
P1-Cu-N2	123.64	131.61	120.50	125.30
P2-Cu-N1	101.04	97.62	103.40	98.41
P2-Cu-N2	104.19	97.87	106.74	100.84
N1-Cu-N2	78.70	77.55	78.86	77.37
<i>Dihedral angle</i> (deg)				
P1-P2-N2-N1	-77.17	-78.36	-78.55	-81.02
τ_4	0.801	0.698	0.828	0.736

The τ_4 geometry index is defined as: $\tau_4 = \{360^\circ - (\theta + \varphi)\} / 141^\circ$, where θ and φ correspond to the two largest angles that pass through the metal center in the four-coordinate geometry [16-18]. The values of τ_4 can range from 1 (for a perfect tetrahedral geometry) to zero (for a perfect square planar geometry), and $\tau_4=0.85$ correspond to a trigonal pyramidal geometry.

S7. Pauli repulsion energy

ΔE_{PAULI} values were obtained by the second-generation energy decomposition analysis based on absolutely localized molecular orbitals (ALMO-EDA) of the Q-Chem5.2 program [19], which is expressed as:

$$\Delta E_{PAULI} = \sum (E[\tilde{P}_F] - E[P_F]) + (E_{xc}^{DF}[P_{FRZ}] - \sum E_{xc}^{DF}[\tilde{P}_F])$$

where the energies are obtained from a set of fragment-localized orthogonal orbitals \mathbf{P} (the tildes indicate that these fragment density matrices, and the corresponding densities are modified from the isolated fragment quantities, P_F). In this framework, $E[P_F]$ stands for the energy obtained from fragment molecular contributions, while $E[P_{FRZ}]$ is the energy obtained for the sum of fragment contributions, where the FRZ term stand for the frozen component (the interaction energy of the complex with constraints on the orbitals to prevent polarization and charge transfer. E_{xc}^{DF} energies are obtained with the use of a dispersion-free exchange-correlation method (xc), where the Hartree-Fock energy is recommended for hybrid functionals (this is to prevent Pauli energy of dispersion contributions). For a detailed description of these quantities, see reference 20 [20].

S8. Other Complexes:

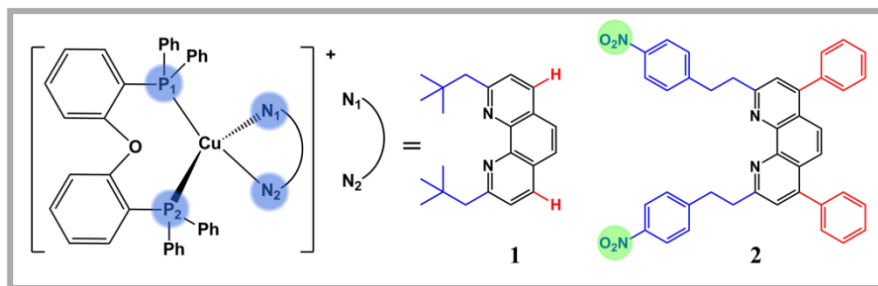


Figure S2. Cu(I) complexes according to diimine (N^N) ligand: (1) neopentyl and (2) nitro group.

The frontier molecular orbitals of complexes **1** and **2** shown in Fig. S2 follow the same trend as the complexes in the manuscript, namely, the HOMO is distributed between the central metal (32 % to 34 %) and POP ligand (54 % to 58 %) and the LUMO is mainly localized entirely on the N^N ligand (up to 98%), see Fig. S3 and Table S7. Note that the presence of an electron-withdrawing group (complex **2**) in the N^N ligand does not show significant change in the contribution of the metal in the HOMO.

Complex **1** has similar characteristics to **A3**, which suggests that the addition of an extra methyl group in the substituent at position 2,9 of phen would not produce significant changes in the molecular properties of the complexes. On the other hand, complex **2** experiences a reduction of Δ_{HL} with respect to **B4**, because of the presence of the electron withdrawing group in the ligand N^N that mainly affects the LUMO, stabilizing its energy, following the trend observed in **B4-1** and **B4-2**.

Table S7. Contribution to molecular orbitals (%) HOMO and LUMO in the ground state (S_0), obtained at the PBE0/6-31G(d,p)/LANL2DZ level of theory.

Orbital	1			2		
	Cu	P^P	N^N	Cu	P^P	N^N
L	2	2	96	0	0	100
H	34	58	8	32	54	14

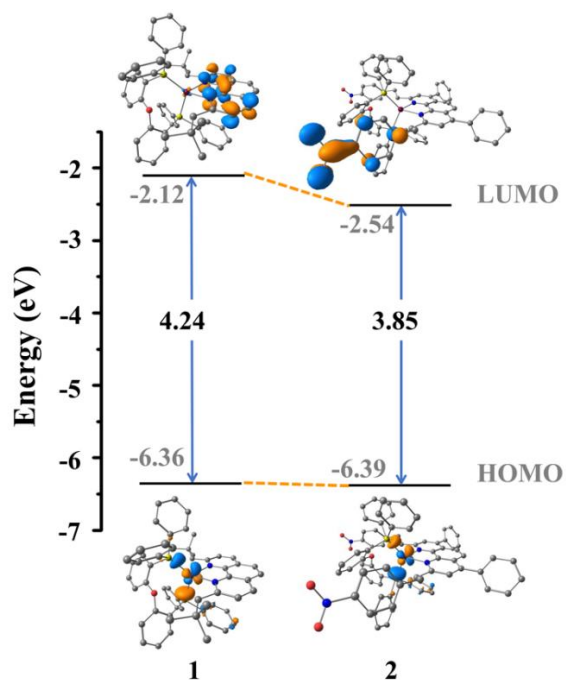


Figure S3. Molecular orbital diagrams of complexes **1** and **2**.

The obtained results suggest that the emission properties will not experience significant changes with respect to the series of complexes presented in the main manuscript. However, the presence of an electron-withdrawing group (complex **2**) is reported to induce an important red shift,[21] according to the energy gap law, could lead to a decrease in photoluminescence quantum yield.

S9. Prediction of radiative (k_r) and non-radiative constants (k_{nr})

Table S8. k_{nr} , k_r and Φ experimental and predicted obtained through relationships.

Complexes	$k_{nr}(x10^4)$ <i>predicted</i>	$k_r(x10^4)$ <i>predicted</i>	Φ <i>predicted</i>
A1	6.53	1.08	0.14
A2	4.01	1.48	0.27
A3	3.92	2.52	0.39
A4	19.57	1.98	0.09
B1	4.14	1.58	0.28
B2	7.45	1.33	0.15
B3	6.70	2.55	0.28
B4	36.69	2.04	0.05
B4-1	8.40	2.88	0.26
B4-2	10.42	3.12	0.23

S10. XYZ coordinates of the optimized molecular structures (S₀ and T₁)

XYZ Coordinates of the S ₀ states.				6	-0.753214000	0.229983000	3.253410000
				6	-0.345846000	1.435263000	-3.403372000
A1				6	2.614729000	0.787681000	1.596081000
				6	2.480345000	-0.499076000	2.136156000
29	-0.454922000	0.338109000	-0.139773000	6	3.103188000	-0.861767000	3.324590000
15	1.751422000	1.177008000	0.018960000	6	3.898240000	0.066901000	3.990309000
15	-0.591768000	-2.024533000	-0.210592000	6	4.051842000	1.350265000	3.472064000
8	1.614102000	-1.389967000	1.532631000	6	3.412118000	1.706451000	2.287918000
7	-1.872037000	1.115939000	1.290421000	6	1.716993000	3.008012000	-0.017820000
7	-1.718313000	1.575072000	-1.402835000	6	2.233955000	3.753718000	-1.081905000
6	-1.911672000	0.913414000	2.604728000	6	2.073982000	5.138510000	-1.113850000
6	-3.002699000	1.352952000	3.386369000	6	1.400686000	5.792346000	-0.086591000
6	-4.049292000	2.009808000	2.790483000	6	0.874955000	5.054970000	0.974127000
6	-4.018105000	2.248090000	1.401441000	6	1.021536000	3.672613000	1.003472000
6	-5.063889000	2.943977000	0.721336000	6	3.024930000	0.697890000	-1.213615000
6	-4.981818000	3.183313000	-0.614013000	6	2.713848000	-0.253882000	-2.188386000
6	-3.849976000	2.739856000	-1.364215000	6	3.672723000	-0.656291000	-3.116256000
6	-3.711035000	3.000392000	-2.743042000	6	4.951935000	-0.110735000	-3.074927000
6	-2.584619000	2.575561000	-3.399196000	6	5.276329000	0.830866000	-2.097935000
6	-1.590311000	1.861401000	-2.694538000	6	4.321570000	1.229377000	-1.169084000
6	-2.809868000	2.022012000	-0.731194000	6	1.072938000	-2.788306000	-0.270064000
6	-2.892430000	1.775870000	0.687899000	6	2.058229000	-2.293987000	0.600551000

6	3.377596000	-2.726283000	0.528332000	8	-0.403884000	-2.263568000	1.460456000
6	3.726114000	-3.678190000	-0.425963000	7	1.801385000	1.433296000	1.077837000
6	2.767522000	-4.194825000	-1.292835000	7	0.789255000	2.172785000	-1.355124000
6	1.450753000	-3.749033000	-1.212645000	6	2.261935000	1.078314000	2.274334000
6	-1.392759000	-2.758006000	1.266420000	6	3.431198000	1.658979000	2.815800000
6	-0.778601000	-3.723234000	2.069132000	6	4.110477000	2.615847000	2.107110000
6	-1.441714000	-4.232353000	3.184501000	6	3.627537000	3.018551000	0.844729000
6	-2.722357000	-3.787973000	3.502434000	6	4.274471000	4.025109000	0.065319000
6	-3.342871000	-2.829311000	2.701998000	6	3.763107000	4.404577000	-1.135505000
6	-2.680078000	-2.311828000	1.594081000	6	2.571729000	3.801192000	-1.641816000
6	-1.490535000	-2.827545000	-1.589375000	6	1.996489000	4.188148000	-2.869465000
6	-1.977901000	-4.138239000	-1.502160000	6	0.832640000	3.594166000	-3.283772000
6	-2.646917000	-4.709330000	-2.580438000	6	0.238490000	2.584097000	-2.493948000
6	-2.837782000	-3.979335000	-3.753190000	6	1.919160000	2.781375000	-0.911396000
6	-2.361986000	-2.673934000	-3.845518000	6	2.456963000	2.386228000	0.367370000
6	-1.694965000	-2.099674000	-2.765911000	6	1.516296000	0.025920000	3.038486000
1	-2.997661000	1.162640000	4.454367000	6	1.124949000	0.423386000	4.465688000
1	-4.899021000	2.352467000	3.374406000	6	0.221432000	1.650071000	4.543714000
1	-5.919203000	3.285792000	1.296653000	6	-0.214482000	1.966913000	5.968564000
1	-5.769419000	3.721755000	-1.132834000	6	-1.061506000	1.980134000	-2.929414000
1	-4.491604000	3.544610000	-3.267223000	6	-2.221910000	2.984386000	-2.871845000
1	-2.441963000	2.777375000	-4.455766000	6	-3.564545000	2.388434000	-3.294797000
1	0.253216000	0.784056000	-2.767090000	6	-3.627581000	1.948992000	-4.753287000
1	0.260140000	2.312046000	-3.658112000	6	-2.135548000	-0.755563000	2.135193000
1	-0.576229000	0.917506000	-4.339531000	6	-1.369571000	-1.904586000	2.379885000
1	2.950504000	-1.861739000	3.718229000	6	-1.470471000	-2.607389000	3.574325000
1	4.388624000	-0.212056000	4.917761000	6	-2.363180000	-2.170076000	4.550247000
1	4.665763000	2.079130000	3.991894000	6	-3.131836000	-1.029759000	4.331762000
1	3.521274000	2.715735000	1.902013000	6	-3.015134000	-0.326881000	3.134450000
1	2.765082000	3.258444000	-1.888618000	6	-2.741255000	1.726703000	0.782414000
1	2.482754000	5.705048000	-1.945524000	6	-1.927725000	2.761218000	1.266926000
1	1.281658000	6.871459000	-0.111980000	6	-2.453906000	4.030759000	1.484578000
1	0.344709000	5.556833000	1.778279000	6	-3.793619000	4.288169000	1.198221000
1	0.593985000	3.106570000	1.827248000	6	-4.603468000	3.271427000	0.698376000
1	1.725355000	-0.703296000	-2.207993000	6	-4.083404000	1.994688000	0.493196000
1	3.418955000	-1.400842000	-3.864791000	6	-3.053462000	-0.866197000	-0.542178000
1	5.700384000	-0.422728000	-3.797480000	6	-2.646596000	-1.218226000	-1.832955000
1	6.276579000	1.251937000	-2.057115000	6	-3.491429000	-1.943583000	-2.670122000
1	4.586783000	1.956319000	-0.406379000	6	-4.749849000	-2.333335000	-2.220955000
1	4.120811000	-2.323556000	1.208163000	6	-5.155859000	-2.010466000	-0.926927000
1	4.756097000	-4.016868000	-0.485444000	6	-4.311590000	-1.288285000	-0.089569000
1	3.041725000	-4.940300000	-2.032456000	6	0.172418000	-3.073250000	-0.662832000
1	0.706872000	-4.142732000	-1.898201000	6	-0.666933000	-3.164646000	0.459202000
1	-0.267590000	-0.451643000	2.554671000	6	-1.661651000	-4.131835000	0.549297000
1	-1.071050000	-0.328663000	4.136986000	6	-1.819829000	-5.038434000	-0.495219000
1	-0.012355000	0.970535000	3.578401000	6	-0.990770000	-4.981789000	-1.611998000
1	0.216324000	-4.082645000	1.822966000	6	-0.004443000	-4.002402000	-1.692137000
1	-0.955629000	-4.981772000	3.802519000	6	2.741286000	-2.145310000	0.320396000
1	-3.237355000	-4.187496000	4.371200000	6	3.837245000	-1.275141000	0.395225000
1	-4.342081000	-2.479182000	2.944351000	6	4.921898000	-1.576822000	1.211937000
1	-3.164827000	-1.556742000	0.979862000	6	4.919915000	-2.744927000	1.973496000
1	-1.837565000	-4.709646000	-0.588801000	6	3.833886000	-3.613540000	1.904662000
1	-3.022347000	-5.725614000	-2.504547000	6	2.749745000	-3.318801000	1.079466000
1	-3.363153000	-4.427173000	-4.591641000	6	2.059078000	-1.808174000	-2.436617000
1	-2.516127000	-2.098962000	-4.753930000	6	3.035872000	-2.760834000	-2.754992000
1	-1.337755000	-1.076344000	-2.829528000	6	3.544245000	-2.837720000	-4.048165000
				6	3.084862000	-1.965826000	-5.034747000
				6	2.118219000	-1.012294000	-4.725504000
				6	1.611494000	-0.931352000	-3.430541000
				1	3.783073000	1.334826000	3.789308000
				1	5.013096000	3.071559000	2.504722000
				1	5.177111000	4.484414000	0.457373000
A2							
29	0.324790000	0.408546000	-0.142506000				
15	-1.920924000	0.107628000	0.526619000				
15	1.339420000	-1.662062000	-0.758918000				

1	4.245744000	5.175888000	-1.728507000	6	3.054995000	-3.497611000	3.435037000
1	2.475901000	4.958619000	-3.466733000	6	3.606890000	-2.347108000	3.900022000
1	0.359483000	3.883337000	-4.216573000	6	3.155828000	-1.078738000	3.419680000
1	-0.842948000	-3.479078000	3.731225000	6	3.720290000	0.134412000	3.856946000
1	-2.447982000	-2.716936000	5.484181000	6	3.271056000	1.320886000	3.332752000
1	-3.821442000	-0.682023000	5.094589000	6	2.250077000	1.319764000	2.357995000
1	-3.607427000	0.569661000	2.975122000	6	2.117016000	-0.999889000	2.463885000
1	-0.874402000	2.569214000	1.459879000	6	1.507959000	-2.223375000	1.993658000
1	-1.814651000	4.821801000	1.865670000	6	-1.159512000	-3.084569000	-0.389565000
1	-4.203037000	5.281513000	1.356841000	6	1.732535000	2.603775000	1.767954000
1	-5.645517000	3.469642000	0.465023000	6	0.118474000	-0.548687000	-3.089194000
1	-4.724782000	1.214929000	0.095138000	6	-1.277671000	-0.419996000	-3.078502000
1	-1.654017000	-0.946654000	-2.178680000	6	-2.059639000	-0.866326000	-4.139648000
1	-3.159589000	-2.211971000	-3.668660000	6	-1.447758000	-1.427875000	-5.255055000
1	-5.409029000	-2.899871000	-2.872105000	6	-0.059220000	-1.534370000	-5.306830000
1	-6.129720000	-2.327356000	-0.565518000	6	0.711087000	-1.097995000	-4.234683000
1	-4.629634000	-1.065241000	0.925143000	6	2.513061000	-1.145859000	-1.544884000
1	2.137744000	-0.878740000	3.069838000	6	3.692242000	-0.714613000	-0.919324000
1	0.624109000	-0.228569000	2.461405000	6	4.732958000	-1.605981000	-0.678446000
1	0.612437000	-0.433817000	4.919796000	6	4.609093000	-2.945021000	-1.044206000
1	2.024365000	0.591727000	5.072962000	6	3.436917000	-3.385723000	-1.651922000
1	-0.664214000	1.483933000	3.917010000	6	2.394321000	-2.495010000	-1.898799000
1	0.741994000	2.517880000	4.116669000	6	1.855847000	1.564594000	-2.324797000
1	-0.778643000	1.132828000	6.400656000	6	1.208599000	2.780237000	-2.077020000
1	-0.853308000	2.854765000	6.003936000	6	1.681753000	3.960599000	-2.646954000
1	0.650051000	2.152293000	6.615817000	6	2.816778000	3.941157000	-3.452647000
1	-1.282618000	1.130919000	-2.277525000	6	3.473240000	2.735602000	-3.695812000
1	-0.955250000	1.595171000	-3.951358000	6	2.992587000	1.552173000	-3.143319000
1	-1.990135000	3.847522000	-3.510043000	6	-2.248899000	1.995809000	-0.607584000
1	-2.302181000	3.365066000	-1.846525000	6	-2.090530000	1.471544000	-1.901952000
1	-2.301224000	-4.174770000	1.424509000	6	-2.133155000	2.290595000	-3.025969000
1	-2.596019000	-5.794910000	-0.428370000	6	-2.319335000	3.660656000	-2.862322000
1	-1.113298000	-5.693237000	-2.422446000	6	-2.458556000	4.207448000	-1.590286000
1	0.630473000	-3.950050000	-2.570986000	6	-2.424293000	3.376400000	-0.472811000
1	-3.802876000	1.538501000	-2.642571000	6	-3.545092000	-0.198911000	0.784800000
1	-4.341948000	3.139790000	-3.110456000	6	-4.564494000	-0.067067000	-0.161563000
1	3.844946000	-0.358985000	-0.190510000	6	-5.712184000	-0.853400000	-0.070942000
1	5.766518000	-0.895561000	1.258558000	6	-5.857403000	-1.766889000	0.969466000
1	5.763987000	-2.977598000	2.616151000	6	-4.845218000	-1.900089000	1.919359000
1	3.829580000	-4.528508000	2.490105000	6	-3.691553000	-1.128671000	1.822505000
1	1.913310000	-4.008938000	1.023933000	6	-2.338995000	1.827299000	2.307144000
1	-3.373304000	2.775438000	-5.426806000	6	-3.533994000	2.533187000	2.506751000
1	-4.632993000	1.604991000	-5.014822000	6	-3.752186000	3.219209000	3.696443000
1	-2.939097000	1.124000000	-4.964563000	6	-2.790805000	3.191812000	4.707417000
1	3.400539000	-3.439387000	-1.988791000	6	-1.614081000	2.470921000	4.528747000
1	4.301851000	-3.578658000	-4.286136000	6	-1.389909000	1.790050000	3.332679000
1	3.485835000	-2.026635000	-6.042277000	1	-0.047791000	-5.422975000	0.612672000
1	1.764517000	-0.325309000	-5.488779000	1	1.772462000	-5.599493000	2.279145000
1	0.871947000	-0.174816000	-3.183287000	1	3.402175000	-4.464915000	3.786027000
				1	4.405496000	-2.368297000	4.635615000
				1	4.512597000	0.119730000	4.600297000
				1	3.701586000	2.260494000	3.658346000
				1	0.889327000	2.939460000	2.388171000
				1	1.305718000	2.370606000	0.784071000
				1	-3.138249000	-0.764263000	-4.076331000
				1	-2.055616000	-1.774934000	-6.084824000
				1	0.424624000	-1.960299000	-6.180128000
				1	1.791600000	-1.195850000	-4.281097000
				1	3.802774000	0.325224000	-0.623950000
				1	5.643064000	-1.251398000	-0.203308000
				1	5.421990000	-3.640072000	-0.856147000
				1	3.329574000	-4.427274000	-1.940633000
A3							
29	0.089321000	-0.121042000	0.527157000				
15	1.108405000	0.027173000	-1.646195000				
15	-2.028272000	0.841473000	0.793797000				
8	-1.912754000	0.110818000	-1.972731000				
7	0.490099000	-2.144232000	1.105235000				
7	1.685778000	0.180886000	1.954882000				
6	-0.062333000	-3.258467000	0.625678000				
6	0.400578000	-4.528782000	1.028152000				
6	1.414666000	-4.627981000	1.949458000				
6	2.000966000	-3.459991000	2.470732000				

1	1.490785000	-2.859039000	-2.378006000	6	-1.324523000	-1.917476000	-2.697127000
1	0.325890000	2.807453000	-1.443792000	6	-1.414634000	-3.184067000	-3.291738000
1	1.161862000	4.894793000	-2.455657000	1	-0.742990000	-3.980489000	-2.982982000
1	3.190633000	4.862209000	-3.890120000	6	-2.352922000	-3.426072000	-4.289468000
1	4.359594000	2.714261000	-4.323173000	1	-2.418541000	-4.412263000	-4.739494000
1	3.511221000	0.619431000	-3.344050000	6	-3.198198000	-2.403152000	-4.720012000
1	-2.012760000	1.863983000	-4.015732000	1	-3.925612000	-2.593922000	-5.503528000
1	-2.349059000	4.300148000	-3.739254000	6	-3.097509000	-1.135166000	-4.155175000
1	-2.594930000	5.276688000	-1.463903000	1	-3.740048000	-0.330255000	-4.500127000
1	-2.524566000	3.807372000	0.517936000	6	-2.163952000	-0.893898000	-3.147622000
1	-0.686764000	-2.710630000	-1.308929000	1	-2.070159000	0.099060000	-2.717484000
1	-1.807507000	-2.267419000	-0.046986000	6	-0.352152000	-2.709821000	-0.062353000
1	-4.474605000	0.657434000	-0.964960000	6	-1.400775000	-3.633878000	-0.025563000
1	-6.498627000	-0.741249000	-0.811737000	1	-2.056549000	-3.731641000	-0.884218000
1	-6.756331000	-2.371806000	1.042775000	6	-1.627974000	-4.417745000	1.102977000
1	-4.952142000	-2.608451000	2.735778000	1	-2.450477000	-5.125796000	1.111911000
1	-2.906309000	-1.242202000	2.566626000	6	-0.801209000	-4.283363000	2.213734000
1	-4.298744000	2.537306000	1.734611000	1	-0.970490000	-4.889754000	3.098400000
1	-4.677939000	3.768623000	3.839927000	6	0.248055000	-3.368319000	2.207665000
1	-2.966889000	3.724081000	5.637601000	1	0.889514000	-3.257088000	3.075063000
1	-0.870854000	2.432324000	5.319745000	6	0.463743000	-2.587998000	1.076487000
1	-0.481702000	1.209111000	3.196425000	6	2.010050000	-1.132761000	2.144623000
6	-2.012234000	-4.308745000	-0.739491000	6	3.138095000	-1.729774000	2.695540000
1	-1.341694000	-5.119536000	-1.058865000	1	3.563628000	-2.601907000	2.210708000
6	-2.848649000	-4.797886000	0.442044000	6	3.712971000	-1.184621000	3.838415000
1	-3.410522000	-5.697495000	0.170542000	1	4.597062000	-1.647206000	4.265539000
1	-3.569155000	-4.028709000	0.739837000	6	3.159602000	-0.047620000	4.422388000
1	-2.239472000	-5.037992000	1.319057000	1	3.601968000	0.378931000	5.317259000
6	-2.917353000	-3.975602000	-1.924649000	6	2.043556000	0.553662000	3.850325000
1	-3.526322000	-4.841257000	-2.204096000	1	1.635322000	1.454104000	4.299210000
1	-2.337365000	-3.671077000	-2.802067000	6	1.451121000	0.030794000	2.693232000
1	-3.598959000	-3.154535000	-1.671884000	6	-1.382671000	0.222493000	2.984379000
6	2.733801000	3.759936000	1.641582000	6	-1.540835000	0.704996000	4.291074000
1	3.134972000	3.982401000	2.640011000	1	-0.878082000	1.476185000	4.672920000
6	3.900421000	3.413600000	0.718755000	6	-2.555574000	0.210438000	5.103055000
1	3.541535000	3.206173000	-0.295819000	1	-2.672182000	0.594156000	6.112477000
1	4.451720000	2.534715000	1.069821000	6	-3.420324000	-0.773576000	4.623132000
1	4.608346000	4.246526000	0.659239000	1	-4.214187000	-1.154961000	5.258960000
6	2.009066000	5.016190000	1.162932000	6	-3.265698000	-1.264068000	3.330260000
1	1.578165000	4.861945000	0.167707000	1	-3.938418000	-2.024445000	2.945021000
1	2.700051000	5.862626000	1.098653000	6	-2.250071000	-0.767871000	2.514747000
1	1.197367000	5.293698000	1.843879000	1	-2.130176000	-1.162760000	1.510441000

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29	-0.095853000	0.632698000	-0.484670000	6	0.133072000	2.583022000	2.272076000
15	-0.070982000	-1.515334000	-1.419023000	6	1.369477000	3.237269000	2.193906000
15	-0.018884000	0.795393000	1.894531000	1	2.281151000	2.667021000	2.042779000
8	1.479628000	-1.668781000	0.985095000	6	1.448569000	4.620884000	2.327003000
7	1.263330000	2.088895000	-1.293222000	1	2.417420000	5.109280000	2.276204000
7	-1.480485000	2.136470000	-1.178079000	6	0.294318000	5.374302000	2.527669000
6	1.448617000	-2.113803000	-2.258337000	1	0.357587000	6.453266000	2.632812000
6	1.951445000	-3.406391000	-2.081464000	6	-0.941180000	4.734684000	2.594254000
1	1.494293000	-4.073312000	-1.355602000	1	-1.847246000	5.312456000	2.752474000
6	3.032925000	-3.847282000	-2.842092000	6	-1.023397000	3.350838000	2.464491000
1	3.413682000	-4.854852000	-2.702065000	1	-1.994350000	2.867514000	2.524948000
6	3.621131000	-3.001997000	-3.780844000	6	0.604424000	3.119811000	-1.874777000
1	4.461342000	-3.349240000	-4.374745000	6	1.276644000	4.172880000	-2.537437000
6	3.134308000	-1.706283000	-3.950007000	6	2.681055000	4.108973000	-2.582759000
1	3.594241000	-1.040587000	-4.674531000	1	3.237404000	4.891864000	-3.090630000
6	2.055887000	-1.262166000	-3.189485000	6	3.334734000	3.064812000	-1.974825000
1	1.677326000	-0.251387000	-3.324680000	1	4.416193000	3.014787000	-1.998220000
				6	2.596247000	2.059603000	-1.316023000
				6	3.272879000	0.936882000	-0.574602000
				1	2.684074000	0.024289000	-0.719517000

1	3.210462000	1.158918000	0.499590000	6	-2.327821000	-0.908631000	-0.085446000
6	4.738733000	0.687684000	-0.944853000	6	-2.269197000	0.445181000	-0.595909000
1	4.804304000	0.471229000	-2.018433000	6	0.388220000	2.656118000	-1.837778000
1	5.326668000	1.594021000	-0.764232000	6	0.115127000	-3.545752000	0.698645000
6	5.358687000	-0.443120000	-0.162304000	6	3.229561000	0.314487000	-2.317839000
6	5.133251000	-1.773451000	-0.529601000	6	3.600496000	1.461082000	-1.601164000
1	4.507694000	-1.991911000	-1.390880000	6	4.295762000	2.503271000	-2.201221000
6	5.713731000	-2.818454000	0.184581000	6	4.646559000	2.405203000	-3.545596000
1	5.534474000	-3.845079000	-0.123876000	6	4.286907000	1.278012000	-4.279324000
6	6.529572000	-2.549276000	1.282773000	6	3.580369000	0.243463000	-3.669951000
1	6.989700000	-3.363453000	1.835641000	6	1.644582000	-2.046535000	-2.798231000
6	6.757839000	-1.227838000	1.660168000	6	2.262513000	-3.209128000	-3.209128000
1	7.396890000	-1.006499000	2.510632000	6	1.675302000	-3.947563000	-4.296675000
6	6.176289000	-0.185296000	0.941475000	6	0.473381000	-3.531265000	-4.862851000
1	6.367164000	0.844450000	1.235964000	6	-0.152363000	-2.377432000	-4.392866000
6	0.541262000	5.251053000	-3.120820000	6	0.422915000	-1.645969000	-3.359107000
1	1.091697000	6.039076000	-3.626192000	6	3.659474000	-1.968557000	-0.682039000
6	-0.813272000	5.292509000	-3.031992000	6	3.514763000	-2.424841000	0.631325000
1	-1.376047000	6.115000000	-3.463200000	6	4.524333000	-3.168419000	1.237833000
6	-1.529372000	4.251759000	-2.363148000	6	5.692234000	-3.456676000	0.537474000
6	-0.838416000	3.155097000	-1.798046000	6	5.855258000	-2.988893000	-0.765947000
6	-2.931091000	4.265877000	-2.232023000	6	4.848620000	-2.243680000	-1.371561000
1	-3.499638000	5.093122000	-2.647640000	6	3.183026000	0.913867000	1.936881000
6	-3.564071000	3.238133000	-1.576498000	6	3.906518000	1.181896000	0.763516000
1	-4.641659000	3.243356000	-1.462019000	6	5.289923000	1.055296000	0.713806000
6	-2.806926000	2.168498000	-1.055279000	6	5.974004000	0.659840000	1.860030000
6	-3.456416000	1.028585000	-0.320524000	6	5.283548000	0.398138000	3.039975000
1	-3.529641000	1.296632000	0.742451000	6	3.897146000	0.523541000	3.073208000
1	-2.772352000	0.173666000	-0.365108000	6	0.934541000	2.744628000	1.853799000
6	-4.844077000	0.614757000	-0.828731000	6	1.896707000	3.755187000	1.937673000
1	-5.550479000	1.442660000	-0.708318000	6	1.509600000	5.094238000	1.939603000
1	-4.785635000	0.397956000	-1.901971000	6	0.161881000	5.435130000	1.863154000
6	-5.374755000	-0.590244000	-0.093125000	6	-0.803368000	4.432084000	1.783943000
6	-4.976954000	-1.880536000	-0.459612000	6	-0.419953000	3.095064000	1.773895000
1	-4.303499000	-2.011368000	-1.304013000	6	0.805168000	0.429473000	3.508288000
6	-5.444142000	-2.994439000	0.233495000	6	0.975053000	1.235043000	4.642567000
1	-5.129111000	-3.989555000	-0.068809000	6	0.539646000	0.791856000	5.887350000
6	-6.322918000	-2.835120000	1.304255000	6	-0.074850000	-0.454252000	6.012105000
1	-6.694665000	-3.703695000	1.840332000	6	-0.258528000	-1.255417000	4.888544000
6	-6.728824000	-1.554946000	1.675472000	6	0.177055000	-0.812291000	3.641448000
1	-7.418525000	-1.420876000	2.504188000	1	-1.989587000	3.941435000	-2.078286000
6	-6.255790000	-0.443136000	0.981829000	1	-5.632945000	1.108233000	-0.642673000
1	-6.579737000	0.553241000	1.274471000	1	-5.736112000	-1.193161000	0.159355000

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29	0.549116000	-0.220237000	-0.063945000	1	-0.038978000	-4.624770000	0.759037000
15	2.296834000	-1.002483000	-1.440123000	1	4.543242000	3.382037000	-1.614040000
15	1.353193000	0.957496000	1.842538000	1	5.191181000	3.216157000	-4.019087000
8	3.153743000	1.607954000	-0.302583000	1	4.550789000	1.203472000	-5.329653000
7	-1.048606000	0.946825000	-0.902168000	1	3.289746000	-0.627030000	-4.251220000
7	-1.154187000	-1.553475000	0.127102000	1	3.197924000	-3.547031000	-2.835874000
6	-0.964935000	2.155392000	-1.453273000	1	2.161502000	-4.851119000	-4.652789000
6	-2.107971000	2.945573000	-1.663989000	1	0.019986000	-4.108737000	-5.663144000
6	-3.364574000	2.493493000	-1.309478000	1	-1.095367000	-2.053425000	-4.823510000
6	-3.468251000	1.172941000	-0.787141000	1	-0.081676000	-0.763389000	-2.971687000
6	-4.717876000	0.547332000	-0.491406000	1	2.616443000	-2.176067000	1.187427000
6	-4.775814000	-0.737726000	-0.053184000	1	4.400672000	-3.513086000	2.260192000
6	-3.589798000	-1.511581000	0.135648000	1	6.481226000	-4.034912000	1.009388000
6	-3.610205000	-2.871927000	0.553064000	1	6.771162000	-3.199346000	-1.310323000
6	-2.395110000	-3.503366000	0.735226000	1	4.995126000	-1.865678000	-2.379697000
6	-1.183256000	-2.826594000	0.515063000	1	5.822442000	1.263670000	-0.208110000

1	7.054659000	0.559537000	1.825010000	6	0.270692000	-4.407421000	-4.468989000
1	5.819815000	0.092478000	3.932712000	6	0.305321000	3.529352000	-0.357286000
1	3.360253000	0.304898000	3.990812000	6	0.495134000	4.256252000	-1.696805000
1	1.066522000	2.613436000	-0.981746000	6	1.860210000	4.930253000	-1.835130000
1	0.343413000	3.683730000	-2.202952000	6	2.104242000	6.067334000	-0.849311000
1	0.813791000	2.026650000	-2.626429000	6	3.279621000	-1.338871000	-1.681313000
1	2.949811000	3.499281000	2.007836000	6	3.466382000	-2.239635000	-0.622712000
1	2.265581000	5.871428000	2.005461000	6	4.084436000	-3.469584000	-0.812282000
1	-0.137007000	6.479259000	1.865380000	6	4.543083000	-3.814257000	-2.081780000
1	-1.856553000	4.690717000	1.722842000	6	4.364891000	-2.938449000	-3.149482000
1	-1.178402000	2.318771000	1.706559000	6	3.734134000	-1.712148000	-2.950090000
1	1.443614000	2.211108000	4.549429000	6	2.030392000	0.914841000	-2.988138000
1	0.675996000	1.421443000	6.761738000	6	0.775065000	0.556008000	-3.499937000
1	-0.416931000	-0.795307000	6.984873000	6	0.366484000	1.009276000	-4.750458000
1	-0.747058000	-2.221178000	4.979167000	6	1.197545000	1.845676000	-5.493944000
1	0.014913000	-1.422375000	2.757900000	6	2.437839000	2.222056000	-4.984417000
6	-4.535747000	3.381089000	-1.490329000	6	2.856676000	1.757826000	-3.738801000
6	-5.404959000	3.659686000	-0.426748000	6	3.853492000	1.263830000	-0.721763000
6	-4.754505000	4.003608000	-2.725738000	6	3.677444000	2.095002000	0.389103000
6	-6.470769000	4.537266000	-0.599636000	6	4.727846000	2.877336000	0.863630000
1	-5.230660000	3.205408000	0.544668000	6	5.969641000	2.829324000	0.236710000
6	-5.826334000	4.873855000	-2.897973000	6	6.163672000	1.986074000	-0.856362000
1	-4.089032000	3.788963000	-3.557340000	6	5.115675000	1.202644000	-1.329155000
6	-6.686726000	5.142972000	-1.835790000	6	2.848361000	-0.642355000	2.551278000
1	-7.130748000	4.751877000	0.235638000	6	3.619683000	-1.314923000	1.589745000
1	-5.989941000	5.341157000	-3.864511000	6	5.006894000	-1.363223000	1.671116000
1	-7.521615000	5.824346000	-1.969903000	6	5.643706000	-0.738954000	2.740144000
6	-4.863422000	-3.628487000	0.777024000	6	4.902829000	-0.080826000	3.717808000
6	-5.056613000	-4.308526000	1.986005000	6	3.514927000	-0.033313000	3.618461000
6	-5.842006000	-3.727081000	-0.221277000	6	0.348249000	-2.100639000	2.795925000
6	-6.210477000	-5.056344000	2.198949000	6	-1.044986000	-2.250341000	2.772291000
1	-4.304197000	-4.234797000	2.766336000	6	-1.630984000	-3.453532000	3.151260000
6	-6.990533000	-4.483157000	-0.008788000	6	-0.832254000	-4.527477000	3.542694000
1	-5.690328000	-3.229953000	-1.175181000	6	0.552875000	-4.387032000	3.564532000
6	-7.179979000	-5.145386000	1.202465000	6	1.142483000	-3.178195000	3.197925000
1	-6.352169000	-5.569525000	3.145472000	6	0.494998000	0.642224000	3.597083000
1	-7.736420000	-4.559117000	-0.794387000	6	0.291644000	0.212841000	4.914918000
1	-8.079094000	-5.731529000	1.367765000	6	-0.112196000	1.117728000	5.892411000
				6	-0.316066000	2.457822000	5.566000000
				6	-0.119112000	2.892661000	4.257680000
				6	0.279387000	1.987195000	3.277445000

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29	0.501482000	0.087158000	0.006762000	1	-2.379228000	-4.280234000	-0.786286000
15	2.441021000	0.258207000	-1.327096000	1	-5.761432000	-0.903347000	-0.088061000
15	1.043329000	-0.488823000	2.264537000	1	-5.680685000	1.531428000	0.083888000
8	2.902924000	-1.942613000	0.602287000	1	-2.084769000	4.746111000	-0.161128000
7	-1.194319000	-1.156248000	-0.499329000	1	4.188799000	-4.146725000	0.029676000
7	-1.101679000	1.539855000	-0.276304000	1	5.029260000	-4.772700000	-2.235014000
6	-1.206309000	-2.479385000	-0.630816000	1	4.712751000	-3.209293000	-4.141470000
6	-2.412786000	-3.203527000	-0.655706000	1	3.585453000	-1.038954000	-3.789545000
6	-3.631804000	-2.567574000	-0.542794000	1	0.113214000	-0.070722000	-2.905827000
6	-3.626309000	-1.151207000	-0.383902000	1	-0.605818000	0.719694000	-5.138272000
6	-4.813583000	-0.385386000	-0.179554000	1	0.875384000	2.209868000	-6.465073000
6	-4.768616000	0.970059000	-0.083580000	1	3.084790000	2.880909000	-5.556208000
6	-3.532633000	1.678226000	-0.179010000	1	3.822589000	2.066019000	-3.351473000
6	-3.449123000	3.099816000	-0.135362000	1	2.721244000	2.113147000	0.902981000
6	-2.191586000	3.665696000	-0.171139000	1	4.576409000	3.514794000	1.729645000
6	-1.034839000	2.867557000	-0.249226000	1	6.790063000	3.437317000	0.606457000
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6	-2.373017000	-0.493846000	-0.382839000	1	5.286858000	0.530216000	-2.165316000
6	0.107536000	-3.192208000	-0.748829000	1	0.275334000	-3.754388000	0.179252000
6	0.228278000	-4.139190000	-1.946750000	1	0.888601000	-2.429482000	-0.794932000
6	0.065944000	-3.452949000	-3.299560000	1	1.217068000	-4.611957000	-1.896846000

1	-0.499551000	-4.956988000	-1.860584000	6	-3.243586000	2.968175000	0.383356000
1	0.784032000	-2.625761000	-3.370492000	6	-3.374668000	1.560075000	0.529339000
1	-0.932506000	-2.999922000	-3.364471000	6	-4.630978000	0.911054000	0.732058000
1	1.277973000	-4.838508000	-4.451288000	6	-4.715804000	-0.441375000	0.830071000
1	0.143301000	-3.897898000	-5.429092000	6	-3.554942000	-1.265535000	0.709243000
1	-0.444895000	-5.236494000	-4.434038000	6	-3.605449000	-2.686488000	0.753025000
1	1.077200000	2.762456000	-0.249927000	6	-2.411228000	-3.377061000	0.678118000
1	0.423809000	4.241181000	0.469161000	6	-1.186605000	-2.703386000	0.525376000
1	-0.295478000	5.008470000	-1.819513000	6	-2.283223000	-0.658020000	0.577821000
1	0.366063000	3.529830000	-2.508142000	6	-2.189323000	0.786906000	0.517922000
1	5.579169000	-1.882297000	0.909540000	6	0.564460000	3.210981000	0.268639000
1	6.727012000	-0.774282000	2.806329000	6	0.112025000	-3.456263000	0.418151000
1	5.401941000	0.399889000	4.553133000	6	2.274770000	1.214222000	-2.664570000
1	2.939933000	0.494247000	4.373010000	6	3.325307000	1.630521000	-1.834245000
1	2.648284000	4.173704000	-1.728966000	6	4.229929000	2.608558000	-2.236815000
1	1.945740000	5.315489000	-2.858429000	6	4.114043000	3.171610000	-3.503134000
1	-1.675879000	-1.420481000	2.462923000	6	3.100362000	2.750269000	-4.361564000
1	-2.712679000	-3.552568000	3.138060000	6	2.194133000	1.782057000	-3.943624000
1	-1.289170000	-5.469060000	3.832978000	6	-0.518038000	0.405162000	-2.829172000
1	1.180213000	-5.217605000	3.875157000	6	-1.480524000	-0.597827000	-3.018505000
1	2.222743000	-3.074456000	3.233629000	6	-2.766644000	-0.274862000	-3.439634000
1	1.317651000	6.827326000	-0.919826000	6	-3.118601000	1.054781000	-3.664572000
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6	-5.011126000	-4.491892000	0.232697000	6	4.162068000	-0.050666000	-0.384238000
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1	-7.833347000	-3.606735000	-2.259759000	6	4.326642000	1.804741000	2.441449000
1	-6.251207000	-6.142151000	0.825842000	6	4.744647000	2.918422000	3.168609000
1	-8.070666000	-5.577965000	-0.768097000	6	3.885092000	3.525508000	4.080011000
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B3

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1	5.802197000	2.095154000	0.367173000				
6	5.181657000	0.071266000	0.286720000				
1	6.194463000	-0.312468000	0.326728000				
6	4.096106000	-0.853455000	0.206398000				
6	2.769822000	-0.362191000	0.138811000				
6	4.281900000	-2.263310000	0.161908000				
6	3.161926000	-3.056551000	-0.002420000				
1	3.278434000	-4.133273000	-0.047251000				
6	1.876294000	-2.493550000	-0.060440000				
6	0.650082000	-3.348321000	-0.231363000				
1	0.421896000	-3.417940000	-1.303687000				
1	-0.193672000	-2.809262000	0.214683000				
6	0.737199000	-4.762453000	0.356507000				
1	1.514842000	-5.335466000	-0.159355000				
1	1.034954000	-4.696430000	1.410012000				
6	-0.569797000	-5.506906000	0.244202000				
6	-1.603147000	-5.273179000	1.158152000				
1	-1.447775000	-4.564707000	1.969140000				
6	-2.816702000	-5.947617000	1.050153000				
1	-3.605368000	-5.758254000	1.773335000				
6	-3.015209000	-6.872457000	0.025572000				
1	-3.958160000	-7.405808000	-0.054367000				
6	-1.992459000	-7.114600000	-0.888959000				
1	-2.135257000	-7.837512000	-1.687366000				
6	-0.781273000	-6.434689000	-0.779223000				
				B4-1			
				29	0.217313000	-0.152947000	-0.325376000
				15	1.899952000	-0.609813000	-1.878088000
				15	0.780952000	-0.119475000	2.012053000
				8	3.237027000	0.547367000	0.378236000
				7	-1.036261000	1.572497000	-0.468731000
				7	-1.732363000	-1.052735000	-0.383910000
				6	2.656822000	0.785391000	-2.799496000
				6	4.037970000	0.908752000	-2.983663000
				1	4.714250000	0.193887000	-2.523052000
				6	4.550893000	1.945930000	-3.760528000
				1	5.624565000	2.032520000	-3.900648000
				6	3.691376000	2.866388000	-4.356124000
				1	4.093662000	3.674482000	-4.959771000
				6	2.314579000	2.751918000	-4.171292000
				1	1.640911000	3.470695000	-4.628314000
				6	1.798872000	1.718927000	-3.393835000
				1	0.724351000	1.636813000	-3.246293000
				6	1.522451000	-1.765751000	-3.250618000
				6	2.462218000	-2.083131000	-4.241863000
				1	3.459417000	-1.652823000	-4.205727000
				6	2.120694000	-2.939359000	-5.282944000
				1	2.856155000	-3.182427000	-6.044164000
				6	0.835082000	-3.476694000	-5.355151000
				1	0.570606000	-4.141967000	-6.171864000
				6	-0.110393000	-3.149552000	-4.388139000
				1	-1.116611000	-3.553800000	-4.447652000
				6	0.231600000	-2.295024000	-3.341285000
				1	-0.510889000	-2.021837000	-2.597569000
				6	3.298726000	-1.371791000	-0.976867000
				6	3.836409000	-2.628348000	-1.271387000
				1	3.482103000	-3.168572000	-2.143657000
				6	4.812073000	-3.200367000	-0.458052000
				1	5.220472000	-4.174764000	-0.706616000
				6	5.256889000	-2.517142000	0.669221000
				1	6.012714000	-2.956938000	1.312841000
				6	4.742239000	-1.262554000	0.985155000

1	5.089260000	-0.729467000	1.863436000	6	-3.387222000	-2.783815000	-0.377487000
6	3.775231000	-0.696118000	0.160483000	1	-3.607710000	-3.845131000	-0.384832000
6	3.289056000	1.098738000	1.645597000	6	-2.046084000	-2.350695000	-0.297374000
6	4.390814000	1.875096000	1.991855000	6	-0.940863000	-3.289958000	-0.159910000
1	5.190005000	2.008482000	1.270794000	1	0.042464000	-2.852851000	-0.318612000
6	4.440099000	2.474660000	3.245021000	6	-1.062543000	-4.589768000	0.175713000
1	5.297625000	3.082441000	3.516567000	1	-2.048877000	-4.983824000	0.415661000
6	3.390597000	2.295803000	4.144132000	6	0.026405000	-5.552975000	0.299467000
1	3.426201000	2.758658000	5.125398000	6	-0.198690000	-6.740877000	1.012784000
6	2.290012000	1.527370000	3.782588000	1	-1.178928000	-6.921806000	1.446843000
1	1.470634000	1.406800000	4.484752000	6	0.816488000	-7.675663000	1.181987000
6	2.211092000	0.920153000	2.521881000	1	0.625384000	-8.584904000	1.744240000
6	1.070961000	-1.646586000	2.991952000	6	2.074043000	-7.447058000	0.627185000
6	0.810467000	-1.718537000	4.367032000	1	2.867195000	-8.178229000	0.752407000
1	0.366361000	-0.872904000	4.883956000	6	2.305688000	-6.280827000	-0.104160000
6	1.103921000	-2.878211000	5.076809000	1	3.278525000	-6.105630000	-0.554008000
1	0.893712000	-2.924789000	6.141452000	6	1.293496000	-5.344533000	-0.269932000
6	1.665885000	-3.975810000	4.425295000	1	1.480383000	-4.454575000	-0.863579000
1	1.892037000	-4.880526000	4.982208000	6	-5.807442000	-2.381710000	-0.641258000
6	1.932715000	-3.911389000	3.060934000	6	-8.395975000	-3.418889000	-0.909676000
1	2.362180000	-4.763827000	2.542913000	6	-6.308540000	-3.295131000	0.294554000
6	1.634723000	-2.751973000	2.347494000	6	-6.617891000	-2.000471000	-1.719117000
1	1.850923000	-2.705789000	1.283840000	6	-7.902096000	-2.519037000	-1.852091000
6	-0.661798000	0.666965000	2.821969000	6	-7.596333000	-3.805625000	0.163504000
6	-0.769401000	2.059026000	2.931195000	1	-5.688673000	-3.591195000	1.136451000
1	0.064054000	2.694882000	2.647166000	1	-6.231432000	-1.314065000	-2.467275000
6	-1.943455000	2.641639000	3.402542000	1	-8.516087000	-2.222788000	-2.697397000
1	-2.007654000	3.722583000	3.488297000	1	-7.975728000	-4.505299000	0.902325000
6	-3.028288000	1.845705000	3.762375000	1	-9.400177000	-3.819117000	-1.012988000
1	-3.941354000	2.301945000	4.133644000	6	-3.941771000	4.734446000	-0.387126000
6	-2.935129000	0.460541000	3.643836000	6	-5.702272000	6.908557000	-0.252221000
1	-3.775914000	-0.169096000	3.920400000	6	-4.899222000	4.811005000	0.633213000
6	-1.763979000	-0.125587000	3.172199000	6	-3.872084000	5.764746000	-1.332487000
1	-1.706671000	-1.206987000	3.084093000	6	-4.751056000	6.841779000	-1.267832000
6	-2.353632000	1.264968000	-0.479188000	6	-5.771349000	5.893189000	0.699711000
6	-3.372322000	2.249226000	-0.473662000	1	-4.942454000	4.031361000	1.388933000
6	-2.970901000	3.616346000	-0.437555000	1	-3.135125000	5.710242000	-2.129097000
6	-1.622736000	3.892763000	-0.447103000	1	-4.693057000	7.629152000	-2.013515000
1	-1.295613000	4.926046000	-0.440949000	1	-6.502940000	5.945362000	1.500620000
6	-0.663272000	2.856470000	-0.441337000	1	-6.386366000	7.750405000	-0.200937000
6	0.766449000	3.139958000	-0.395172000				
1	1.411763000	2.294919000	-0.625964000				
6	1.294965000	4.335717000	-0.060682000				
1	0.626560000	5.135176000	0.256044000				
6	2.708902000	4.696131000	-0.052445000				
6	3.686053000	3.952249000	-0.733541000				
1	3.400783000	3.072758000	-1.301803000				
6	5.017047000	4.348721000	-0.709679000				
1	5.757208000	3.768729000	-1.253826000				
6	5.402240000	5.489245000	-0.004005000				
1	6.444021000	5.796186000	0.010053000				
6	4.441722000	6.240939000	0.670241000				
1	4.731445000	7.134616000	1.215187000				
6	3.107338000	5.852556000	0.637378000				
1	2.358332000	6.445712000	1.156473000				
6	-4.737898000	1.846673000	-0.5329820000				
1	-5.507699000	2.609373000	-0.553689000				
6	-5.084923000	0.530963000	-0.553528000				
1	-6.130856000	0.248064000	-0.579998000				
6	-4.094879000	-0.493312000	-0.522180000				
6	-2.724429000	-0.136617000	-0.469624000				
6	-4.419257000	-1.881907000	-0.511228000				
				B4-2			
				29	0.109358000	-0.229013000	-0.152199000
				15	0.370287000	1.477955000	-1.709691000
				15	-0.249332000	0.401045000	2.134772000
				8	-1.308344000	2.605434000	0.315553000
				7	-1.242203000	-1.854489000	-0.434791000
				7	1.452943000	-1.892160000	-0.129449000
				6	-1.005639000	1.963811000	-2.823754000
				6	-1.348055000	3.296343000	-3.070488000
				1	-0.856951000	4.095095000	-2.521500000
				6	-2.311845000	3.605453000	-4.028773000
				1	-2.569509000	4.643853000	-4.216496000
				6	-2.936912000	2.589225000	-4.748483000
				1	-3.683036000	2.833320000	-5.498773000
				6	-2.609080000	1.257610000	-4.496567000
				1	-3.099645000	0.460903000	-5.048192000
				6	-1.653681000	0.945304000	-3.533076000
				1	-1.402171000	-0.094841000	-3.337270000
				6	1.717966000	1.302776000	-2.942925000
				6	2.071665000	2.333163000	-3.825335000

1	1.573036000	3.296901000	-3.766906000	1	-5.197608000	-1.056042000	-1.077363000
6	3.051816000	2.125310000	-4.789907000	6	-5.189468000	1.060408000	-0.899426000
1	3.322883000	2.931528000	-5.465224000	6	-4.830081000	2.271366000	-1.494803000
6	3.673624000	0.880887000	-4.901122000	1	-4.046447000	2.285551000	-2.247742000
1	4.432409000	0.719417000	-5.661200000	6	-5.458893000	3.466521000	-1.167242000
6	3.310365000	-0.155749000	-4.046033000	1	-5.149044000	4.370773000	-1.678989000
1	3.781134000	-1.130346000	-4.136847000	6	-6.484419000	3.508933000	-0.199307000
6	2.337843000	0.055926000	-3.069235000	6	-6.858623000	2.283168000	0.390168000
1	2.046360000	-0.753528000	-2.405587000	1	-7.661539000	2.246795000	1.117353000
6	0.759754000	2.980898000	-0.746633000	6	-6.217900000	1.099550000	0.045422000
6	1.965727000	3.683278000	-0.830976000	1	-6.542252000	0.175523000	0.521021000
1	2.706613000	3.393309000	-1.568070000	6	-0.589487000	-5.507945000	-0.584000000
6	2.249579000	4.729355000	0.044266000	1	-1.133161000	-6.438962000	-0.696365000
1	3.199532000	5.249549000	-0.029546000	6	0.765712000	-5.523255000	-0.480033000
6	1.319741000	5.087679000	1.015040000	1	1.297690000	-6.467515000	-0.492435000
1	1.529655000	5.903913000	1.699757000	6	1.510678000	-4.313096000	-0.334346000
6	0.116068000	4.396726000	1.130776000	6	0.820867000	-3.077716000	-0.300195000
1	-0.603437000	4.664438000	1.896930000	6	2.926093000	-4.282363000	-0.185547000
6	-0.151037000	3.344584000	0.260655000	6	3.526768000	-3.056398000	0.033146000
6	-1.986166000	2.533953000	1.518562000	1	4.603224000	-3.005800000	0.152611000
6	-3.054631000	3.401003000	1.720931000	6	2.771549000	-1.871225000	0.055651000
1	-3.319894000	4.098577000	0.933719000	6	3.413782000	-0.530824000	0.281407000
6	-3.768255000	3.345767000	2.912859000	1	3.413961000	-0.322965000	1.360200000
1	-4.605392000	4.019186000	3.068799000	1	2.760529000	0.227599000	-0.165066000
6	-3.403331000	2.433211000	3.900325000	6	4.839648000	-0.371130000	-0.266520000
1	-3.947173000	2.394965000	4.839033000	1	5.526157000	-1.018771000	0.291982000
6	-2.344952000	1.558754000	3.679582000	1	4.863605000	-0.707840000	-1.309425000
1	-2.081345000	0.839385000	4.449012000	6	5.320062000	1.055288000	-0.188270000
6	-1.625829000	1.574512000	2.476393000	6	5.299956000	1.893589000	-1.305484000
6	1.080810000	1.040330000	3.231204000	1	4.962349000	1.500549000	-2.262360000
6	1.084165000	0.809390000	4.613460000	6	5.709413000	3.220276000	-1.238368000
1	0.317773000	0.186061000	5.064819000	1	5.687768000	3.815567000	-2.144079000
6	2.077794000	1.361783000	5.415078000	6	6.150087000	3.784621000	-0.023127000
1	2.072899000	1.172831000	6.484700000	6	6.199489000	2.929379000	1.098727000
6	3.075499000	2.154393000	4.848249000	1	6.570563000	3.293945000	2.049798000
1	3.850430000	2.583702000	5.476818000	6	5.788279000	1.605165000	1.007854000
6	3.078292000	2.390255000	3.476559000	1	5.843350000	0.982119000	1.898628000
1	3.855412000	2.997691000	3.022506000	6	3.767193000	-5.499622000	-0.252431000
6	2.087068000	1.833281000	2.670257000	6	5.440523000	-7.742729000	-0.392176000
1	2.098320000	2.022169000	1.600564000	6	4.679102000	-5.772636000	0.774968000
6	-0.750456000	-1.166888000	2.944295000	6	3.710805000	-6.361519000	-1.356092000
6	-2.085349000	-1.568341000	3.067483000	6	4.544713000	-7.473222000	-1.424847000
1	-2.888452000	-0.886648000	2.806069000	6	5.505522000	-6.889944000	0.707529000
6	-2.402008000	-2.840378000	3.540562000	1	4.726156000	-5.113062000	1.637100000
1	-3.444269000	-3.130649000	3.636740000	1	3.028843000	-6.145730000	-2.173756000
6	-1.391946000	-3.731254000	3.892097000	1	4.497604000	-8.127124000	-2.290596000
1	-1.640567000	-4.720731000	4.264391000	1	6.200336000	-7.094933000	1.516571000
6	-0.058874000	-3.344070000	3.765716000	1	6.087662000	-8.613143000	-0.445861000
1	0.737374000	-4.030857000	4.037992000	6	-3.594722000	-5.431483000	-0.686736000
6	0.260300000	-2.076136000	3.290625000	6	-5.286863000	-7.662432000	-0.769306000
1	1.304399000	-1.790133000	3.194412000	6	-3.508413000	-6.425935000	0.296870000
6	-0.621048000	-3.059100000	-0.437614000	6	-4.546271000	-5.564942000	-1.705397000
6	-1.322477000	-4.282436000	-0.547636000	6	-5.382395000	-6.676446000	-1.748876000
6	-2.741940000	-4.221840000	-0.627846000	6	-4.351741000	-7.531881000	0.255548000
6	-3.335754000	-2.974900000	-0.631485000	1	-2.795634000	-6.317484000	1.109690000
1	-4.416896000	-2.906900000	-0.670523000	1	-4.617209000	-4.799783000	-2.473602000
6	-2.568828000	-1.800250000	-0.527238000	1	-6.108779000	-6.772349000	-2.550468000
6	-3.222830000	-0.449329000	-0.413222000	1	-4.281473000	-8.290522000	1.029439000
1	-2.478569000	0.317573000	-0.656770000	1	-5.941298000	-8.528435000	-0.802184000
1	-3.475961000	-0.298091000	0.645512000	7	6.510998000	5.115591000	0.066739000
6	-4.495249000	-0.232573000	-1.244761000	6	7.189680000	5.578694000	1.256558000
1	-4.234365000	-0.250931000	-2.309389000	1	8.151825000	5.071717000	1.427786000

1	6.567009000	5.432426000	2.145935000	6	-2.620938000	-3.978393000	1.534041000
1	7.379638000	6.648870000	1.164511000	6	-1.297144000	-3.569231000	1.394541000
6	6.690113000	5.876278000	-1.150012000	6	1.455773000	-2.556758000	-1.308320000
1	7.482100000	5.470491000	-1.798180000	6	0.827801000	-3.500809000	-2.124037000
1	6.952374000	6.903260000	-0.892368000	6	1.420743000	-3.891066000	-3.323720000
1	5.762136000	5.912061000	-1.731097000	6	2.640947000	-3.344287000	-3.713853000
7	-7.090676000	4.698719000	0.160713000	6	3.275940000	-2.407404000	-2.899397000
6	-6.866911000	5.870964000	-0.655508000	6	2.684142000	-2.012623000	-1.703859000
1	-7.201473000	5.740904000	-1.696446000	6	1.723079000	-2.705192000	1.540874000
1	-5.805405000	6.141424000	-0.673601000	6	2.045430000	-4.067880000	1.502484000
1	-7.409725000	6.713847000	-0.225453000	6	2.815846000	-4.630498000	2.513949000
6	-8.297234000	4.655452000	0.956237000	6	3.276505000	-3.836042000	3.565532000
1	-9.121843000	4.120538000	0.459849000	6	2.970430000	-2.478877000	3.603514000
1	-8.626019000	5.675321000	1.160698000	6	2.196357000	-1.913645000	2.590772000
1	-8.114038000	4.172007000	1.922008000	1	3.050696000	1.006138000	-4.451809000

XYZ Coordinates of the triplet excited states.

A1 (T₁)

29	0.440081000	0.508935000	0.170612000
15	-1.909522000	1.071982000	0.041843000
15	0.721280000	-1.907670000	0.239449000
8	-1.477878000	-1.429477000	-1.529880000
7	1.886750000	1.278518000	-1.296006000
7	1.753061000	1.751525000	1.379243000
6	1.907122000	1.008460000	-2.632520000
6	3.053861000	1.257857000	-3.397076000
6	4.165507000	1.825008000	-2.813857000
6	4.140737000	2.166202000	-1.424540000
6	5.183570000	2.789548000	-0.760863000
6	5.070877000	3.131673000	0.666285000
6	3.932837000	2.810532000	1.388226000
6	3.755293000	3.106440000	2.775638000
6	2.586544000	2.731369000	3.410817000
6	1.590241000	2.052415000	2.707291000
6	2.844232000	2.124847000	0.743449000
6	2.935708000	1.829401000	-0.714122000
6	0.657865000	0.425986000	-3.213738000
6	0.302562000	1.619000000	3.329567000
6	-2.650401000	0.673041000	-1.590552000
6	-2.363235000	-0.573729000	-2.163376000
6	-2.854377000	-0.935824000	-3.410233000
6	-3.659808000	-0.040785000	-4.110969000
6	-3.958754000	1.204373000	-3.563955000
6	-3.454579000	1.558516000	-2.313907000
6	-2.133586000	2.882159000	0.182997000
6	-3.212604000	3.499452000	0.821850000
6	-3.285097000	4.890392000	0.880997000
6	-2.287731000	5.670550000	0.301496000
6	-1.205063000	5.060706000	-0.331175000
6	-1.122238000	3.672930000	-0.380885000
6	-3.116661000	0.312911000	1.190258000
6	-2.633853000	-0.401800000	2.289065000
6	-3.517352000	-1.035157000	3.160332000
6	-4.888855000	-0.959229000	2.935190000
6	-5.378417000	-0.258434000	1.832901000
6	-4.497072000	0.369632000	0.959186000
6	-0.923418000	-2.699171000	0.367091000
6	-1.915923000	-2.261751000	-0.522870000
6	-3.241505000	-2.659570000	-0.395847000
6	-3.588351000	-3.515857000	0.645666000

6	-2.620938000	-3.978393000	1.534041000
6	-1.297144000	-3.569231000	1.394541000
6	1.455773000	-2.556758000	-1.308320000
6	0.827801000	-3.500809000	-2.124037000
6	1.420743000	-3.891066000	-3.323720000
6	2.640947000	-3.344287000	-3.713853000
6	3.275940000	-2.407404000	-2.899397000
6	2.684142000	-2.012623000	-1.703859000
6	1.723079000	-2.705192000	1.540874000
6	2.045430000	-4.067880000	1.502484000
6	2.815846000	-4.630498000	2.513949000
6	3.276505000	-3.836042000	3.565532000
6	2.970430000	-2.478877000	3.603514000
6	2.196357000	-1.913645000	2.590772000
1	3.050696000	1.006138000	-4.451809000
1	5.058646000	2.032290000	-3.393872000
1	6.092367000	3.042127000	-1.294376000
1	5.895911000	3.637651000	1.154005000
1	4.540839000	3.628635000	3.310921000
1	2.432017000	2.958458000	4.459737000
1	0.217451000	0.525562000	3.314950000
1	-0.548789000	2.022308000	2.767284000
1	0.228963000	1.954470000	4.364787000
1	-2.589652000	-1.906194000	-3.816924000
1	-4.046004000	-0.316049000	-5.086305000
1	-4.580320000	1.904684000	-4.110942000
1	-3.678855000	2.536660000	-1.897803000
1	-3.993126000	2.900573000	1.280025000
1	-4.123543000	5.363065000	1.381744000
1	-2.349047000	6.752731000	0.349061000
1	-0.421253000	5.665064000	-0.775657000
1	-0.265373000	3.194862000	-0.853853000
1	-1.561844000	-0.490704000	2.443832000
1	-3.131799000	-1.599705000	4.002924000
1	-5.577881000	-1.456141000	3.610358000
1	-6.446677000	-0.209017000	1.649542000
1	-4.881853000	0.891948000	0.086819000
1	-3.988426000	-2.291745000	-1.091213000
1	-4.623645000	-3.819486000	0.759901000
1	-2.896688000	-4.646589000	2.342354000
1	-0.549538000	-3.913801000	2.101855000
1	0.402070000	-0.516021000	-2.714782000
1	0.768949000	0.238285000	-4.282834000
1	-0.182824000	1.114694000	-3.062910000
1	-0.125820000	-3.927967000	-1.827252000
1	0.926239000	-4.622761000	-3.954264000
1	3.096488000	-3.646558000	-4.651090000
1	4.224609000	-1.974001000	-3.199539000
1	3.173521000	-1.266520000	-1.079741000
1	1.692117000	-4.683476000	0.678839000
1	3.062065000	-5.686633000	2.482281000
1	3.880501000	-4.277343000	4.351507000
1	3.336645000	-1.858639000	4.414840000
1	1.970551000	-0.849783000	2.604836000

A2 (T₁)

29	0.437583000	0.420868000	-0.167486000
15	-1.845166000	0.190902000	0.619943000
15	1.258720000	-1.781114000	-0.796280000
8	-0.385798000	-2.234749000	1.529622000
7	2.089220000	1.354333000	0.939065000

7	0.850801000	2.243794000	-1.322683000	1	0.006905000	4.189974000	-3.951828000
6	2.684636000	0.845546000	2.057627000	1	-0.687002000	-3.313795000	3.865958000
6	3.936597000	1.321254000	2.479855000	1	-2.122695000	-2.416800000	5.708461000
6	4.565931000	2.329950000	1.788196000	1	-3.455724000	-0.354489000	5.333335000
6	3.932659000	2.902787000	0.638306000	1	-3.362393000	0.803810000	3.150763000
6	4.458018000	3.957309000	-0.087085000	1	-0.591426000	2.688191000	1.132974000
6	3.732737000	4.511834000	-1.241905000	1	-1.390274000	5.013108000	1.383290000
6	2.525759000	3.968639000	-1.651539000	1	-3.807656000	5.530048000	1.142541000
6	1.774168000	4.451034000	-2.768231000	1	-5.422413000	3.703035000	0.686333000
6	0.591435000	3.832673000	-3.110446000	1	-4.640945000	1.376090000	0.478804000
6	0.133060000	2.726096000	-2.383474000	1	-1.735594000	-0.910001000	-2.069859000
6	1.969228000	2.840781000	-0.953666000	1	-3.328259000	-2.197662000	-3.444827000
6	2.672521000	2.322241000	0.255830000	1	-5.550370000	-2.816370000	-2.527263000
6	1.928316000	-0.180496000	2.842989000	1	-6.156226000	-2.164730000	-0.210217000
6	1.277793000	0.420466000	4.103256000	1	-4.561025000	-0.893073000	1.177447000
6	0.383069000	1.618543000	3.795382000	1	2.604604000	-0.998675000	3.121819000
6	-0.389977000	2.110383000	5.014090000	1	1.153470000	-0.607453000	2.198260000
6	-1.154273000	2.039243000	-2.728549000	1	0.682419000	-0.362571000	4.589696000
6	-2.391440000	2.945742000	-2.613270000	1	2.058551000	0.716769000	4.815908000
6	-3.701599000	2.179998000	-2.814613000	1	-0.323394000	1.333759000	3.006665000
6	-3.810031000	1.480749000	-4.167890000	1	0.988922000	2.436828000	3.383977000
6	-2.006913000	-0.610849000	2.263198000	1	-1.018943000	1.311064000	5.418563000
6	-1.259523000	-1.773136000	2.501063000	1	-1.039013000	2.952370000	4.757091000
6	-1.293114000	-2.424646000	3.727183000	1	0.291199000	2.436919000	5.806312000
6	-2.092021000	-1.914052000	4.748031000	1	-1.275301000	1.182042000	-2.058762000
6	-2.840492000	-0.758374000	4.536579000	1	-1.089048000	1.641816000	-3.750037000
6	-2.794305000	-0.109913000	3.303609000	1	-2.320364000	3.752484000	-3.354044000
6	-2.564980000	1.863494000	0.826153000	1	-2.395616000	3.418959000	-1.623847000
6	-1.655823000	2.904659000	1.065200000	1	-2.580113000	-3.788178000	1.534084000
6	-2.102732000	4.216843000	1.194499000	1	-3.267486000	-5.222552000	-0.371291000
6	-3.459259000	4.505983000	1.058020000	1	-1.898900000	-5.282984000	-2.443934000
6	-4.367020000	3.480060000	0.802637000	1	0.121820000	-3.873177000	-2.629360000
6	-3.924839000	2.163294000	0.692632000	1	-3.807350000	1.436282000	-2.014972000
6	-3.058694000	-0.764607000	-0.370310000	1	-4.534005000	2.882328000	-2.693196000
6	-2.715494000	-1.156640000	-1.668029000	1	3.854475000	-0.689795000	-0.290794000
6	-3.610211000	-1.891451000	-2.442653000	1	5.705125000	-1.292992000	1.227958000
6	-4.853420000	-2.243440000	-1.924506000	1	5.508759000	-3.284554000	2.701866000
6	-5.195281000	-1.876563000	-0.623375000	1	3.461575000	-4.683043000	2.621375000
6	-4.299708000	-1.148543000	0.153632000	1	1.614730000	-4.098465000	1.086727000
6	-0.066717000	-3.037099000	-0.657346000	1	-3.637960000	2.183180000	-4.990539000
6	-0.844855000	-3.040437000	0.509613000	1	-4.801606000	1.040356000	-4.301027000
6	-1.989615000	-3.820389000	0.624657000	1	-3.081108000	0.669411000	-4.259965000
6	-2.367721000	-4.621414000	-0.449286000	1	2.999493000	-3.843518000	-2.061771000
6	-1.602003000	-4.654139000	-1.611929000	1	3.821026000	-4.101680000	-4.385138000
6	-0.459913000	-3.864180000	-1.713066000	1	3.215688000	-2.427428000	-6.110902000
6	2.611929000	-2.359357000	0.291790000	1	1.794307000	-0.484603000	-5.513363000
6	3.771277000	-1.574994000	0.338082000	1	0.982199000	-0.215169000	-3.183222000
6	4.813218000	-1.910592000	1.196575000				
6	4.700656000	-3.026659000	2.025279000				
6	3.549911000	-3.810887000	1.981829000				
6	2.507914000	-3.481606000	1.116291000				
6	1.923701000	-2.020765000	-2.479103000				
6	2.732768000	-3.111446000	-2.819731000				
6	3.194063000	-3.255554000	-4.124266000				
6	2.852472000	-2.312848000	-5.094893000				
6	2.053459000	-1.222395000	-4.761242000				
6	1.593174000	-1.074421000	-3.454010000				
1	4.395773000	0.879657000	3.358675000				
1	5.531921000	2.710848000	2.103066000				
1	5.406889000	4.394257000	0.201201000				
1	4.157354000	5.351758000	-1.779191000				
1	2.147028000	5.301293000	-3.329316000				
				A3 (T1)			
				29	-0.046144000	-0.145381000	-0.705559000
				15	-1.017243000	0.159287000	1.577517000
				15	2.216966000	0.602004000	-0.865251000
				8	1.973601000	-0.233302000	1.870497000
				7	-0.843442000	-2.114213000	-1.138192000
				7	-1.829874000	0.306832000	-1.895344000
				6	-0.337805000	-3.284946000	-0.644093000
				6	-1.027022000	-4.487164000	-0.836188000
				6	-2.215966000	-4.501193000	-1.538426000
				6	-2.756284000	-3.281634000	-2.049814000
				6	-3.955606000	-3.191095000	-2.737266000
				6	-4.462950000	-1.887634000	-3.194905000

6	-3.766379000	-0.720688000	-2.932538000	1	-0.495384000	4.973019000	2.467116000
6	-4.222020000	0.582546000	-3.304733000	1	-2.538042000	5.167697000	3.871184000
6	-3.496408000	1.693187000	-2.930785000	1	-3.958498000	3.172779000	4.267556000
6	-2.308809000	1.552443000	-2.199226000	1	-3.343495000	0.993230000	3.286598000
6	-2.516089000	-0.770747000	-2.223095000	1	2.098294000	1.431826000	3.978777000
6	-1.989501000	-2.094667000	-1.785303000	1	2.532476000	3.864393000	3.809079000
6	0.926057000	-3.142247000	0.152790000	1	2.870547000	4.920810000	1.584617000
6	-1.491039000	2.718804000	-1.718231000	1	2.807040000	3.534117000	-0.459867000
6	-0.134513000	-0.641230000	2.978998000	1	0.656967000	-2.703036000	1.128509000
6	1.262735000	-0.741717000	2.946126000	1	1.553526000	-2.385949000	-0.340227000
6	1.974254000	-1.374480000	3.959857000	1	4.594664000	0.314009000	0.962424000
6	1.286482000	-1.910280000	5.044210000	1	6.508422000	-1.240477000	0.922150000
6	-0.101672000	-1.800234000	5.114845000	1	6.686447000	-2.960450000	-0.857416000
6	-0.801490000	-1.170741000	4.090682000	1	4.917531000	-3.129642000	-2.592293000
6	-2.555722000	-0.815173000	1.387044000	1	2.973984000	-1.605012000	-2.534846000
6	-3.650748000	-0.201940000	0.762924000	1	4.654073000	2.108037000	-1.682099000
6	-4.761063000	-0.952375000	0.385281000	1	5.154252000	3.467920000	-3.689703000
6	-4.788929000	-2.326078000	0.618395000	1	3.443587000	3.742925000	-5.463734000
6	-3.702998000	-2.944221000	1.234874000	1	1.231786000	2.642821000	-5.238360000
6	-2.590414000	-2.196373000	1.613418000	1	0.727249000	1.280234000	3.225542000
6	-1.573693000	1.749363000	2.304641000	6	1.766495000	-4.399871000	0.386354000
6	-0.785980000	2.881314000	2.072048000	1	1.155217000	-5.143602000	0.915585000
6	-1.122740000	4.105390000	2.647163000	6	2.260018000	-5.003499000	-0.929479000
6	-2.266007000	4.212733000	3.433778000	1	2.867449000	-5.893539000	-0.742186000
6	-3.065277000	3.091183000	3.657047000	1	2.883784000	-4.275038000	-1.457960000
6	-2.717031000	1.861913000	3.105261000	1	1.438812000	-5.287473000	-1.592995000
6	2.429746000	1.694120000	0.586860000	6	2.951447000	-4.031148000	1.280720000
6	2.212964000	1.125025000	1.852822000	1	3.589630000	-4.899752000	1.466012000
6	2.262036000	1.893494000	3.011567000	1	2.611895000	-3.641252000	2.245655000
6	2.503916000	3.261671000	2.907646000	1	3.561366000	-3.256840000	0.797850000
6	2.694087000	3.853870000	1.662845000	6	-2.252548000	4.025722000	-1.457516000
6	2.661117000	3.069776000	0.510019000	1	-2.714674000	4.355108000	-2.397652000
6	3.653660000	-0.537940000	-0.783791000	6	-3.350394000	3.849511000	-0.405976000
6	4.652728000	-1.644615000	0.187954000	1	-2.922356000	3.493864000	0.538288000
6	5.737845000	-1.319661000	0.162341000	1	-4.111734000	3.131675000	-0.726055000
6	5.838296000	-2.284242000	-0.836835000	1	-3.850630000	4.802171000	-0.209120000
6	4.845369000	-2.379757000	-1.811015000	6	-1.255762000	5.103898000	-1.030288000
6	3.752696000	-1.517950000	-1.778956000	1	-0.749887000	4.808221000	-0.104412000
6	2.643356000	1.634868000	-2.310282000	1	-1.762876000	6.055141000	-0.847171000
6	3.899742000	2.237775000	-2.454559000	1	-0.491876000	5.264369000	-1.797280000
6	4.182123000	2.998193000	-3.583667000				
6	3.218629000	3.151122000	-4.582578000				
6	1.976212000	2.537216000	-4.456144000				
6	1.690414000	1.777229000	-3.322155000				
1	-0.623437000	-5.407863000	-0.430026000	29	-0.033161000	0.533045000	-0.721015000
1	-2.758597000	-5.427185000	-1.698053000	15	-0.659847000	-1.707122000	-1.110266000
1	-4.536872000	-4.084253000	-2.934252000	15	0.440238000	1.050602000	1.657541000
1	-5.403057000	-1.845917000	-3.732720000	8	1.180263000	-1.831206000	1.082863000
1	-5.148828000	0.681068000	-3.860128000	7	1.420456000	1.780263000	-1.688195000
1	-3.851514000	2.684785000	-3.187237000	7	-1.199814000	2.294813000	-1.249862000
1	-0.689952000	2.917509000	-2.445748000	6	0.506135000	-2.923135000	-1.830507000
1	-0.982407000	2.412332000	-0.790904000	6	0.808926000	-4.145043000	-1.227512000
1	3.054901000	-1.432278000	3.881775000	1	0.371083000	-4.403458000	-0.267504000
1	1.836102000	-2.405884000	5.837027000	6	1.667563000	-5.041318000	-1.863287000
1	-0.638572000	-2.207853000	5.964157000	1	1.894146000	-5.992977000	-1.392881000
1	-1.884743000	-1.102942000	4.141395000	6	2.229039000	-4.721977000	-3.097459000
1	-3.631075000	0.867207000	0.558802000	1	2.897686000	-5.421969000	-3.587411000
1	-5.598384000	-0.462781000	-0.102087000	6	1.932940000	-3.499638000	-3.701333000
1	-5.649596000	-2.912931000	0.314173000	1	2.370595000	-3.244337000	-4.660664000
1	-3.713021000	-4.014897000	1.412257000	6	1.079257000	-2.601422000	-3.067690000
1	-1.744378000	-2.697005000	2.076717000	1	0.852245000	-1.645893000	-3.537109000
1	0.093253000	2.810413000	1.436379000	6	-2.147379000	-1.962234000	-2.145441000
				6	-2.738733000	-3.220081000	-2.321072000

A4 (T1)

1	-2.360072000	-4.078062000	-1.770738000	1	4.911472000	-0.329928000	-2.364114000
6	-3.796348000	-3.377267000	-3.210577000	1	5.209705000	0.596395000	-0.896938000
1	-4.251938000	-4.353256000	-3.340962000	6	4.938419000	-1.493701000	-0.557610000
6	-4.255833000	-2.286215000	-3.951445000	6	4.263370000	-2.689529000	-0.830108000
1	-5.070595000	-2.415828000	-4.656256000	1	3.482747000	-2.715098000	-1.587228000
6	-3.668902000	-1.034210000	-3.788127000	6	4.591292000	-3.860119000	-0.151172000
1	-4.023647000	-0.184330000	-4.362213000	1	4.061200000	-4.778323000	-0.385015000
6	-2.621766000	-0.871043000	-2.880758000	6	5.593036000	-3.854550000	0.819492000
1	-2.158021000	0.105877000	-2.754036000	1	5.849486000	-4.768273000	1.346135000
6	-1.063520000	-2.348624000	0.551349000	6	6.260923000	-2.667217000	1.107073000
6	-2.338703000	-2.756506000	0.951921000	1	7.039612000	-2.648480000	1.863449000
1	-3.148791000	-2.788867000	0.229892000	6	5.932811000	-1.498002000	0.422566000
6	-2.592659000	-3.095539000	2.280879000	1	6.458712000	-0.574604000	0.651237000
1	-3.590807000	-3.402631000	2.572093000	6	1.249298000	5.202768000	-2.962921000
6	-1.569803000	-3.026724000	3.221047000	1	1.869830000	5.971570000	-3.408431000
1	-1.760778000	-3.288838000	4.256341000	6	-0.171697000	5.494543000	-2.700827000
6	-0.293812000	-2.606416000	2.850971000	1	-0.563264000	6.473695000	-2.951705000
1	0.501938000	-2.535710000	3.584105000	6	-1.001701000	4.539396000	-2.138209000
6	-0.052803000	-2.261332000	1.525226000	6	-0.474153000	3.245844000	-1.806873000
6	2.023330000	-1.237691000	2.010848000	6	-2.384735000	4.744925000	-1.829995000
6	3.092664000	-1.983360000	2.489340000	1	-2.840911000	5.701741000	-2.061816000
1	3.232097000	-2.995286000	2.124892000	6	-3.112751000	3.741230000	-1.229654000
6	3.970610000	-1.408167000	3.402576000	1	-4.154839000	3.899162000	-0.974490000
1	4.813402000	-1.985738000	3.767576000	6	-2.503003000	2.511062000	-0.928605000
6	3.769890000	-0.100246000	3.839732000	6	-3.188876000	1.404660000	-0.178707000
1	4.448875000	0.346808000	4.557479000	1	-3.160242000	1.639415000	0.895809000
6	2.701860000	0.640634000	3.342727000	1	-2.595552000	0.489417000	-0.298482000
1	2.565638000	1.669444000	3.664555000	6	-4.638095000	1.106883000	-0.589070000
6	1.815112000	0.091557000	2.408878000	1	-5.281246000	1.959748000	-0.344524000
6	-0.775234000	1.208206000	3.020166000	1	-4.687297000	0.961485000	-1.673700000
6	-0.587841000	2.086003000	4.095335000	6	-5.138943000	-0.133594000	0.114828000
1	0.273140000	2.748665000	4.112810000	6	-5.394912000	-1.307250000	-0.596282000
6	-1.510456000	2.123546000	5.135730000	1	-5.253955000	-1.320800000	-1.673053000
1	-1.361721000	2.808915000	5.963598000	6	-5.830442000	-2.459360000	0.058535000
6	-2.621149000	1.278818000	5.117220000	1	-6.025928000	-3.360492000	-0.515160000
1	-3.335435000	1.305853000	5.933654000	6	-6.011252000	-2.452337000	1.439048000
6	-2.813400000	0.404967000	4.050947000	1	-6.354323000	-3.345708000	1.951404000
1	-3.672013000	-0.259117000	4.027742000	6	-5.752107000	-1.286088000	2.160317000
6	-1.898595000	0.375533000	2.999509000	1	-5.899038000	-1.270332000	3.236397000
1	-2.062317000	-0.303607000	2.165102000	6	-5.318940000	-0.138024000	1.502981000
6	1.113537000	2.741006000	1.446516000	1	-5.126291000	0.768534000	2.072932000
6	2.453600000	2.964995000	1.107138000				
1	3.175764000	2.154442000	1.161713000				
6	2.871868000	4.223001000	0.679539000				
1	3.911993000	4.377683000	0.410667000				
6	1.959386000	5.271470000	0.581245000				
1	2.284735000	6.246795000	0.233897000				
6	0.625464000	5.060107000	0.924663000				
1	-0.093533000	5.869784000	0.848392000				
6	0.204108000	3.803049000	1.350912000				
1	-0.843929000	3.643855000	1.596220000				
6	0.965386000	2.957016000	-2.051223000				
6	1.797014000	3.970236000	-2.641175000				
6	3.166824000	3.613310000	-2.835950000				
1	3.840653000	4.329853000	-3.293231000				
6	3.625997000	2.372067000	-2.419825000				
1	4.670508000	2.111326000	-2.546014000				
6	2.750456000	1.466313000	-1.825144000				
6	3.131272000	0.137078000	-1.240221000				
1	2.522163000	-0.643000000	-1.719821000				
1	2.815293000	0.136296000	-0.185665000				
6	4.613980000	-0.223633000	-1.312995000				
				B1 (T1)			
				29	0.505364000	-0.286917000	-0.051080000
				15	2.415524000	-1.154796000	-1.255594000
				15	1.240742000	1.158879000	1.762466000
				8	3.059321000	1.633179000	-0.397317000
				7	-1.120799000	0.788714000	-1.070849000
				7	-1.220212000	-1.564507000	0.254808000
				6	-1.007717000	2.000113000	-1.680636000
				6	-2.124503000	2.820234000	-1.851928000
				6	-3.383847000	2.427733000	-1.422548000
				6	-3.524480000	1.095989000	-0.877623000
				6	-4.733244000	0.481826000	-0.596341000
				6	-4.790881000	-0.882520000	-0.076885000
				6	-3.645397000	-1.631785000	0.133081000
				6	-3.625797000	-2.987525000	0.636785000
				6	-2.385020000	-3.535119000	0.975433000
				6	-1.206543000	-2.834300000	0.785448000
				6	-2.363594000	-1.004838000	-0.076546000
				6	-2.308342000	0.348550000	-0.692209000

6	0.365418000	2.413866000	-2.098361000	1	3.212989000	0.563859000	3.968140000
6	0.140716000	-3.402383000	1.096086000	1	1.005266000	2.545311000	-1.217279000
6	3.264277000	0.124146000	-2.263816000	1	0.344497000	3.351087000	-2.656584000
6	3.516407000	1.372716000	-1.678346000	1	0.822608000	1.638185000	-2.723658000
6	4.117439000	2.404102000	-2.386862000	1	2.854868000	3.695193000	1.573877000
6	4.487316000	2.194073000	-3.713488000	1	2.185061000	6.016989000	1.048375000
6	4.247253000	0.962919000	-4.318041000	1	-0.197132000	6.566304000	0.634700000
6	3.637264000	-0.062679000	-3.598038000	1	-1.920676000	4.777776000	0.759796000
6	1.867379000	-2.385256000	-2.493411000	1	-1.256713000	2.456692000	1.276078000
6	2.601604000	-3.513853000	-2.869082000	1	1.476461000	2.696060000	4.297139000
6	2.088615000	-4.394406000	-3.820178000	1	0.640766000	2.244195000	6.584916000
6	0.846712000	-4.153022000	-4.402592000	1	-0.669061000	0.189813000	7.046476000
6	0.106153000	-3.033163000	-4.026569000	1	-1.153839000	-1.412261000	5.216596000
6	0.608727000	-2.158561000	-3.068485000	1	-0.324858000	-0.957489000	2.921832000
6	3.820190000	-1.912970000	-0.358988000	6	-4.523330000	3.359194000	-1.523052000
6	3.664113000	-2.207595000	0.997671000	6	-5.402252000	3.546099000	-0.444954000
6	4.723820000	-2.739506000	1.728932000	6	-4.710120000	4.117799000	-2.687516000
6	5.946728000	-2.976409000	1.107713000	6	-6.440981000	4.466383000	-0.533462000
6	6.114630000	-2.672750000	-0.243322000	1	-5.251752000	2.985079000	0.472618000
6	5.058894000	-2.136875000	-0.973317000	6	-5.755602000	5.030113000	-2.776095000
6	3.064674000	1.077789000	1.885067000	1	-4.043483000	3.971501000	-3.532141000
6	3.794389000	1.231322000	0.696698000	6	-6.623772000	5.207046000	-1.700040000
6	5.164703000	1.005432000	0.643282000	1	-7.105359000	4.609325000	0.312204000
6	5.826220000	0.615105000	1.804465000	1	-5.895236000	5.601032000	-3.688001000
6	5.129682000	0.470398000	3.001582000	1	-7.438086000	5.920494000	-1.769370000
6	3.756587000	0.698951000	3.038545000	6	-4.848348000	-3.795123000	0.775008000
6	0.844236000	2.922457000	1.466473000	6	-5.034445000	-4.600038000	1.910071000
6	1.808927000	3.930526000	1.399090000	6	-5.821998000	-3.824557000	-0.237143000
6	1.430776000	5.238721000	1.101686000	6	-6.165578000	-5.398013000	2.035255000
6	0.091933000	5.547716000	0.871720000	1	-4.296755000	-4.577153000	2.706652000
6	-0.875940000	4.546763000	0.945051000	6	-6.947254000	-4.631147000	-0.113039000
6	-0.500427000	3.239487000	1.237554000	1	-5.676220000	-3.234683000	-1.136898000
6	0.650050000	0.882937000	3.467996000	6	-7.126022000	-5.416277000	1.024921000
6	0.907905000	1.792186000	4.501998000	1	-6.300288000	-6.003683000	2.925273000
6	0.437278000	1.539279000	5.785706000	1	-7.682981000	-4.652252000	-0.910123000
6	-0.300365000	0.382557000	6.044342000	1	-8.007614000	-6.040843000	1.122722000
6	-0.571320000	-0.518577000	5.018923000				
6	-0.098618000	-0.267155000	3.731366000				
1	-1.986279000	3.809939000	-2.275482000				
1	-5.665536000	0.992773000	-0.801033000				
1	-5.760955000	-1.291555000	0.175421000				
1	-2.336271000	-4.553320000	1.347796000				
1	0.651605000	-2.788274000	1.847190000				
1	0.769169000	-3.413513000	0.196763000				
1	0.063668000	-4.420314000	1.480127000				
1	4.275660000	3.357137000	-1.893126000				
1	4.955735000	2.995949000	-4.273631000				
1	4.528474000	0.799884000	-5.352604000				
1	3.438255000	-1.016376000	-4.078672000				
1	3.568240000	-3.713390000	-2.417597000				
1	2.661907000	-5.270489000	-4.104765000				
1	0.451986000	-4.840854000	-5.143040000				
1	-0.865979000	-2.847171000	-4.471081000				
1	0.021177000	-1.296223000	-2.756046000				
1	2.720820000	-1.988501000	1.490933000				
1	4.596900000	-2.951506000	2.785482000				
1	6.774619000	-3.385451000	1.677620000				
1	7.071189000	-2.845159000	-0.725522000				
1	5.202533000	-1.876283000	-2.018958000				
1	5.698022000	1.118019000	-0.294650000				
1	6.893213000	0.422363000	1.767290000				
1	5.650673000	0.167471000	3.903101000				
				B2 (T1)			
				29	0.407050000	0.024890000	0.104082000
				15	2.294497000	0.558925000	-1.328697000
				15	1.266148000	-1.093722000	2.087573000
				8	2.912672000	-2.059154000	-0.071622000
				7	-1.369072000	-1.106701000	-0.498902000
				7	-1.200218000	1.511526000	0.158490000
				6	-1.386669000	-2.440554000	-0.777748000
				6	-2.591774000	-3.145231000	-0.821887000
				6	-3.808447000	-2.515678000	-0.612735000
				6	-3.792142000	-1.104093000	-0.296065000
				6	-4.913635000	-0.359933000	0.028717000
				6	-4.826328000	1.078220000	0.279035000
				6	-3.618099000	1.750826000	0.231112000
				6	-3.463780000	3.174117000	0.441582000
				6	-2.169207000	3.674301000	0.543963000
				6	-1.055308000	2.854553000	0.401961000
				6	-2.406711000	0.990079000	0.048923000
				6	-2.501229000	-0.465198000	-0.265753000
				6	-0.085830000	-3.099436000	-1.122396000
				6	0.062764000	-3.325859000	-2.638498000
				6	-0.120571000	-2.046467000	-3.451380000
				6	0.185281000	-2.236886000	-4.932887000
				6	0.338229000	3.408301000	0.462949000

6	0.644693000	4.433796000	-0.641867000	1	-1.146114000	-1.673801000	-3.328304000
6	2.113070000	4.865795000	-0.656501000	1	1.213844000	-2.584585000	-5.071347000
6	2.591131000	5.484226000	0.655492000	1	0.069234000	-1.299314000	-5.484016000
6	3.047753000	-0.888681000	-2.170422000	1	-0.484271000	-2.978319000	-5.380281000
6	3.302038000	-2.032789000	-1.401125000	1	1.042977000	2.574450000	0.382490000
6	3.843990000	-3.183212000	-1.959403000	1	0.501403000	3.871698000	1.444445000
6	4.146903000	-3.202115000	-3.319294000	1	0.004660000	5.314579000	-0.503456000
6	3.898691000	-2.079012000	-4.105083000	1	0.384507000	3.999081000	-1.614591000
6	3.349272000	-0.932103000	-3.534278000	1	5.579140000	-1.730091000	-0.188897000
6	1.714105000	1.652233000	-2.680083000	1	6.946039000	-0.817116000	1.671110000
6	0.356702000	1.551382000	-3.019377000	1	5.861057000	-0.144202000	3.802450000
6	-0.187812000	2.370765000	-4.004458000	1	3.410534000	-0.333794000	4.052723000
6	0.611464000	3.319466000	-4.639651000	1	2.739401000	3.997211000	-0.894734000
6	1.956425000	3.438830000	-4.295470000	1	2.254224000	5.580305000	-1.475319000
6	2.508936000	2.605871000	-3.324701000	1	-1.354131000	-2.216915000	2.291286000
6	3.780823000	1.371126000	-0.622590000	1	-2.239414000	-4.521643000	2.317911000
6	3.724612000	1.878684000	0.679341000	1	-0.683240000	-6.455808000	2.188324000
6	4.840169000	2.490675000	1.246558000	1	1.763686000	-6.065670000	2.074917000
6	6.022017000	2.596033000	0.518312000	1	2.658205000	-3.761632000	2.079111000
6	6.094386000	2.072408000	-0.771891000	1	1.940488000	6.309936000	0.963276000
6	4.982820000	1.455257000	-1.336882000	1	3.607624000	5.873643000	0.555461000
6	3.096553000	-1.149363000	2.087956000	1	2.605289000	4.747129000	1.464555000
6	3.738188000	-1.543693000	0.904580000	1	1.326137000	-2.181391000	4.861111000
6	5.114412000	-1.432589000	0.745043000	1	0.754543000	-1.155837000	7.043477000
6	5.872893000	-0.919205000	1.793569000	1	-0.058795000	1.184235000	7.141886000
6	5.264965000	-0.539976000	2.987641000	1	-0.311833000	2.501229000	5.055665000
6	3.884596000	-0.653300000	3.130119000	1	0.246788000	1.472163000	2.866589000
6	0.713661000	-2.835660000	2.188799000	6	-5.064303000	-3.283178000	-0.735044000
6	-0.667004000	-3.060957000	2.255193000	6	-7.395896000	-4.813086000	-1.029398000
6	-1.167758000	-4.358683000	2.263282000	6	-5.172600000	-4.543745000	-0.131541000
6	-0.293676000	-5.443085000	2.190702000	6	-6.140287000	-2.804990000	-1.497972000
6	1.080613000	-5.224001000	2.125094000	6	-7.294211000	-3.566785000	-1.645513000
6	1.585712000	-3.924553000	2.127406000	6	-6.331385000	-5.299676000	-0.273113000
6	0.839968000	-0.412268000	3.726210000	1	-4.347499000	-4.920764000	0.465447000
6	0.972349000	-1.154529000	4.906128000	1	-6.058226000	-1.845285000	-1.999110000
6	0.650762000	-0.578522000	6.130754000	1	-8.113372000	-3.189087000	-2.248344000
6	0.193344000	0.738852000	6.185110000	1	-6.404198000	-6.268283000	0.210151000
6	0.052356000	1.480008000	5.014872000	1	-8.299215000	-5.403397000	-1.141031000
6	0.371348000	0.903603000	3.786517000	6	-4.617554000	4.086991000	0.527805000
1	-2.568443000	-4.202906000	-1.069089000	6	-6.755746000	5.899757000	0.652558000
1	-5.882648000	-0.835528000	0.104644000	6	-5.678690000	4.006760000	-0.388304000
1	-5.736568000	1.610363000	0.523558000	6	-4.644124000	5.096689000	1.501580000
1	-2.019881000	4.738957000	0.698007000	6	-5.706650000	5.991223000	1.565702000
1	4.010846000	-4.047180000	-1.324574000	6	-6.735232000	4.908097000	-0.327068000
1	4.569819000	-4.096751000	-3.763089000	1	-5.656876000	3.251188000	-1.167752000
1	4.125042000	-2.095472000	-5.165759000	1	-3.835947000	5.161609000	2.224061000
1	3.138276000	-0.065679000	-4.155459000	1	-5.717929000	6.758318000	2.332872000
1	-0.279862000	0.840302000	-2.496154000	1	-7.541240000	4.840456000	-1.050184000
1	-1.238281000	2.280952000	-4.260896000	1	-7.583673000	6.599022000	0.702344000
1	0.185126000	3.970411000	-5.395783000				
1	2.578788000	4.183077000	-4.781148000				
1	3.554520000	2.719915000	-3.056483000				
1	2.814865000	1.775670000	1.265951000	29	-0.646255000	-0.103205000	-0.509438000
1	4.786286000	2.872460000	2.260954000	15	-0.690902000	-0.250423000	1.985789000
1	6.891512000	3.071659000	0.960119000	15	-2.823499000	-0.143931000	-1.491248000
1	7.019217000	2.137223000	-1.335532000	8	-3.248934000	1.093044000	1.067151000
1	5.055517000	1.022374000	-2.331360000	7	0.893899000	1.402150000	-0.700378000
1	-0.008094000	-4.055144000	-0.588745000	7	1.164869000	-1.278728000	-0.860119000
1	0.729518000	-2.463050000	-0.764163000	6	0.685297000	2.744006000	-0.519758000
1	1.061961000	-3.737463000	-2.829229000	6	1.761931000	3.619302000	-0.452242000
1	-0.661984000	-4.080194000	-2.971348000	6	3.074079000	3.169401000	-0.582393000
1	0.538154000	-1.272683000	-3.039470000	6	3.287108000	1.763209000	-0.838559000

B3 (T₁)

6	4.511424000	1.186935000	-1.126267000	1	-3.200220000	-4.395685000	2.843069000
6	4.653699000	-0.259824000	-1.278463000	1	-2.012587000	-4.950118000	4.956577000
6	3.575711000	-1.114582000	-1.118396000	1	-0.205418000	-3.465065000	5.782912000
6	3.656052000	-2.555925000	-1.154158000	1	0.406945000	-1.431820000	4.525236000
6	2.470523000	-3.277044000	-1.061166000	1	-4.683792000	-0.006690000	3.058438000
6	1.241411000	-2.644185000	-0.890444000	1	-5.878842000	-2.168426000	2.885934000
6	2.261602000	-0.551103000	-0.946862000	1	-5.787683000	-3.481622000	0.777012000
6	2.113850000	0.926910000	-0.827167000	1	-4.530295000	-2.610050000	-1.162332000
6	-0.745444000	3.140359000	-0.298707000	1	-1.025330000	2.829418000	0.721821000
6	-0.054342000	-3.388320000	-0.714484000	1	-1.371762000	2.533064000	-0.967171000
6	-1.651355000	1.038266000	2.880515000	1	-5.420810000	1.215949000	-0.785924000
6	-2.819008000	1.554143000	2.301871000	1	-6.509386000	3.231186000	-1.702221000
6	-3.559068000	2.556790000	2.919431000	1	-5.420865000	4.525933000	-3.517262000
6	-3.141558000	3.053923000	4.150141000	1	-3.214196000	3.802235000	-4.398168000
6	-1.997720000	2.540238000	4.759573000	1	-2.098116000	1.808389000	-3.459812000
6	-1.263104000	1.541951000	4.128193000	1	-5.204704000	-0.978274000	-3.074773000
6	1.060480000	0.133922000	2.360417000	1	-5.439398000	-2.472857000	-5.033989000
6	1.997496000	-0.904649000	2.268361000	1	-3.440816000	-3.573463000	-6.005810000
6	3.362011000	-0.633025000	2.320314000	1	-1.198611000	-3.166391000	-5.025775000
6	3.809183000	0.680204000	2.456704000	1	-0.961185000	-1.669469000	-3.060020000
6	2.884873000	1.719724000	2.542699000	6	-1.112610000	4.614132000	-0.488304000
6	1.518516000	1.450663000	2.490385000	1	-0.524036000	5.221378000	0.212920000
6	-1.042525000	-1.766433000	2.957910000	6	-0.833376000	5.089215000	-1.915072000
6	-2.048726000	-2.617038000	2.489219000	1	-1.120022000	6.137763000	-2.035840000
6	-2.408691000	-3.751711000	3.213936000	1	-1.420738000	4.495528000	-2.623689000
6	-1.743878000	-4.060086000	4.397158000	1	0.221344000	4.992693000	-2.187617000
6	-0.727381000	-3.225174000	4.862448000	6	-2.592975000	4.791179000	-0.146191000
6	-0.383821000	-2.077531000	4.154007000	1	-2.905075000	5.831394000	-0.275360000
6	-3.902009000	-0.807808000	-0.171093000	1	-2.796254000	4.496683000	0.888461000
6	-3.943314000	-0.098616000	1.040900000	1	-3.209469000	4.165587000	-0.804011000
6	-4.660618000	-0.573375000	2.134478000	6	0.036902000	-4.798975000	-0.117018000
6	-5.327651000	-1.792189000	2.030764000	1	0.648012000	-5.422866000	-0.782867000
6	-5.277956000	-2.527466000	0.850499000	6	0.672964000	-4.794350000	1.275084000
6	-4.571054000	-2.032342000	-0.244742000	1	0.096459000	-4.158243000	1.956465000
6	-3.686279000	1.373129000	-2.061113000	1	1.702628000	-4.424896000	1.254421000
6	-4.927356000	1.783493000	-1.569195000	1	0.688680000	-5.805024000	1.693223000
6	-5.545443000	2.919438000	-2.090824000	6	-1.365620000	-5.407379000	-0.071676000
6	-4.934885000	3.645622000	-3.109944000	1	-2.021024000	-4.802517000	0.565117000
6	-3.696159000	3.239725000	-3.604966000	1	-1.339817000	-6.420511000	0.338782000
6	-3.070022000	2.114709000	-3.076542000	1	-1.811228000	-5.452607000	-1.070182000
6	-3.069241000	-1.257083000	-2.919195000	6	4.942625000	-3.273372000	-1.241947000
6	-4.329583000	-1.470019000	-3.493030000	6	7.340218000	-4.723696000	-1.359754000
6	-4.461065000	-2.306233000	-4.595754000	6	6.025668000	-2.931783000	-0.417221000
6	-3.334875000	-2.924100000	-5.143046000	6	5.078901000	-4.358960000	-2.118959000
6	-2.076820000	-2.699280000	-4.592493000	6	6.270036000	-5.073903000	-2.180904000
6	-1.944359000	-1.863877000	-3.483503000	6	7.212181000	-3.654526000	-0.474517000
1	1.582455000	4.668938000	-0.243631000	1	5.924235000	-2.112499000	0.288536000
1	5.393377000	1.803900000	-1.240830000	1	4.250474000	-4.625508000	-2.768593000
1	5.633159000	-0.655890000	-1.513302000	1	6.364033000	-5.903184000	-2.874113000
1	2.515326000	-4.360962000	-1.060967000	1	8.036443000	-3.386347000	0.177997000
1	-0.563349000	-3.450783000	-1.687442000	1	8.268789000	-5.282625000	-1.407289000
1	-0.707408000	-2.774860000	-0.074621000	6	4.189889000	4.116692000	-0.413442000
1	-4.451685000	2.926567000	2.425643000	6	6.248327000	5.979968000	-0.014205000
1	-3.714381000	3.836581000	4.635493000	6	4.128987000	5.387244000	-1.005080000
1	-1.676066000	2.919593000	5.723106000	6	5.297324000	3.798489000	0.388903000
1	-0.362996000	1.157147000	4.599633000	6	6.314383000	4.724965000	0.589290000
1	1.659550000	-1.931924000	2.144378000	6	5.152670000	6.307843000	-0.811272000
1	4.073532000	-1.450115000	2.249676000	1	3.282329000	5.639990000	-1.637017000
1	4.873672000	0.890316000	2.497774000	1	5.341119000	2.828202000	0.875396000
1	3.225426000	2.746624000	2.638956000	1	7.157512000	4.469024000	1.222350000
1	0.811320000	2.274319000	2.541366000				
1	-2.553438000	-2.397199000	1.551776000				

B4 (T₁)

29	0.227874000	-0.077821000	-0.336623000	1	-1.445039000	2.741089000	2.230619000
15	2.264182000	-0.291952000	-1.500136000	6	-3.396014000	1.898336000	2.519781000
15	0.419908000	0.365833000	2.083450000	1	-3.892329000	2.860643000	2.433344000
8	2.691129000	1.668263000	0.546082000	6	-4.142988000	0.741190000	2.726678000
7	-1.516020000	1.130437000	-0.730434000	1	-5.223783000	0.795648000	2.815099000
7	-1.353041000	-1.531424000	-0.344263000	6	-3.495884000	-0.489874000	2.824651000
6	2.882698000	1.039185000	-2.594779000	1	-4.069245000	-1.398235000	2.980031000
6	4.193736000	1.518715000	-2.553413000	6	-2.110097000	-0.559689000	2.718640000
1	4.883194000	1.155268000	-1.796089000	1	-1.617410000	-1.527426000	2.786654000
6	4.620512000	2.458008000	-3.491766000	6	-2.648272000	0.447377000	-0.698365000
1	5.640886000	2.826288000	-3.458153000	6	-3.942849000	1.066141000	-0.761456000
6	3.744662000	2.917025000	-4.473896000	6	-3.959717000	2.509231000	-0.809392000
1	4.082088000	3.644557000	-5.204540000	6	-2.744616000	3.177861000	-0.847976000
6	2.430532000	2.450603000	-4.509624000	1	-2.741827000	4.262891000	-0.844963000
1	1.741787000	2.816030000	-5.264144000	6	-1.530420000	2.486987000	-0.787290000
6	1.997398000	1.522766000	-3.566026000	6	-0.206177000	3.184147000	-0.623119000
1	0.969534000	1.165352000	-3.585809000	1	0.601601000	2.464872000	-0.813434000
6	2.468604000	-1.756313000	-2.580784000	1	-0.103165000	3.481628000	0.432506000
6	3.697074000	-2.108423000	-3.154431000	6	0.016263000	4.431579000	-1.491149000
1	4.595650000	-1.553201000	-2.896644000	1	0.045639000	4.133664000	-2.545480000
6	3.768012000	-3.154157000	-4.068920000	1	-0.816431000	5.131656000	-1.372242000
1	4.723064000	-3.423686000	-4.507582000	6	1.304589000	5.123315000	-1.109382000
6	2.609692000	-3.840699000	-4.438808000	6	2.526984000	4.658492000	-1.601628000
1	2.666491000	-4.646146000	-5.163654000	1	2.539280000	3.806739000	-2.274354000
6	1.382765000	-3.490747000	-3.880926000	6	3.721186000	5.281191000	-1.247958000
1	0.480043000	-4.020576000	-4.167342000	1	4.658353000	4.911867000	-1.654407000
6	1.313833000	-2.455323000	-2.948797000	6	3.710669000	6.369895000	-0.376223000
1	0.354543000	-2.176635000	-2.515987000	1	4.639391000	6.858951000	-0.100017000
6	3.494337000	-0.442216000	-0.158007000	6	2.498302000	6.827319000	0.137236000
6	4.279642000	-1.575024000	0.073535000	1	2.480343000	7.673095000	0.817725000
1	4.244799000	-2.409812000	-0.620087000	6	1.304521000	6.208141000	-0.229692000
6	5.085878000	-1.662628000	1.208532000	1	0.360874000	6.574789000	0.167196000
1	5.681259000	-2.553797000	1.372880000	6	-5.066333000	0.254851000	-0.808282000
6	5.109753000	-0.615874000	2.124198000	1	-6.047963000	0.688170000	-0.951298000
1	5.734692000	-0.677819000	3.008830000	6	-4.963288000	-1.200860000	-0.706232000
6	4.318843000	0.514616000	1.928683000	1	-5.881148000	-1.773465000	-0.663257000
1	4.318404000	1.324418000	2.649878000	6	-3.738444000	-1.840079000	-0.624930000
6	3.510361000	0.588406000	0.799648000	6	-2.546661000	-1.032791000	-0.566329000
6	2.262005000	2.428054000	1.625316000	6	-3.547977000	-3.271934000	-0.513843000
6	2.838693000	3.678594000	1.803594000	6	-2.261177000	-3.741816000	-0.222366000
1	3.601743000	4.008898000	1.107458000	1	-2.101881000	-4.809581000	-0.110811000
6	2.408993000	4.486992000	2.851714000	6	-1.183216000	-2.878908000	-0.124230000
1	2.849643000	5.470054000	2.980478000	6	0.210911000	-3.289470000	0.258383000
6	1.422748000	4.035031000	3.725823000	1	0.329175000	-3.168497000	1.346433000
1	1.095003000	4.657554000	4.551085000	1	0.913944000	-2.575829000	-0.189397000
6	0.845351000	2.783731000	3.530585000	6	0.637402000	-4.705601000	-0.144423000
1	0.057538000	2.446764000	4.198387000	1	0.066659000	-5.448203000	0.424649000
6	1.236951000	1.964308000	2.465208000	1	0.412744000	-4.862305000	-1.205536000
6	1.033273000	-0.768152000	3.386049000	6	2.117551000	-4.896585000	0.094846000
6	0.587097000	-0.691298000	4.711785000	6	3.010220000	-4.962728000	-0.976656000
1	-0.188154000	0.019540000	4.984676000	1	2.630050000	-4.902524000	-1.992198000
6	1.123294000	-1.534225000	5.679202000	6	4.380115000	-5.107383000	-0.758984000
1	0.771068000	-1.472317000	6.703575000	1	5.055316000	-5.158883000	-1.608075000
6	2.114678000	-2.454126000	5.334020000	6	4.876225000	-5.183555000	0.539835000
1	2.535803000	-3.106045000	6.092418000	1	5.941076000	-5.302455000	0.713955000
6	2.559516000	-2.536896000	4.018067000	6	3.993507000	-5.111187000	1.618075000
1	3.332430000	-3.246288000	3.739392000	1	4.373475000	-5.179931000	2.633312000
6	2.013989000	-1.703135000	3.042731000	6	2.626364000	-4.967197000	1.396643000
1	2.361594000	-1.779907000	2.014135000	1	1.944279000	-4.917288000	2.242972000
6	-1.347936000	0.599959000	2.513744000	6	-4.654655000	-4.225736000	-0.691205000
6	-2.007947000	1.829309000	2.407493000	6	-6.703883000	-6.110056000	-1.055786000
				6	-4.774078000	-5.331384000	0.166071000

6	-5.579148000	-4.086248000	-1.739859000	1	4.044043000	3.345206000	1.827089000
6	-6.590617000	-5.022711000	-1.920727000	6	2.812494000	3.555179000	3.595841000
6	-5.791812000	-6.260820000	-0.012228000	1	3.364865000	4.407157000	3.977764000
1	-4.077304000	-5.444337000	0.991220000	6	1.724245000	3.046170000	4.302802000
1	-5.481773000	-3.255690000	-2.432367000	1	1.425129000	3.495522000	5.243427000
1	-7.288063000	-4.906777000	-2.743687000	6	1.016860000	1.959506000	3.799238000
1	-5.876706000	-7.101974000	0.667752000	1	0.160262000	1.575959000	4.346079000
1	-7.497167000	-6.836747000	-1.195416000	6	1.373743000	1.365638000	2.581972000
6	-5.216482000	3.281804000	-0.754222000	6	0.938780000	-1.483404000	2.862706000
6	-7.546635000	4.829592000	-0.585271000	6	0.487185000	-1.668173000	4.176000000
6	-6.205623000	2.981084000	0.194244000	1	-0.202065000	-0.954415000	4.619468000
6	-5.409263000	4.375008000	-1.610176000	6	0.902560000	-2.775811000	4.907350000
6	-6.568804000	5.138469000	-1.529465000	1	0.546155000	-2.915847000	5.922661000
6	-7.359421000	3.752605000	0.279437000	6	1.772714000	-3.706944000	4.336759000
1	-6.051189000	2.153677000	0.880731000	1	2.091027000	-4.571612000	4.910264000
1	-4.652704000	4.610267000	-2.352965000	6	2.226635000	-3.530147000	3.033229000
1	-6.710814000	5.973988000	-2.206787000	1	2.896930000	-4.253260000	2.575998000
1	-8.110704000	3.515645000	1.025358000	6	1.807436000	-2.422059000	2.298478000
1	-8.449735000	5.427352000	-0.521982000	1	2.166931000	-2.289591000	1.279932000

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29	0.279104000	-0.084083000	-0.641767000	6	-1.815635000	1.569244000	2.360418000
15	2.383413000	-0.220050000	-1.715356000	1	-1.153678000	2.428349000	2.289535000
15	0.451090000	-0.040318000	1.841336000	6	-3.188391000	1.770560000	2.486015000
8	2.873854000	1.335846000	0.687090000	1	-3.578373000	2.783629000	2.525745000
7	-1.281552000	1.376084000	-0.844880000	6	-4.056120000	0.681580000	2.540719000
7	-1.489917000	-1.311794000	-0.794078000	1	-5.126971000	0.838740000	2.626293000
6	3.039588000	1.278556000	-2.530785000	6	-3.543499000	-0.613466000	2.483491000
6	4.378098000	1.671917000	-2.440738000	1	-4.213082000	-1.467782000	2.517005000
1	5.074790000	1.097876000	-1.835500000	6	-2.170877000	-0.818078000	2.371809000
6	4.817306000	2.803133000	-3.125956000	1	-1.781586000	-1.832624000	2.317701000
1	5.858143000	3.103446000	-3.058202000	6	-2.518237000	0.848583000	-0.892967000
6	3.923765000	3.549864000	-3.892345000	6	-3.696185000	1.631063000	-0.859997000
1	4.268441000	4.434695000	-4.417044000	6	-3.541372000	3.047929000	-0.719127000
6	2.586741000	3.165019000	-3.979016000	6	-2.269902000	3.559746000	-0.631554000
1	1.887547000	3.749174000	-4.567826000	1	-2.135286000	4.628914000	-0.510380000
6	2.144404000	2.034282000	-3.297365000	6	-1.130263000	2.708500000	-0.680665000
1	1.097578000	1.741092000	-3.349229000	6	0.202108000	3.198912000	-0.510310000
6	2.610952000	-1.516137000	-2.985113000	1	1.003148000	2.497482000	-0.740146000
6	3.820045000	-1.690695000	-3.671691000	6	0.525669000	4.453850000	0.016774000
1	4.663443000	-1.037634000	-3.460957000	1	-0.270462000	5.065557000	0.433981000
6	3.944099000	-2.698456000	-4.621215000	6	1.848503000	4.980914000	0.130773000
1	4.883397000	-2.831875000	-5.147390000	6	2.960880000	4.416923000	-0.545811000
6	2.860739000	-3.533949000	-4.900121000	1	2.819868000	3.567852000	-1.205790000
1	2.961401000	-4.319786000	-5.641439000	6	4.227493000	4.951975000	-0.380642000
6	1.650312000	-3.353469000	-4.238280000	1	5.064771000	4.511599000	-0.912530000
1	0.802955000	-3.992566000	-4.462830000	6	4.433380000	6.045603000	0.467385000
6	1.523335000	-2.341991000	-3.286288000	1	5.430181000	6.452719000	0.598992000
1	0.571794000	-2.186466000	-2.782721000	6	3.345691000	6.621209000	1.136531000
6	3.599752000	-0.632636000	-0.410232000	1	3.500182000	7.474033000	1.789210000
6	4.363877000	-1.803430000	-0.404803000	6	2.073393000	6.108183000	0.961506000
1	4.351967000	-2.451570000	-1.275781000	1	1.229043000	6.553662000	1.479942000
6	5.126489000	-2.159399000	0.706176000	6	-4.968541000	0.984608000	-0.944291000
1	5.707310000	-3.074966000	0.694185000	1	-5.864277000	1.592578000	-0.983588000
6	5.134471000	-1.337660000	1.827871000	6	-5.072590000	-0.373798000	-0.950848000
1	5.719932000	-1.608669000	2.699884000	1	-6.051154000	-0.838118000	-0.971444000
6	4.390704000	-0.160618000	1.847475000	6	-3.911872000	-1.205186000	-0.892118000
1	4.394014000	0.478884000	2.722639000	6	-2.629701000	-0.605578000	-0.889623000
6	3.629332000	0.183805000	0.734631000	6	-3.974019000	-2.631661000	-0.765132000
6	2.480319000	1.887963000	1.900305000	6	-2.801835000	-3.320693000	-0.571859000
6	3.199905000	2.970059000	2.395085000	1	-2.828351000	-4.399271000	-0.461437000
				6	-1.549054000	-2.645471000	-0.580086000
				6	-0.306021000	-3.311869000	-0.363615000

1	0.576484000	-2.698810000	-0.530798000	1	1.451826000	-4.858534000	-5.335277000
6	-0.135197000	-4.611917000	0.112951000	6	0.361087000	-3.596069000	-3.977171000
1	-1.003381000	-5.176240000	0.443441000	1	-0.604112000	-4.030872000	-4.215993000
6	1.138803000	-5.239526000	0.282584000	6	0.446287000	-2.570135000	-3.035902000
6	1.233859000	-6.415830000	1.066838000	1	-0.455350000	-2.203998000	-2.547977000
1	0.328830000	-6.828856000	1.502719000	6	2.960224000	-0.854534000	-0.340975000
6	2.456668000	-7.019484000	1.301354000	6	3.632750000	-2.068458000	-0.179871000
1	2.509875000	-7.911322000	1.916667000	1	3.475325000	-2.873218000	-0.890846000
6	3.623899000	-6.483560000	0.744207000	6	4.481319000	-2.277342000	0.908387000
1	4.581657000	-6.960156000	0.922552000	1	4.994266000	-3.229442000	1.008451000
6	3.547780000	-5.339506000	-0.058367000	6	4.658153000	-1.266280000	1.847516000
1	4.448143000	-4.941421000	-0.515780000	1	5.315410000	-1.419057000	2.697238000
6	2.330219000	-4.721942000	-0.288965000	6	3.983425000	-0.052720000	1.721720000
1	2.286923000	-3.852876000	-0.939772000	1	4.104895000	0.730080000	2.462260000
6	-5.259722000	-3.372761000	-0.812520000	6	3.134543000	0.141068000	0.637447000
6	-7.637708000	-4.843784000	-0.922601000	6	2.141212000	2.090005000	1.556954000
6	-5.587753000	-4.266782000	0.212074000	6	2.888028000	3.245871000	1.741566000
6	-6.133141000	-3.227452000	-1.897299000	1	3.666711000	3.487267000	1.026486000
6	-7.314028000	-3.960962000	-1.951580000	6	2.603098000	4.079873000	2.818138000
6	-6.772770000	-4.995396000	0.158641000	1	3.176241000	4.992158000	2.949572000
1	-4.915277000	-4.378095000	1.057874000	6	1.589153000	3.744947000	3.713302000
1	-5.875189000	-2.550318000	-2.706600000	1	1.371220000	4.387469000	4.559365000
1	-7.979488000	-3.846536000	-2.800746000	6	0.844085000	2.585938000	3.514718000
1	-7.020689000	-5.679745000	0.963178000	1	0.039419000	2.341625000	4.202576000
1	-8.560578000	-5.412599000	-0.964870000	6	1.092133000	1.744631000	2.423375000
6	-4.701344000	3.970599000	-0.625134000	6	0.614775000	-0.958439000	3.309486000
6	-6.819637000	5.785650000	-0.394351000	6	0.236147000	-0.853222000	4.654259000
6	-5.705177000	3.771354000	0.331030000	1	-0.445443000	-0.066883000	4.967091000
6	-4.766964000	5.093011000	-1.457480000	6	0.718934000	-1.761985000	5.589497000
6	-5.822998000	5.992705000	-1.345390000	1	0.419130000	-1.677186000	6.628842000
6	-6.756617000	4.675430000	0.445899000	6	1.591319000	-2.776654000	5.192648000
1	-5.649778000	2.911800000	0.993698000	1	1.972897000	-3.479767000	5.925885000
1	-3.992560000	5.249494000	-2.202686000	6	1.967822000	-2.888214000	3.857679000
1	-5.867784000	6.854632000	-2.002780000	1	2.647941000	-3.670907000	3.537196000
1	-7.524593000	4.514696000	1.195183000	6	1.473084000	-1.988528000	2.914238000
1	-7.642041000	6.487738000	-0.306307000	1	1.765979000	-2.089662000	1.870604000

B4-2 (Ti)

29	-0.267425000	-0.129923000	-0.362473000	6	-3.519976000	2.204650000	2.635759000
15	1.687693000	-0.539910000	-1.613309000	1	-3.908409000	3.216878000	2.569130000
15	0.079165000	0.260291000	2.049555000	6	-4.384393000	1.136078000	2.861978000
8	2.425752000	1.307989000	0.446874000	1	-5.449356000	1.309169000	2.983058000
7	-1.877984000	1.268676000	-0.680187000	6	-3.875591000	-0.159910000	2.935682000
7	-2.008050000	-1.398524000	-0.321769000	1	-4.541246000	-0.999752000	3.107829000
6	2.395452000	0.745235000	-2.709758000	6	-2.510532000	-0.383114000	2.782884000
6	3.755004000	1.064598000	-2.734498000	1	-2.126287000	-1.399951000	2.829844000
1	4.436724000	0.596843000	-2.029082000	6	-3.078900000	0.720156000	-0.613041000
6	4.238596000	1.977365000	-3.671161000	6	-4.295677000	1.483723000	-0.629273000
1	5.296012000	2.221459000	-3.688287000	6	-4.147891000	2.919023000	-0.677041000
6	3.370479000	2.569281000	-4.587029000	6	-2.865604000	3.444291000	-0.751921000
1	3.751354000	3.275796000	-5.316955000	1	-2.738909000	4.521755000	-0.750727000
6	2.009900000	2.263780000	-4.556137000	6	-1.737367000	2.619404000	-0.730142000
1	1.328785000	2.733986000	-5.257768000	6	-0.337368000	3.155929000	-0.601791000
6	1.521693000	1.363241000	-3.612851000	1	0.375311000	2.357295000	-0.848474000
1	0.458439000	1.132577000	-3.579309000	1	-0.160684000	3.398899000	0.457979000
6	1.682938000	-1.993670000	-2.727323000	6	0.000970000	4.403258000	-1.431618000
6	2.837032000	-2.458062000	-3.371237000	1	-0.039322000	4.144890000	-2.496509000
1	3.799190000	-1.998243000	-3.158793000	1	-0.743150000	5.187718000	-1.260041000
6	2.753935000	-3.494735000	-4.294846000	6	1.368201000	4.930992000	-1.068556000
1	3.652184000	-3.851931000	-4.787615000	6	2.525733000	4.355317000	-1.594492000
6	1.514821000	-4.059505000	-4.603854000	1	2.438077000	3.534296000	-2.299573000

6	3.792671000	4.809823000	-1.252018000	1	7.086851000	-6.197771000	-0.297304000
1	4.652751000	4.333469000	-1.707975000	1	6.020016000	-5.286784000	-1.366232000
6	3.957584000	5.859106000	-0.323330000	7	5.217991000	6.280825000	0.072488000
6	2.788166000	6.445676000	0.202256000	6	6.362446000	5.859902000	-0.713220000
1	2.854639000	7.271748000	0.899500000	1	6.284431000	6.158101000	-1.768946000
6	1.530114000	5.981701000	-0.165597000	1	6.481581000	4.772725000	-0.675005000
1	0.651291000	6.460184000	0.261511000	1	7.263883000	6.304935000	-0.292710000
6	-5.505884000	0.807387000	-0.639035000	6	5.327987000	7.524043000	0.811148000
1	-6.435473000	1.352567000	-0.741887000	1	4.914767000	8.382755000	0.261987000
6	-5.566942000	-0.651883000	-0.555439000	1	6.379221000	7.719865000	1.021317000
1	-6.542308000	-1.117168000	-0.488834000	1	4.806632000	7.452009000	1.770947000
6	-4.421356000	-1.427826000	-0.526019000				
6	-3.143428000	-0.763368000	-0.497389000				
6	-4.392624000	-2.874187000	-0.446473000				
6	-3.160945000	-3.492583000	-0.202640000				
1	-3.120639000	-4.573563000	-0.114555000				
6	-1.987857000	-2.759798000	-0.125194000				
6	-0.640047000	-3.335853000	0.203609000				
1	-0.480529000	-3.264650000	1.290985000				
1	0.126953000	-2.689678000	-0.242015000				
6	-0.377833000	-4.777340000	-0.250682000				
1	-1.016350000	-5.470508000	0.309362000				
1	-0.641938000	-4.874925000	-1.310204000				
6	1.078448000	-5.125924000	-0.055298000				
6	1.950806000	-5.247119000	-1.136868000				
1	1.565345000	-5.144451000	-2.147656000				
6	3.308760000	-5.494600000	-0.963756000				
1	3.935668000	-5.579980000	-1.843505000				
6	3.861348000	-5.610473000	0.326741000				
6	2.973022000	-5.528102000	1.419973000				
1	3.337181000	-5.664712000	2.431200000				
6	1.620048000	-5.282789000	1.223330000				
1	0.970498000	-5.214387000	2.094224000				
6	-5.604921000	-3.691265000	-0.617784000				
6	-7.863031000	-5.318352000	-0.987466000				
6	-5.832754000	-4.801448000	0.211098000				
6	-6.527925000	-3.416335000	-1.640556000				
6	-7.643158000	-4.225403000	-1.824424000				
6	-6.953719000	-5.603184000	0.030255000				
1	-5.136578000	-5.018249000	1.015840000				
1	-6.349897000	-2.581563000	-2.311520000				
1	-8.338649000	-4.006300000	-2.627796000				
1	-7.120788000	-6.449547000	0.688246000				
1	-8.736629000	-5.945815000	-1.128824000				
6	-5.305730000	3.831407000	-0.595594000				
6	-7.436874000	5.639856000	-0.392321000				
6	-6.296659000	3.658635000	0.382352000				
6	-5.394759000	4.928533000	-1.463395000				
6	-6.455923000	5.821825000	-1.365723000				
6	-7.351384000	4.559487000	0.484194000				
1	-6.220253000	2.827647000	1.077767000				
1	-4.636665000	5.064962000	-2.228977000				
1	-6.518959000	6.659455000	-2.052334000				
1	-8.104518000	4.420523000	1.252663000				
1	-8.263344000	6.338407000	-0.315430000				
7	5.224582000	-5.768909000	0.519540000				
6	5.701845000	-6.141991000	1.837430000				
1	5.275958000	-7.092331000	2.189764000				
1	5.457550000	-5.366471000	2.571349000				
1	6.786779000	-6.237717000	1.807280000				
6	6.053375000	-6.092487000	-0.625976000				
1	5.746341000	-7.025056000	-1.120526000				
				1 (S₀)			
				29	-0.102964000	-0.114107000	-0.473421000
				15	0.171345000	-1.166638000	1.678843000
				15	-0.138699000	2.227613000	-0.552094000
				8	1.330818000	1.635169000	1.824577000
				7	1.177547000	-1.257841000	-1.762005000
				7	-1.560139000	-1.340926000	-1.499678000
				6	2.509766000	-1.211545000	-1.845206000
				6	3.200091000	-2.068543000	-2.726547000
				6	2.505027000	-2.962868000	-3.505035000
				6	1.104291000	-3.029760000	-3.413982000
				6	0.330185000	-3.957300000	-4.178122000
				6	-1.018620000	-4.013144000	-4.034249000
				6	-1.687725000	-3.141071000	-3.120026000
				6	-3.078095000	-3.187775000	-2.916445000
				6	-3.666489000	-2.335118000	-2.014043000
				6	-2.881484000	-1.398990000	-1.309392000
				6	-0.960183000	-2.192678000	-2.364682000
				6	0.478098000	-2.140394000	-2.510305000
				6	3.167182000	-0.200612000	-0.938055000
				6	-3.430757000	-0.447285000	-0.277168000
				6	1.522902000	-0.567031000	2.777209000
				6	1.917409000	0.777113000	2.733213000
				6	2.938130000	1.265038000	3.544593000
				6	3.569008000	0.410857000	4.442205000
				6	3.174700000	-0.923163000	4.527791000
				6	2.162421000	-1.402110000	3.704066000
				6	0.644394000	-2.885930000	1.257124000
				6	-0.367890000	-3.784254000	0.888491000
				6	-0.049955000	-5.052448000	0.412670000
				6	1.282395000	-5.440083000	0.283303000
				6	2.294223000	-4.550396000	0.633247000
				6	1.979571000	-3.281205000	1.114007000
				6	-1.196099000	-1.362297000	2.894276000
				6	-2.095933000	-0.301974000	3.052341000
				6	-3.098048000	-0.365202000	4.018586000
				6	-3.219536000	-1.493021000	4.825907000
				6	-2.329513000	-2.554662000	4.671839000
				6	-1.318920000	-2.488922000	3.717196000
				6	-0.588270000	2.793494000	1.127769000
				6	0.210144000	2.338802000	2.191232000
				6	-0.120218000	2.612947000	3.514610000
				6	-1.273097000	3.344514000	3.788800000
				6	-2.086307000	3.797164000	2.754284000
				6	-1.741558000	3.522078000	1.432817000
				6	1.367280000	3.190728000	-0.984617000
				6	1.963056000	4.113113000	-0.121271000
				6	3.077816000	4.841977000	-0.533857000
				6	3.601556000	4.662314000	-1.811125000
				6	3.008088000	3.746842000	-2.679792000

6	1.901613000	3.010960000	-2.267553000	1	-4.418148000	2.010705000	0.340343000
6	-1.345558000	3.016098000	-1.683342000	6	-5.424227000	0.423388000	-1.624368000
6	-1.498780000	4.408519000	-1.752615000	1	-5.427041000	-0.379697000	-2.366589000
6	-2.369102000	4.972844000	-2.678313000	1	-4.804418000	1.237394000	-2.014457000
6	-3.079381000	4.156504000	-3.559337000	1	-6.450943000	0.796068000	-1.540972000
6	-2.916956000	2.775345000	-3.512190000	6	5.429111000	-1.247409000	-0.381264000
6	-2.054983000	2.206119000	-2.574744000	1	5.058690000	-1.537839000	0.608663000
1	4.277687000	-2.028995000	-2.791693000	1	6.500467000	-1.040448000	-0.284612000
1	3.030591000	-3.626392000	-4.186243000	1	5.322336000	-2.112886000	-1.040358000
1	0.846438000	-4.619981000	-4.866333000				
1	-1.612531000	-4.721883000	-4.603761000				
1	-3.677490000	-3.905211000	-3.469918000	2 (S₀)			
1	-4.733342000	-2.382351000	-1.847619000	29	-0.155769000	0.153669000	-0.147756000
1	-2.816422000	0.459787000	-0.348879000	15	0.194248000	-1.429435000	-1.825330000
1	-3.185570000	-0.875415000	0.705276000	15	0.414165000	-0.435423000	2.102890000
1	3.222948000	2.308956000	3.460561000	8	2.125627000	-2.070716000	0.190294000
1	4.364375000	0.789198000	5.076776000	7	0.561256000	2.153651000	-0.362692000
1	3.657038000	-1.591843000	5.233749000	7	-1.986030000	1.273090000	-0.062748000
1	1.869148000	-2.445470000	3.772506000	6	1.662715000	-1.305910000	-2.921325000
1	-1.411834000	-3.496395000	0.979652000	6	2.481923000	-2.398277000	-2.219983000
1	-0.847187000	-5.738739000	0.142265000	1	2.312109000	-3.355504000	-2.734987000
1	1.529420000	-6.430234000	-0.087975000	6	3.511182000	-2.267697000	-4.150948000
1	3.336037000	-4.841864000	0.536068000	1	4.139165000	-3.123503000	-4.381159000
1	2.783553000	-2.603360000	1.383757000	6	3.728763000	-1.048927000	-4.790451000
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References

- [1] A.D. Becke, The Journal of Chemical Physics, 98 (1993) 5648-5652.
[2] J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, C. Fiolhais, Physical Review B, 46 (1992) 6671-6687.

- [3] J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, C. Fiolhais, *Physical Review B*, 48 (1993) 4978-4978.
- [4] J.P. Perdew, K. Burke, Y. Wang, *Physical Review B*, 54 (1996) 16533-16539.
- [5] J.P. Perdew, K. Burke, Y. Wang, *Physical Review B*, 57 (1998) 14999-14999.
- [6] B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chemical Physics Letters*, 157 (1989) 200-206.
- [7] Y. Zhao, D.G. Truhlar, *Theoretical Chemistry Accounts*, 120 (2008) 215-241.
- [8] X. Shang, D. Han, D. Li, S. Guan, Z. Wu, *Chemical Physics Letters*, 588 (2013) 68-75.
- [9] J.-D. Chai, M. Head-Gordon, *Physical Chemistry Chemical Physics*, 10 (2008) 6615-6620.
- [10] C. Adamo, V. Barone, *The Journal of Chemical Physics*, 110 (1999) 6158-6170.
- [11] N. Armaroli, G. Accorsi, M. Holler, O. Moudam, J.F. Nierengarten, Z. Zhou, R.T. Wegh, R. Welter, *Advanced Materials*, 18 (2006) 1313-1316.
- [12] X. Shang, D. Han, Q. Zhan, D. Zhou, G. Zhang, *New Journal of Chemistry*, 39 (2015) 2588-2595.
- [13] Q. Zhang, L. Wang, X. Wang, Y. Li, J. Zhang, *Organic Electronics*, 28 (2016) 100-110.
- [14] K. Zhang, D. Zhang, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 124 (2014) 341-348.
- [15] A. Hagfeldt, G. Boschloo, L. Sun, L. Kloo, H. Pettersson, *Chemical Reviews*, 110 (2010) 6595-6663.
- [16] L. Yang, D.R. Powell, R.P. Houser, *Journal of the Chemical Society. Dalton Transactions*, (2007) 955-964.
- [17] M.G. Fraser, H. Van Der Salm, S.A. Cameron, A.G. Blackman, K.C. Gordon, *Inorganic Chemistry*, 52 (2013) 2980-2992.
- [18] S. Wei, K. Li, X. Lu, Z. Zhao, Y. Shao, Y. Dang, S. Li, W. Guo, *Materials Chemistry and Physics*, 173 (2016) 139-145.
- [19] Y. Shao, Z. Gan, E. Epifanovsky, A.T.B. Gilbert, M. Wormit, J. Kussmann, A.W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P.R. Horn, L.D. Jacobson, I. Kaliman, R.Z. Khaliullin, T. Kuś, A. Landau, J. Liu, E.I. Proynov, Y.M. Rhee, R.M. Richard, M.A. Rohrdanz, R.P. Steele, E.J. Sundstrom, H.L. Woodcock, P.M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G.J.O. Beran, Y.A. Bernard, E. Berquist, K. Brandhorst, K.B. Bravaya, S.T. Brown, D. Casanova, C.-M. Chang, Y. Chen, S.H. Chien, K.D. Closser, D.L. Crittenden, M. Diedenhofen, R.A. DiStasio, H. Do, A.D. Dutoi, R.G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M.W.D. Hanson-Heine, P.H.P. Harbach, A.W. Hauser, E.G. Hohenstein, Z.C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyayev, J. Kim, J. Kim, R.A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C.M. Krauter, K.U. Lao, A.D. Laurent, K.V. Lawler, S.V. Levchenko, C.Y. Lin, F. Liu, E. Livshits, R.C. Lochan, A. Luenser, P. Manohar, S.F. Manzer, S.-P. Mao, N. Mardirossian, A.V. Marenich, S.A. Maurer, N.J. Mayhall, E. Neuscamman, C.M. Oana, R. Olivares-Amaya, D.P. O'Neill, J.A. Parkhill, T.M. Perrine, R. Peverati, A. Prociuk, D.R. Rehn, E. Rosta, N.J. Russ, S.M. Sharada, S. Sharma, D.W. Small, A. Sodt, T. Stein, D. Stück, Y.-C. Su, A.J.W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M.A. Watson, J. Wenzel, A. White, C.F. Williams, J. Yang, S. Yeganeh, S.R. Yost, Z.-Q. You, I.Y. Zhang, X. Zhang, Y. Zhao, B.R. Brooks, G.K.L. Chan, D.M. Chipman, C.J. Cramer, W.A. Goddard, M.S. Gordon, W.J. Hehre, A. Klamt, H.F. Schaefer, M.W. Schmidt, C.D. Sherrill, D.G. Truhlar, A. Warshel, X. Xu, A. Aspuru-Guzik, R. Baer, A.T. Bell, N.A. Besley, J.-D. Chai, A. Dreuw, B.D. Dunietz, T.R. Furlani, S.R. Gwaltney, C.-P. Hsu,

Y. Jung, J. Kong, D.S. Lambrecht, W. Liang, C. Ochsenfeld, V.A. Rassolov, L.V. Slipchenko, J.E. Subotnik, T. Van Voorhis, J.M. Herbert, A.I. Krylov, P.M.W. Gill, M. Head-Gordon, *Molecular Physics*, 113 (2015) 184-215.

[20] P.R. Horn, Y. Mao, M. Head-Gordon, *Physical Chemistry Chemical Physics*, 18 (2016) 23067-23079.

[21] G. Zhang, X. Li, X. Jiang, P. Sun, *Journal of Luminescence*, 130 (2010) 976-980.