

Electronic supporting information

Protonated Bisphosphines: A New Class of Powerful Hydride Donors Capable of CO₂ Reduction

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Computational Details

All DFT calculations were carried out using the Gaussian16 computational chemistry package¹. Conformational ensembles of the molecules studied were generated and analyzed using the CREST (Conformer-Rotamer Ensemble Sampling Tool) program, developed by Grimme and coworkers². This tool uses the GFN2-xTB semiempirical tight-binding method for geometry optimization and relative energy assessment³. The lowest-energy conformers were selected as starting points for further calculations. The geometries of the minima and transition-state (TS) structures were optimized with the ω B97XD functional^{4,5} and the Pople 6-31G(d,p) basis set⁶ within the PCM solvation model⁷ in acetonitrile at 298 K. All structures were fully optimized without any geometric constraints and vibrational frequency analyses were conducted at the same level of theory to confirm proper convergence (all positive eigenvalues for minima and a single negative eigenvalue for TS structures).

For all calculations, we used the default SCF and geometry optimization convergence thresholds, as well as the default integration grid, in Gaussian 16. Single point energy is calculated at ω B97XD/6-311++G(d,p) level of theory; therefore, the applied theoretical model can be written as (PCM) ω B97XD/6-311++G(d,p)//(PCM) ω B97XD/6-31G(d,p).

The thermodynamic hydricity was determined as relative hydricity by calculating $\Delta_r G$ for the following reaction:



and taking experimental value for hydricity of $HCOO^-$ as 44 kcal mol⁻¹. (Here, **P** = phosphine framework; PH^+ = protonated hydride-donating species.)

The Gibbs energy of reaction (1) is easily obtained by calculating the absolute values of the Gibbs energy of solvated reactants and products. However, it cannot directly provide the hydricity of PH^+ .

Equation (1), i.e., hydride transfer from PH^+ to $HCOO^-$, can be written as a combination of two reactions:



The Gibbs energy of reaction (2) is the hydricity of PH^+ , while the Gibbs energy of reaction (3) is a negative value of the hydricity of $HCOO^-$. Taking into account the known hydricity of $HCOO^-$, it is possible to combine it with the Gibbs energy of (1) to obtain the hydricity of PH^+ . Namely:

$$\Delta_r G(1) = \Delta_r G(2) + \Delta_r G(3) = \Delta_r G_H^-(PH^+) - \Delta G_H^-(HCOO^-) \quad (4)$$

Thus, the hydricity of PH^+ can be obtained according to reaction (5):

$$\Delta_r G_H^-(PH^+) = \Delta_r G(1) + \Delta G_H^-(HCOO^-) \quad (5)$$

Phosphine	NBO charge
1a	-0.0287
1b	-0.0568
1c	-0.0633
1d	-0.0660
1e	-0.0735
1f	-0.0803

Table S1. NBO charges on the H atom bonded to the central phosphorus atom.

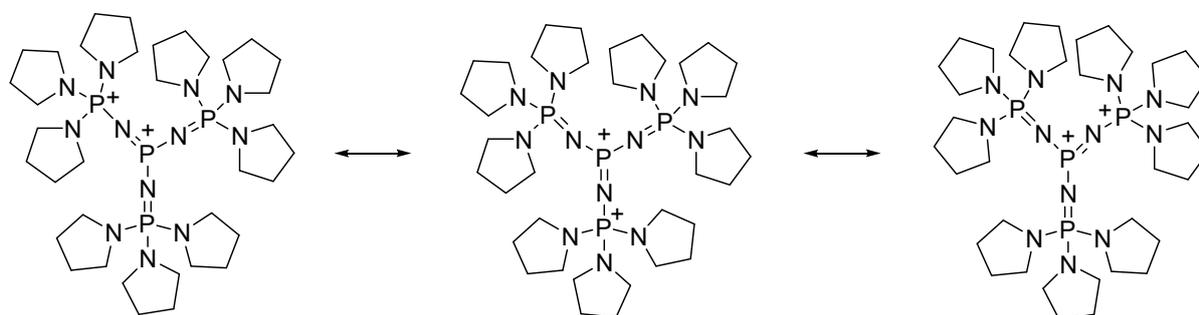


Figure S1. The most significant resonance structures of the dication of **1f**, as determined by NRT analysis.

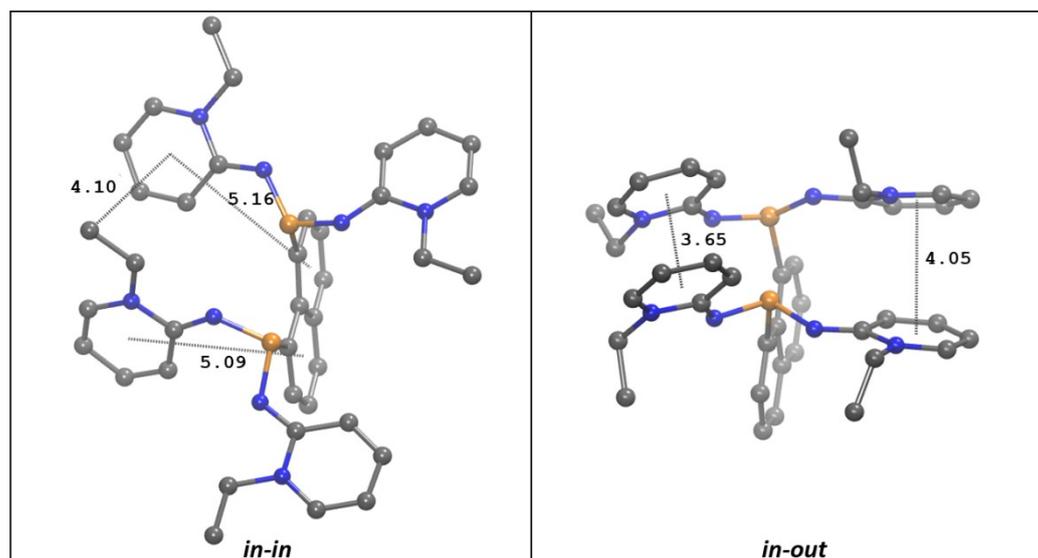


Figure S2. Optimized geometries of *in-in* and *in-out* protonated bisphosphine **2d**. The *in-in* conformer features two weak T-shaped π - π interactions ($d > 5 \text{ \AA}$) between a pyridine unit and the naphthalene core, together with an alkyl- π contact (4.1 \AA). The *in-out* conformer exhibits two strong parallel π - π stacking interactions ($d \leq 4 \text{ \AA}$) between the pyridine rings.

BisPhosphine	P...P distance/Å
2a	2.213
2b	2.242
2c	2.221
2d	2.234
2e	2.221
2f	2.220

Table S2. P...P distances in dications obtained from bisphosphines **2a-2f**.

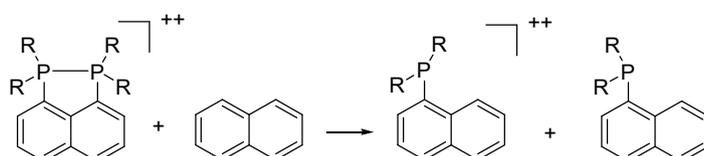


Figure S3. Homodesmotic reaction scheme used to evaluate the stabilization energy of the dicationic bisphosphine species

BisPhosphine dication	$\Delta_r G/\text{kcal mol}^{-1}$
2a⁺⁺	56.3
2b⁺⁺	60.2
2c⁺⁺	68.9
2d⁺⁺	64.6
2e⁺⁺	70.9
2f⁺⁺	75.1

Table S3. Calculated Gibbs reaction energies* for the homodesmotic reaction depicted in Fig. S3.

*The Gibbs free energies obtained from the homodesmotic reaction described above are comparable to the differences in hydricity between phosphines **3a-3f** and **2a-2f** (Table 1 in the main text), indicating that the dominant contribution to the hydricity of the bisphosphines arises from stabilization of the dication upon formation of the P-P bond.

Comparison of stability of *in-in* vs. *in-out* conformers

To determine why **2a** and **2d**, unlike the other species, adopt the *in-out* conformation, we analyzed their geometries and performed NBO analyses of both the *in-out* and *in-in* conformers for all bisphosphine species **2a–2f**. The first notable observation is that the two phosphorus atoms in **2a** are much closer (2.52 Å) than in **2d** (3.23 Å), suggesting that the factors favoring the *in-out* arrangement are likely different between the two compounds. Note that in all other protonated bisphosphines, the P...P distances lie between 3.23 and 3.32 Å. Using NBO analysis, Dudding established that in the Janus proton sponge, there is donation of the nitrogen lone pair into the antibonding orbital of cyclopropenimine π -system; however, interaction is quite weak, being 3.1 kcal·mol⁻¹.²¹ Performed NBO analysis of **2a** and identified the following donor→acceptor interactions and their stabilization energies: LP(P1)→BD*(P2–H)=44.9 kcal·mol⁻¹; LP(P1)→BD*(P2–N3)= 14.7 kcal·mol⁻¹; LP(P1)→BD*(P2–N4)=17.5 kcal·mol⁻¹, where P1 is the phosphorus atom bearing the lone pair, P2 is the protonated phosphorus atom, and N3 and N4 are the nitrogens directly bonded to P2. In the less stable *in-in* conformation of **2a**, the two phosphine groups are significantly farther apart (3.23 Å), and the corresponding interactions are much weaker, being LP(P1)→BD*(P2–H)=3.8 kcal·mol⁻¹; LP(P1)→BD*(P2–N3)=1.5 kcal·mol⁻¹; LP(P1)→BD*(P2–N4)=1.4 kcal·mol⁻¹. By contrast, in the *in-out* conformation of protonated **2d**, the separation between phosphine groups is substantially greater than in the *in-out* conformation of **2a**, as noted above. Consequently, NBO second-order perturbation energies are much smaller: LP(P1)→BD*(P2–H)=3.8 kcal·mol⁻¹, LP(P1)→BD*(P2–N3)=1.5 kcal·mol⁻¹, and LP(P1)→BD*(P2–N4)=1.4 kcal·mol⁻¹. These values suggest that the electronic donor→acceptor stabilization, which probably drives the *in-out* arrangement in **2a**, is not operative in **2d**. Instead, comparison of the *in-in* and *in-out* geometries for **2d** reveals that the *in-out* conformer is stabilized by a pronounced π – π stacking interaction (see Fig. S2). Interestingly, no significant differences are observed in the donor–acceptor interactions between the lone pair on P1 and the antibonding σ (P2–H), σ (P2–N2), and σ^* (P2–N1) orbitals for species **2b**, **2e**, and **2f**, with **2c** being an exception. In the case of **2c**, the LP(P1) → σ^* (P2–H) interaction in the *in-in* conformation is substantially stronger than in the *in-out* conformation. However, it should be emphasized that the preference for the *in-in* or *in-out* conformation results from the interplay of several factors, and the orbital interactions discussed here represent only one of them. Substituents may interact attractively through dispersion forces or π – π

stacking when positioned at optimal distances; however, if they are forced too close due to the rigidity of the aromatic naphthalene ring and the bulkiness of substituents, such attractive interactions may become repulsive.

Table S4. Gibbs energy difference between *in-in* and *in-out* conformers, expressed as $G(in-in)-G(in-$

BisPhosphine	$\Delta G/kcal\ mol^{-1}$
2a	-0.1
2b	2.2
2c	4.2
2d	-15.4
2e	5.8
2f	4.5

out).

Table S5 Natural Bond Orbital (NBO) analysis of *in-in* and *in-out* conformers of bisphosphine species **2a-2f**.

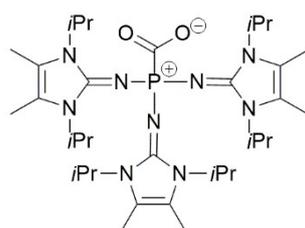
BisPhosphine	Conformer	Donor \rightarrow Akceptor	E^2 (kcal/mol)
2a	<i>in-out</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	44.9
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	14.7
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	17.5
2a	<i>in-in</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	3.8
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	1.5
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	1.4
2b	<i>in-out</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	2.4
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	0.7
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	0.6
2b	<i>in-in</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	1.2
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	4.4
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	0.6
2c	<i>in-out</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	1.9
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	0.6
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	0.6
2c	<i>in-in</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	12.2
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	0.9
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	-
2d	<i>in-out</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	3.8
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	1.5
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	1.4
2d	<i>in-in</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	0.6

		LP(P1) \rightarrow $\sigma^*(P2-N1)$	2.3
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	-
		LP(N1) \rightarrow $\sigma^*(P2-H)$	7.1
2e	<i>in-out</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	2.9
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	0.8
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	1.0
2e	<i>in-in</i>	LP(P1) \rightarrow $\sigma^*(P2-H)$	1.7
		LP(P1) \rightarrow $\sigma^*(P2-N1)$	2.9
		LP(P1) \rightarrow $\sigma^*(P2-N2)$	-

BisPhosphine	$\Delta_r G(\text{binding})/\text{kcal mol}^{-1}$
2a	15.0
2b	10.9
2c	0.2
2d	14.1
2e	-0.1
2f	3.9

Table S6. Gibbs energy of CO₂ binding.

Figure S4. CO₂ capture in Tris(imidazolin-2-ylidnamino)phosphine



For clarity, three conceptually distinct processes involving CO₂ are defined below: CO₂ capture, CO₂ reduction, and combined capture-reduction processes.

Carbon dioxide (CO₂) capture refers to processes in which CO₂ is reversibly taken up from a gas or solution phase through physical adsorption or chemical binding, without altering its molecular structure or oxidation state. In CO₂ capture, the carbon center remains in the +4 oxidation state, and no net electron transfer occurs. Typical capture mechanisms include physisorption driven by weak intermolecular forces and chemisorption involving reversible Lewis acid-base or Brønsted acid-base interactions (as it is shown in Fig. S4), leading to the formation of molecular adducts.

In contrast, CO₂ reduction involves the chemical conversion of CO₂ into more reduced carbon-containing species, such as carbon monoxide, formate, methanol, or hydrocarbons. This process necessarily entails electron transfer and a decrease in the oxidation state of carbon, and therefore constitutes a redox reaction.

A third class of processes combines CO₂ capture and CO₂ reduction within a single system or reaction sequence. In such cases, CO₂ is first captured through reversible binding, which can increase its local concentration and facilitate activation. Subsequent electron and/or hydride transfer steps then reduce the bound CO₂ to a chemically transformed product. In these capture-assisted reduction processes, CO₂ capture and CO₂ reduction are mechanistically distinct but sequentially linked steps: capture serves as a prerequisite for, but is not itself equivalent to, reduction.

Although we anticipated that the studied protonated bisphosphines might enable a combined process involving CO₂ capture followed by CO₂ reduction to formate, where CO₂ would first bind to the neutral phosphine unit within the protonated bisphosphine, the results show that CO₂ binding is not thermodynamically favourable (Table S6). The investigation therefore involves direct hydride transfer to CO₂, leading to formate formation, and is appropriately described as a CO₂ reduction process.

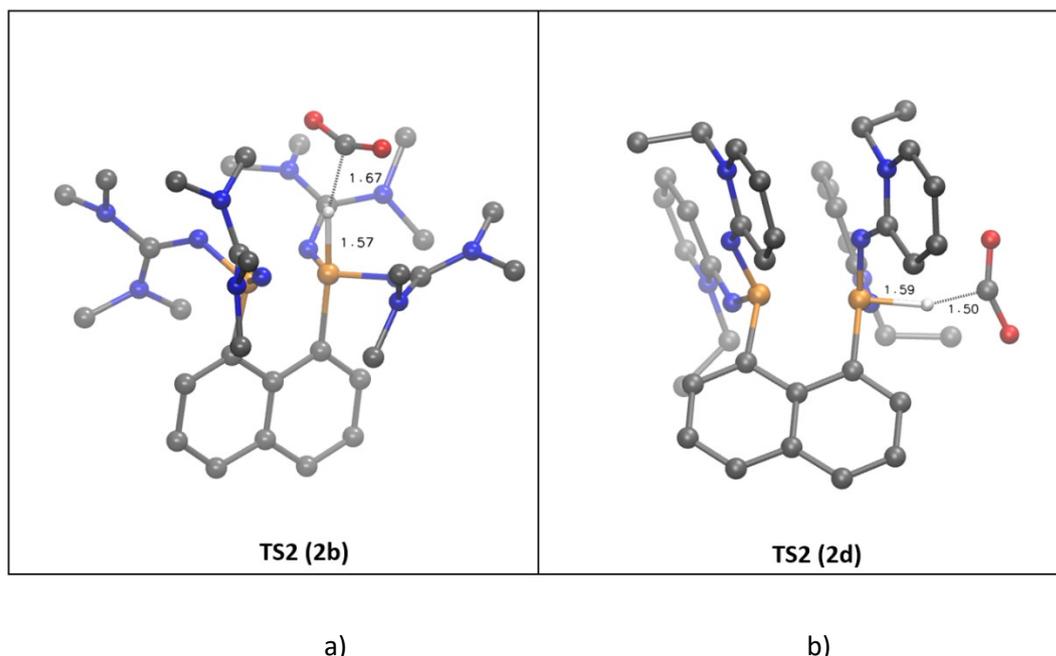


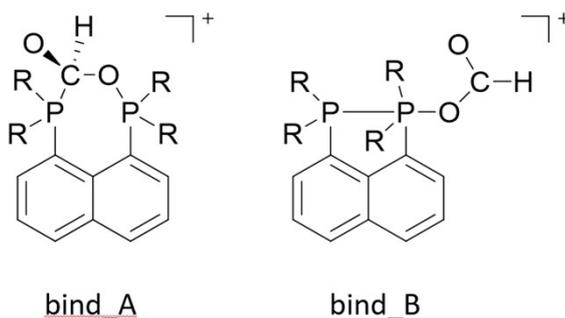
Figure S5. Optimized geometries of the **TS2** structures for bisphosphines **2b** and **2d**. In **2b**, CO₂ adopts a top approach toward the hydride, whereas in **2d** it approaches laterally.

Table S7. Gibbs energy of formate binding to the phosphine dication, expressed as relative energy

BisPhosphine dication	$\Delta_r G/\text{kcal mol}^{-1}$
2a⁺⁺	5.8 ^{bind_B}
2b⁺⁺	17.9 ^{bind_A}
2c⁺⁺	4.7 ^{bind_A}
2d⁺⁺	8.1 ^{bind_B}
2e⁺⁺	4.7 ^{bind_A}
2f⁺⁺	7.5 ^{bind_A}

with respect to the reactants (**2a-2f** + CO₂).^a

^aTwo possible binding modes were investigated, bind_A and bind_B (see schematic below). For each compound, the $\Delta_r G$ value corresponding to the more stable binding mode is reported.



Cartesian Coordinates of Optimized Structures

1a (protonated form)				1a (dication)			
C	2.963409	3.000966	-1.446593	C	3.380305	2.077495	1.138320
N	2.427076	2.746008	-0.115901	N	3.608758	0.871677	0.341276
C	2.961450	3.571460	0.962237	C	5.003802	0.433763	0.244291
C	1.481083	1.816834	0.076696	C	2.631840	0.231970	-0.261536
C	1.044959	1.565578	1.501075	C	2.944600	-0.974350	-1.097639
N	0.991147	1.198100	-0.974645	N	1.388521	0.723970	-0.128036
P	-0.144656	0.027877	-0.936172	P	-0.007051	0.036259	-0.209360
N	-1.526251	0.632436	-0.320790	N	-0.090193	-1.518212	-0.170315
C	-2.677539	0.007750	-0.244769	C	-1.106324	-2.386207	-0.304750
C	-2.951666	-1.363215	-0.817308	C	-2.361170	-2.070880	-1.063778
N	0.225512	-1.349156	-0.132918	N	-1.308109	0.890690	-0.146371
C	1.307106	-2.083924	-0.260465	C	-1.546733	2.209222	-0.242268

C	2.451140	-1.785441	-1.201545	C	-0.621856	3.165054	-0.936019
N	1.387993	-3.181301	0.503556	N	-2.681831	2.659291	0.246347
C	2.482730	-4.141122	0.471081	C	-3.063076	4.070329	0.142087
C	0.302417	-3.475504	1.432264	C	-3.628227	1.801497	0.960207
N	-3.697890	0.610688	0.383853	N	-0.951775	-3.589214	0.203659
C	-5.015959	0.001038	0.518867	C	-1.972285	-4.629550	0.050442
C	-3.568232	1.956460	0.926427	C	0.225482	-3.968931	0.985132
H	2.461787	3.857268	-1.908878	H	3.504285	1.838399	2.196928
H	4.029780	3.217838	-1.360405	H	4.118353	2.826476	0.847724
H	2.187977	3.834966	1.682875	H	5.546176	0.846395	1.093084
H	3.339041	4.497554	0.528396	H	5.452101	0.804240	-0.680938
H	3.784070	3.068463	1.480918	H	5.076524	-0.651435	0.283399
H	0.597541	-4.320742	2.053289	H	-3.814044	2.233007	1.945592
H	-0.613664	-3.725874	0.890220	H	-3.217877	0.801830	1.063743
H	0.099720	-2.610006	2.065521	H	-4.564746	1.764427	0.399851
H	2.080514	-5.144104	0.307097	H	-2.534915	4.662153	0.893706
H	3.021935	-4.130190	1.422857	H	-4.134007	4.145094	0.320877
H	3.183198	-3.922526	-0.329788	H	-2.848738	4.459779	-0.852004
H	-2.596902	2.362062	0.656658	H	0.877284	-3.110325	1.113780
H	-3.663719	1.930527	2.016054	H	0.757025	-4.766190	0.461460
H	-4.359843	2.590709	0.517975	H	-0.106816	-4.335201	1.958352
H	-4.943435	-1.060980	0.752934	H	-2.346953	-4.659652	-0.971807
H	-5.612432	0.131086	-0.390148	H	-2.799121	-4.456159	0.743261
H	-5.533681	0.489854	1.344278	H	-1.513381	-5.589036	0.280794
H	-0.303393	-0.269041	-2.300971	H	2.376892	2.453491	0.960705
H	2.817407	2.123975	-2.073026	H	2.099031	-1.224526	-1.733850
H	0.336120	2.338902	1.812163	H	3.822549	-0.803431	-1.721985
H	0.548660	0.600316	1.584711	H	3.145508	-1.830052	-0.445322
H	1.892668	1.580100	2.187557	H	-1.049900	3.443575	-1.904175
H	2.312264	-0.818163	-1.680977	H	-0.487704	4.075981	-0.350222
H	3.401936	-1.758330	-0.664441	H	0.349544	2.705725	-1.102250
H	2.517562	-2.554175	-1.976115	H	-2.340370	-2.587449	-2.028436
H	-3.897962	-1.384365	-1.360527	H	-3.244294	-2.407529	-0.517995
H	-2.157692	-1.673570	-1.493855	H	-2.441922	-1.000952	-1.240224
H	-3.002639	-2.100095	-0.010337				
1b (protonated form)				1b (dication)			
C	-2.936451	-0.904477	2.137336	C	-2.186721	1.392360	-2.175844
N	-2.898546	-1.299666	0.741271	N	-2.367190	2.041342	-0.882771
C	-1.727764	-1.705427	0.171976	C	-1.338849	2.247803	-0.043862
N	-0.528740	-1.443461	0.652794	N	-0.178864	1.545599	-0.131806
P	0.001915	0.001307	1.178276	P	0.001173	-0.005591	-0.151328
N	1.522013	0.264632	0.663381	N	-1.249607	-0.939143	-0.128216
C	2.346623	-0.645371	0.184116	C	-1.277893	-2.295740	-0.058679
N	2.571325	-1.865796	0.750543	N	-2.043975	-2.842145	0.890688
C	2.239475	-2.098241	2.144248	C	-2.490092	-2.038796	2.025627
C	-4.026538	-0.842177	-0.057042	C	-3.759236	2.238646	-0.483009
N	-1.824783	-2.478893	-0.940043	N	-1.398561	3.209771	0.881948
C	-2.928513	-3.400567	-1.170274	C	-2.190566	4.427097	0.715549
C	-0.653232	-2.692059	-1.772534	C	-0.436743	3.235936	1.980378
				N	1.435013	-0.622810	-0.115396

N	-0.985108	1.189170	0.670086	C	2.619643	0.036687	-0.019575
C	-0.613694	2.355899	0.181468	N	2.972560	0.999430	-0.886120
N	0.333933	3.164174	0.736621	C	2.334042	1.128200	-2.190282
C	0.710600	3.004056	2.129176	N	3.459827	-0.355852	0.942875
N	-1.248435	2.827637	-0.922296	C	4.913998	-0.289864	0.807368
C	-1.485830	4.245384	-1.154985	C	2.970684	-1.155197	2.062943
C	-2.034629	1.922631	-1.743100	N	-0.623044	-3.068161	-0.940037
N	3.074018	-0.342356	-0.921416	C	-0.179221	-2.553008	-2.229760
C	2.685652	0.783535	-1.753497	C	-0.100679	-4.388441	-0.592489
C	4.418367	-0.852650	-1.150387	C	-2.725847	-4.124693	0.724355
C	2.720030	-3.070833	-0.052538	C	3.834651	2.118409	-0.510360
C	1.288840	3.903781	-0.075938	H	-2.438402	0.329040	-2.117561
H	-3.920208	-1.155214	2.542702	H	-2.851218	1.876581	-2.893903
H	-2.180800	-1.455612	2.698450	H	-3.826732	2.381204	0.593933
H	-4.232304	0.204965	0.190176	H	-4.310610	1.331603	-0.742774
H	-4.926631	-1.433194	0.140181	H	-4.213999	3.087922	-0.998887
H	-3.786599	-0.898887	-1.117958	H	-1.548322	5.278093	0.952011
H	-2.523907	-4.403413	-1.339100	H	-3.054674	4.441512	1.383815
H	-3.519248	-3.113329	-2.045870	H	-2.520870	4.524178	-0.317044
H	-3.577920	-3.434452	-0.296521	H	-0.908703	3.727788	2.831982
H	-0.979752	-2.832064	-2.806147	H	0.461563	3.791294	1.694671
H	-0.093756	-3.580609	-1.456555	H	-0.157267	2.224814	2.267603
H	0.006674	-1.827702	-1.714637	H	-3.418203	-1.511117	1.786588
H	2.939353	-2.833625	2.549714	H	-1.727062	-1.315451	2.304851
H	1.217898	-2.480295	2.258607	H	-2.663493	-2.710078	2.867678
H	2.346049	-1.171576	2.709535	H	-3.769742	-3.986904	1.014093
H	1.898849	-3.756108	0.184628	H	-2.285515	-4.902277	1.352873
H	3.669986	-3.575516	0.150383	H	-2.699458	-4.433992	-0.318915
H	2.663067	-2.828637	-1.112871	H	-0.289311	-3.347791	-2.969746
H	2.966982	0.567936	-2.787459	H	0.871209	-2.248732	-2.187577
H	3.186724	1.706210	-1.437390	H	-0.798789	-1.711609	-2.537469
H	1.608945	0.935310	-1.693900	H	-0.639612	-5.187517	-1.107280
H	5.094532	-0.008427	-1.317520	H	-0.150450	-4.542780	0.483713
H	4.458548	-1.507384	-2.026655	H	0.949067	-4.419765	-0.894122
H	4.764370	-1.403126	-0.276525	H	1.937069	0.167638	-2.515534
H	0.987891	3.983258	2.528498	H	3.091160	1.446713	-2.909073
H	1.560700	2.320927	2.242223	H	1.533903	1.874140	-2.161911
H	-0.137621	2.625611	2.700891	H	3.329555	3.040824	-0.807409
H	2.299543	3.555142	0.162733	H	4.804539	2.069743	-1.011287
H	1.233985	4.980177	0.115854	H	3.976936	2.140226	0.568423
H	1.108203	3.719206	-1.134093	H	5.346808	0.471246	1.460849
H	-2.556236	4.403158	-1.319471	H	5.188114	-0.088114	-0.226500
H	-0.943249	4.607775	-2.033842	H	5.319624	-1.264943	1.085477
H	-1.182804	4.824704	-0.283789	H	2.979083	-2.220295	1.813129
H	-1.995116	2.266299	-2.779908	H	1.959468	-0.857069	2.331920
H	-3.082275	1.898030	-1.420071	H	3.627856	-0.979473	2.915491
H	-1.627845	0.914577	-1.678599	H	-1.161839	1.514962	-2.524122
H	0.000255	-0.006508	2.589076				
H	-2.766808	0.172158	2.257425				
1c (protonated form)				1c (dication)			
P	-0.220684	0.046734	-1.660960	P	-0.074724	-0.075916	0.050805

N	-0.676042	1.591477	-1.463717	N	-1.533447	-0.599388	0.199082
N	0.931682	-0.218917	-0.556144	N	0.217353	1.449274	-0.034534
N	-1.468974	-0.983130	-1.691961	N	1.118860	-1.079754	-0.054159
C	0.017369	2.377613	-0.638482	C	-1.926800	-1.899399	0.220318
C	1.746276	-1.156089	-0.140833	C	-0.654168	2.484522	0.025963
C	-2.333678	-1.018619	-0.673129	C	2.418467	-0.690263	-0.147678
N	1.160598	3.056185	-0.915367	N	-2.122945	-2.681304	-0.859190
N	-0.311563	2.670601	0.646463	N	-2.289455	-2.588649	1.313677
N	2.483789	-1.006942	1.000154	N	-1.481192	2.897567	-0.954887
N	2.073809	-2.375371	-0.664973	N	-0.746675	3.348588	1.049132
N	-2.275008	-1.842924	0.406036	N	3.336840	-0.921482	0.805323
N	-3.478172	-0.294114	-0.557259	N	3.022505	-0.085820	-1.188025
C	1.582245	3.741978	0.224876	C	-2.604077	-3.920883	-0.432600
C	1.791170	2.985816	-2.242405	C	-1.808629	-2.234327	-2.232374
C	0.663889	3.502814	1.198155	C	-2.708386	-3.859093	0.922053
C	-1.502617	2.090852	1.282361	C	-2.224475	-2.107050	2.710930
C	3.306830	-2.123541	1.170448	C	-2.138778	4.054011	-0.527178
C	2.455900	0.248485	1.764590	C	-1.610652	2.187071	-2.243775
C	3.063261	-2.968062	0.139234	C	-1.679140	4.330668	0.722605
C	1.616221	-2.800797	-1.997256	C	0.003084	3.269178	2.321800
C	-3.396961	-1.633404	1.210703	C	4.565416	-0.425076	0.371288
C	-1.255373	-2.898774	0.513064	C	2.979227	-1.533032	2.103192
C	-4.147498	-0.673214	0.609786	C	4.371127	0.093039	-0.872504
C	-3.963391	0.550290	-1.665532	C	2.330188	0.216156	-2.458223
C	2.812763	4.582146	0.292448	C	-2.947922	-5.049974	-1.344285
C	3.031314	2.094169	-2.236400	C	-2.984191	-2.419545	-3.186627
C	2.051529	4.368478	-2.835708	C	-0.507383	-2.859989	-2.728556
C	0.631280	4.017706	2.597884	C	-3.177080	-4.884164	1.896490
C	-2.409410	3.150315	1.901144	C	-3.051107	-0.839086	2.905808
C	-1.141977	0.962397	2.242482	C	-0.776832	-1.980577	3.178976
C	4.217756	-2.309094	2.336953	C	-3.124682	4.816409	-1.346455
C	3.694516	1.099235	1.490764	C	-1.354490	3.106402	-3.434480
C	2.197440	0.034478	3.253352	C	-2.931969	1.426795	-2.328282
C	3.677546	-4.298989	-0.135972	C	-2.030306	5.439643	1.653244
C	1.268881	-4.286100	-2.082492	C	1.511249	3.294419	2.085658
C	2.606835	-2.356354	-3.070626	C	-0.471587	2.085282	3.158920
C	-3.605194	-2.297731	2.529859	C	5.823795	-0.493155	1.168914
C	-1.862268	-4.268059	0.213701	C	2.895409	-0.475513	3.201382
C	-0.471739	-2.858377	1.820927	C	3.884280	-2.708040	2.459351
C	-5.415312	-0.047288	1.084362	C	5.354057	0.786508	-1.754319
C	-5.018624	-0.203553	-2.472909	C	2.373837	1.702350	-2.796253
C	-4.426786	1.936025	-1.227728	C	2.807904	-0.697975	-3.583189
H	1.026331	2.500636	-2.853701	H	-1.656761	-1.159045	-2.126347
H	-2.031171	1.641451	0.440762	H	-2.692326	-2.901785	3.292744
H	1.599613	0.776733	1.343409	H	-0.795358	1.460875	-2.224415
H	0.675252	-2.271094	-2.149896	H	-0.265436	4.183085	2.852782
H	-0.565592	-2.657176	-0.294188	H	1.977240	-1.928495	1.927551
H	-3.077520	0.683724	-2.286004	H	1.291104	-0.046266	-2.261819
H	3.677386	4.072920	-0.139217	H	-3.065453	-5.963992	-0.761751
H	3.050649	4.802453	1.334079	H	-2.165678	-5.232517	-2.083352
H	2.686017	5.536715	-0.226009	H	-3.886624	-4.869121	-1.874384

H	3.371714	1.939427	-3.263833	H	-2.782169	-1.846909	-4.095097
H	2.797663	1.123379	-1.792649	H	-3.910088	-2.045106	-2.743582
H	3.855063	2.547583	-1.677801	H	-3.123276	-3.461304	-3.479403
H	2.907161	4.864486	-2.372926	H	-0.611626	-3.934430	-2.896073
H	1.172722	5.009884	-2.732838	H	0.298962	-2.693599	-2.009621
H	2.272152	4.256979	-3.900346	H	-0.228788	-2.397173	-3.678779
H	-0.099626	4.822400	2.719932	H	-3.425474	-5.806716	1.372058
H	1.610258	4.416642	2.867192	H	-4.075365	-4.553252	2.425949
H	0.389971	3.231692	3.316774	H	-2.407397	-5.118742	2.637279
H	-2.010614	3.548342	2.836663	H	-4.080496	-0.997798	2.576032
H	-3.378388	2.695082	2.123905	H	-2.632464	0.003883	2.354076
H	-2.572208	3.979314	1.207277	H	-3.063375	-0.587890	3.969042
H	-0.579118	1.314776	3.110797	H	-0.760499	-1.758421	4.248158
H	-0.547640	0.212762	1.716114	H	-0.255004	-1.168706	2.667066
H	-2.059618	0.487934	2.601396	H	-0.227648	-2.909538	3.007085
H	4.850628	-1.434989	2.506765	H	-2.633619	5.395823	-2.132576
H	4.876520	-3.160414	2.163210	H	-3.663962	5.515453	-0.706788
H	3.658829	-2.504576	3.256772	H	-3.864804	4.163908	-1.812419
H	4.605946	0.643794	1.887586	H	-0.456840	3.709051	-3.276685
H	3.570691	2.077624	1.963728	H	-2.197941	3.768927	-3.635439
H	3.821181	1.253321	0.416736	H	-1.202060	2.487561	-4.321892
H	3.071745	-0.354897	3.779023	H	-2.929197	0.806317	-3.228657
H	1.359351	-0.648469	3.415085	H	-3.786854	2.102915	-2.395667
H	1.944536	0.997240	3.706309	H	-3.061913	0.781090	-1.456408
H	2.959178	-5.115669	-0.025287	H	-2.422114	5.058698	2.600788
H	4.490542	-4.477148	0.568560	H	-2.797418	6.071286	1.205671
H	4.100979	-4.353481	-1.142675	H	-1.164431	6.072698	1.867971
H	0.636452	-4.440466	-2.959991	H	2.016786	3.356490	3.052354
H	0.710981	-4.613145	-1.201750	H	1.792648	4.167862	1.492452
H	2.149103	-4.920214	-2.195839	H	1.853802	2.396129	1.569066
H	3.574849	-2.849260	-2.941406	H	0.023037	2.106934	4.132549
H	2.761843	-1.274372	-3.028930	H	-0.225640	1.133345	2.682861
H	2.221381	-2.611949	-4.061159	H	-1.551904	2.125840	3.316181
H	-3.520970	-3.384712	2.466807	H	5.672133	-0.162117	2.198021
H	-4.601485	-2.067865	2.908472	H	6.575001	0.159976	0.724873
H	-2.879518	-1.946299	3.269748	H	6.231534	-1.507085	1.191383
H	-2.610877	-4.557614	0.955014	H	2.484293	-0.931005	4.105759
H	-1.075476	-5.027166	0.227119	H	2.244899	0.351674	2.906643
H	-2.330034	-4.271882	-0.773925	H	3.877919	-0.065212	3.447243
H	-0.141657	-1.842396	2.045435	H	3.414905	-3.268523	3.271231
H	0.419575	-3.483616	1.713139	H	4.867830	-2.386683	2.806209
H	-1.047954	-3.237280	2.667600	H	4.008344	-3.379505	1.606564
H	-5.261606	0.988983	1.398670	H	5.168692	1.863368	-1.788047
H	-5.801012	-0.599703	1.941560	H	5.336809	0.404572	-2.776006
H	-6.190285	-0.054964	0.314103	H	6.361818	0.633336	-1.368501
H	-5.921056	-0.393225	-1.884741	H	1.667530	1.895959	-3.607819
H	-4.622646	-1.161471	-2.819681	H	3.361658	2.019700	-3.135154
H	-5.303990	0.388741	-3.346289	H	2.078809	2.300353	-1.930867
H	-4.556880	2.549295	-2.123088	H	2.159688	-0.554087	-4.451160
H	-3.682471	2.424191	-0.596123	H	2.750125	-1.745599	-3.278488
H	-5.382799	1.917512	-0.701661	H	3.831390	-0.477810	-3.892388

H	0.312226	-0.138068	-2.951757				
	1d (protonated form)				1d (dication)		
C	-1.882312	-2.414208	0.840709	P	0.022528	-0.001069	0.527044
C	-0.717572	-2.505853	0.016311	N	-0.829239	1.303517	0.491716
N	-0.455377	-3.753789	-0.519427	N	-0.684073	-1.389460	0.493442
C	-1.236637	-4.837801	-0.257807	N	1.578599	0.087542	0.508953
C	-2.339632	-4.760777	0.538066	C	2.386783	1.173608	0.472292
C	-2.663642	-3.506599	1.096404	N	3.608624	0.983484	-0.111371
N	0.134483	-1.542352	-0.285916	C	4.518519	1.985885	-0.192939
P	0.006128	-0.006847	0.229969	C	4.262612	3.231508	0.314664
N	-1.386646	0.651210	-0.289040	C	3.027462	3.456529	0.933516
C	-1.798609	1.865890	0.028150	C	2.103033	2.438626	1.014992
N	-3.008386	2.268618	-0.507823	C	3.938188	-0.326135	-0.722430
C	-3.559474	3.482754	-0.232144	H	5.450044	1.735756	-0.683229
C	-2.946655	4.389117	0.579572	H	5.012176	4.006723	0.233831
C	-1.700877	4.036518	1.139395	H	2.795371	4.428886	1.352574
C	-1.142527	2.818069	0.869483	H	1.142237	2.586576	1.489409
C	-3.751057	1.335799	-1.374877	C	3.347966	-0.453704	-2.118704
C	-4.582625	0.350005	-0.566264	H	5.025596	-0.395357	-0.742975
C	0.735762	-3.929749	-1.370114	H	3.556386	-1.099442	-0.058627
C	1.993876	-4.159462	-0.544645	H	2.257748	-0.401277	-2.088747
N	1.272592	0.870572	-0.287136	H	3.725043	0.334040	-2.775598
C	2.530086	0.628843	0.037838	H	3.634586	-1.420293	-2.538558
N	3.480980	1.482184	-0.492187	C	-0.166592	-2.638605	0.433082
C	4.806507	1.364730	-0.203899	N	-0.993583	-3.594581	-0.089735
C	5.286331	0.385595	0.612875	C	-0.602550	-4.888636	-0.196411
C	4.361511	-0.526084	1.163538	C	0.632051	-5.303486	0.226227
C	3.028556	-0.412319	0.881810	C	1.496976	-4.354820	0.784068
C	3.042007	2.584590	-1.367289	C	1.100745	-3.039862	0.889949
C	2.578949	3.794849	-0.568486	C	-2.330666	-3.212231	-0.602718
H	-4.514868	3.675245	-0.703810	H	-1.325817	-5.563643	-0.634649
H	-3.412440	5.345690	0.772523	H	0.909703	-6.343995	0.128150
H	-1.179865	4.734238	1.786268	H	2.478389	-4.650680	1.136623
H	-0.180310	2.549486	1.287173	H	1.749301	-2.287683	1.318402
H	-4.382230	1.941488	-2.026853	C	-2.247959	-2.655747	-2.015966
H	-3.017085	0.813439	-1.987187	H	-2.947342	-4.110008	-0.564510
H	-5.302424	0.873979	0.068539	H	-2.744871	-2.479732	0.087291
H	-5.134505	-0.303299	-1.246449	H	-1.820988	-3.391854	-2.701610
H	-3.937738	-0.269472	0.060104	H	-3.254559	-2.407238	-2.359201
H	5.449192	2.101428	-0.669214	H	-1.640706	-1.748673	-2.043743
H	6.346369	0.320887	0.816242	C	-2.172331	1.462745	0.432894
H	4.706848	-1.323701	1.812575	N	-2.607680	2.606552	-0.176676
H	2.317561	-1.118289	1.292257	C	-3.928942	2.892067	-0.286127
H	3.886875	2.836616	-2.009994	C	-4.888814	2.056524	0.219081
H	2.234896	2.198931	-1.988940	C	-4.477376	0.886412	0.868030
H	2.291701	4.594709	-1.255358	C	-3.135406	0.596221	0.977713
H	1.712692	3.538641	0.044591	C	-1.626574	3.539321	-0.780456
H	3.378656	4.166290	0.078061	H	-4.168391	3.815824	-0.796008
H	-0.920175	-5.760877	-0.727028	H	-5.933320	2.316517	0.115347
H	-2.938961	-5.642149	0.720320	H	-5.210633	0.207803	1.288397
H	-3.537539	-3.404750	1.730973	H	-2.790961	-0.298743	1.478046

H	-2.135063	-1.447426	1.257610	C	-1.197630	3.080341	-2.165885
H	0.535561	-4.778036	-2.026343	H	-2.108558	4.516141	-0.816820
H	0.830510	-3.032416	-1.980238	H	-0.776823	3.598145	-0.102793
H	2.844317	-4.311404	-1.213764	H	-2.055238	3.013504	-2.839798
H	2.201239	-3.292505	0.085661	H	-0.491463	3.805063	-2.576821
H	1.890160	-5.045356	0.087797	H	-0.704204	2.107332	-2.119919
H	0.004829	-0.004571	1.650730				
1e (protonated form)				1e (dication)			
C	4.908410	1.582528	-1.188665	C	-3.400774	3.003659	-0.530894
N	3.639161	0.882687	-1.364160	N	-2.248729	3.316027	0.314685
C	3.536160	0.218133	-2.659468	P	-0.759527	2.789156	-0.138904
P	2.793422	0.247351	-0.067034	N	0.207203	3.038890	1.174325
N	3.588083	-0.966166	0.755532	C	-0.135750	2.421076	2.454915
C	4.960452	-0.762867	1.200034	C	-2.475595	4.414676	1.252052
N	1.440738	-0.389086	-0.545119	N	-0.192841	3.614263	-1.443636
P	0.009619	0.047740	-1.117994	C	-0.337051	5.068598	-1.496558
N	-1.143918	-1.007174	-0.710425	N	-0.962777	1.228773	-0.563712
P	-1.177847	-2.447414	-0.067182	P	-0.004335	0.006630	-0.526614
N	-1.113470	-2.446240	1.593508	N	1.533701	0.225555	-0.565919
C	-0.096808	-1.653108	2.270144	P	2.779477	-0.730651	-0.130469
N	-0.383571	1.578353	-0.810479	N	3.211920	-1.650692	-1.422604
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C	-2.952416	1.637207	-2.473990	N	-0.581689	-1.434260	-0.589213
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C	2.434296	2.858058	0.591658	N	-3.035949	-1.958130	-1.464201
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C	-3.026637	0.676652	1.563391	N	-1.733102	-3.608650	0.264204
N	-1.188791	3.871565	0.077807	C	-0.883554	-4.435525	-0.592356
C	-2.136441	4.801618	0.686260	N	-2.721589	-1.359446	1.160500
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C	0.557870	-3.310148	-2.002308	N	3.983173	0.297238	0.314128
C	2.498034	1.259140	2.419862	C	4.300696	1.432282	-0.552321
C	3.210040	-2.364319	0.604378	N	2.506349	-1.676637	1.192412
C	-1.358029	2.148216	2.539778	C	2.069208	-3.065281	1.064597
C	-0.364280	4.510010	-0.944753	C	5.042083	-0.044478	1.262161
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C	0.407304	-4.656707	0.031066	C	2.153596	-1.058763	2.470013
C	-1.760892	-3.429665	2.452696	C	4.537201	-2.268160	-1.455933
H	0.110260	-0.020010	-2.523251	C	-1.999900	-1.361227	2.432321
H	5.764596	0.900884	-1.279113	C	-4.220189	-2.814170	-1.521672
H	4.947927	2.067733	-0.213501	H	-3.629022	3.836816	-1.205377
H	5.001225	2.354000	-1.960054	H	-4.269854	2.816616	0.106097
H	4.316073	-0.545272	-2.786883	H	-3.206271	2.107508	-1.120278
H	3.650637	0.961614	-3.454627	H	-3.200086	4.100882	2.009557
H	2.561779	-0.257448	-2.766075	H	-2.876387	5.290462	0.728908
H	3.045405	1.973889	3.042552	H	-1.546957	4.696729	1.746419
H	2.795003	0.249106	2.700284	H	0.425574	1.490528	2.605436
H	1.425839	1.381487	2.618367	H	-1.203804	2.203564	2.503048
H	3.037252	3.588906	1.141012	H	0.112323	3.109954	3.266941

H	1.372084	3.050278	0.783057	H	1.821557	3.843141	0.080435
H	2.615993	2.984397	-0.475218	H	2.230563	2.420286	1.064839
H	3.359652	-2.880923	1.559255	H	1.937239	4.002306	1.837872
H	3.820259	-2.870283	-0.157163	H	0.597336	5.573171	-1.225021
H	2.159233	-2.432282	0.323221	H	-1.124546	5.405297	-0.822577
H	5.122092	-1.310050	2.134551	H	-0.612478	5.361003	-2.513492
H	5.147285	0.294369	1.394735	H	0.818604	1.990779	-2.337970
H	5.688773	-1.121438	0.460328	H	1.728638	3.509107	-2.321521
H	-0.673536	2.969492	2.327763	H	0.359063	3.302679	-3.437485
H	-0.777637	1.274274	2.862404	H	0.977031	-3.141088	1.122990
H	-2.015429	2.443671	3.364647	H	2.513380	-3.651696	1.873251
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H	-2.447246	-0.200467	1.875267	H	1.071028	-1.101631	2.642111
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H	-0.972912	4.911086	-1.767859	H	2.145628	-3.250196	-2.304497
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H	0.325747	-4.212882	-2.581227	H	-4.339803	-3.186454	-2.542697
H	1.644812	-3.174462	-1.981629	H	-5.124863	-2.264337	-1.237791
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H	-2.369672	-2.918256	3.207554	H	-0.207518	-3.807996	-1.173258
H	-1.015049	-4.043195	2.974555	H	-1.488020	-5.043891	-1.274732
H	-0.534409	-1.171733	3.152125	H	-0.283712	-5.100035	0.035861
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H	-2.865025	-3.157859	-2.498801	H	-4.239240	-0.359834	0.091178
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1f (protonated form)				1f (dication)			
P	-0.001469	-0.000492	0.961707	C	5.084533	-0.692970	3.045374
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H	-3.702234	-1.100253	-0.130994	P	2.833821	0.462585	0.056959
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C	-2.572910	-0.988762	-3.270447	C	3.501882	3.038801	0.523087
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C	-1.492064	-1.708872	-2.459164	N	0.121060	-1.553205	0.398203
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H	-0.655669	-1.037906	-2.230054	N	-1.929358	-2.913474	1.393194
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C	-1.182684	-4.921729	-1.253234	C	-3.342601	-2.526286	3.240120
H	-0.823337	-4.705157	-2.267915	C	-3.148611	-4.033511	3.055429
H	-2.274136	-4.876530	-1.268234	C	-2.717882	-4.144058	1.593851
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H	-0.008724	-4.782713	1.571752	P	-1.817770	2.220030	0.061217
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N	-2.330444	-2.749574	1.364285	C	-0.568808	2.848916	2.453559
C	-2.639227	-1.757333	2.409225	C	-0.529387	4.157063	3.247412
H	-2.646950	-0.738858	2.009841	C	-1.933121	4.737828	3.058192
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H	-4.000030	-3.788394	0.538312	C	1.028503	3.450862	-2.192398
C	-0.651463	-6.273598	-0.771499	C	0.133603	2.876469	-3.293656
H	-0.577159	-7.000234	-1.583080	C	-0.973454	2.149712	-2.522100
H	-1.316371	-6.685312	-0.004155	N	-3.403534	2.181676	-0.331432
C	0.700073	-5.911861	-0.150515	C	-4.067708	3.055770	-1.319949
H	1.085825	-6.675865	0.527258	C	-5.506161	3.131020	-0.807694
H	1.443079	-5.742743	-0.937384	C	-5.713287	1.762319	-0.154218
C	-4.015720	-2.193536	2.915726	C	-4.379836	1.510867	0.548922
H	-4.187474	-1.896726	3.952294	N	-1.960330	-2.320912	-1.231623
H	-4.799433	-1.742329	2.297191	C	-3.372867	-1.901549	-1.119826
C	-3.999801	-3.710922	2.712994	C	-3.507141	-0.823514	-2.192243
H	-4.995933	-4.157471	2.704811	C	-2.560370	-1.311690	-3.291585
H	-3.414520	-4.190437	3.504291	C	-1.374644	-1.896772	-2.517194
H	-0.001470	-0.001864	2.374633	N	-0.197711	-4.037581	-0.340146
N	1.376717	0.710447	0.519143	C	-0.633972	-5.041390	-1.332436
P	2.804406	0.158112	0.120037	C	0.002798	-6.334146	-0.822669
N	2.911103	-0.826840	-1.213335	C	1.299736	-5.847212	-0.171640
C	3.052683	-2.290651	-1.125998	C	0.870478	-4.560950	0.533745
H	2.803758	-2.653485	-0.127575	N	3.006338	-0.537929	-1.233415
H	4.089083	-2.579803	-1.344559	C	3.327962	-1.975017	-1.113858
C	2.097639	-2.821134	-2.193758	C	2.460397	-2.622657	-2.190031
H	2.398175	-3.803434	-2.566434	C	2.432471	-1.562631	-3.294224
H	1.094011	-2.902404	-1.767808	C	2.363236	-0.237805	-2.526921
C	2.145216	-1.732571	-3.268336	H	0.446928	3.895168	-0.119818
H	1.276265	-1.740346	-3.930705	H	-0.384526	4.873929	-1.341630
H	3.041931	-1.847555	-3.885835	H	1.645491	4.283367	-2.536091

C	2.229288	-0.435847	-2.457914	H	1.686145	2.677715	-1.783927
H	2.783126	0.347857	-2.985478	H	0.660566	2.202922	-3.972469
H	1.230196	-0.045211	-2.231187	H	-0.300067	3.685587	-3.888447
N	3.731368	1.460285	-0.294013	H	-1.932396	2.172200	-3.047146
C	4.854088	1.441207	-1.245326	H	-0.711465	1.095910	-2.355408
H	4.492415	1.649068	-2.261060	H	-4.035256	2.588841	-2.311617
H	5.357776	0.471892	-1.261484	H	-3.581439	4.031069	-1.382924
C	3.772840	2.647780	0.570541	H	-4.366497	1.961189	1.549797
H	4.128161	2.386370	1.577504	H	-4.140382	0.449670	0.648749
H	2.777340	3.087084	0.666914	H	0.406681	2.588951	2.034928
N	3.543915	-0.640001	1.367316	H	-0.916109	2.012942	3.070750
C	2.837665	-1.402960	2.411812	H	-3.305919	4.335690	1.387053
H	1.958827	-1.917277	2.011900	H	-1.816024	5.192325	0.932156
H	2.503692	-0.729915	3.211637	H	-6.214600	3.337278	-1.611800
C	4.988643	-0.910319	1.373012	H	-5.596873	3.924304	-0.058358
H	5.556860	0.020831	1.281587	H	-6.553321	1.737060	0.541659
H	5.277131	-1.568681	0.541399	H	-5.878896	0.999218	-0.921572
C	5.759202	2.573214	-0.754607	H	-0.269170	3.989102	4.293825
H	6.358700	3.000877	-1.560753	H	0.215744	4.831605	2.813358
H	6.441217	2.199459	0.017174	H	-1.988596	5.807208	3.268126
C	4.768212	3.564322	-0.139144	H	-2.649180	4.220013	3.703912
H	5.233851	4.278218	0.543045	H	-3.593837	-1.535862	-0.115889
H	4.257582	4.125835	-0.928996	H	-4.028859	-2.754264	-1.328206
C	3.902027	-2.379165	2.917261	H	-4.537152	-0.711299	-2.536301
H	3.730066	-2.677894	3.953234	H	-3.170663	0.135819	-1.787860
H	3.902136	-3.282228	2.296892	H	-2.244481	-0.520122	-3.973941
C	5.209219	-1.608136	2.716027	H	-3.040399	-2.097213	-3.882390
H	6.093305	-2.248520	2.708016	H	-0.906839	-2.735331	-3.040299
H	5.332216	-0.862113	3.507825	H	-0.599680	-1.135951	-2.350735
N	-1.305811	0.838890	0.520037	H	-0.240513	-4.781907	-2.322616
P	-1.539455	2.351744	0.120870	H	-1.722386	-5.093590	-1.397428
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C	0.453403	3.791566	-1.132956	H	1.679767	-3.833491	0.628385
H	0.892681	3.764536	-0.134656	H	-2.438026	-0.937489	2.030879
H	0.182424	4.831676	-1.357113	H	-1.287500	-1.798577	3.073615
C	1.391589	3.226899	-2.198127	H	-2.107629	-5.028872	1.392377
H	2.090559	3.977972	-2.574170	H	-3.589106	-4.163722	0.927037
H	1.965152	2.401046	-1.768811	H	0.166619	-7.052828	-1.627444
C	0.425843	2.716584	-3.269851	H	-0.644179	-6.800331	-0.072198
H	0.868895	1.966941	-3.929890	H	1.733342	-6.568510	0.522814
H	0.073296	3.547130	-3.889962	H	2.045168	-5.618950	-0.940291
C	-0.735728	2.140043	-2.455515	H	-3.333119	-2.214653	4.285924
H	-1.692130	2.220062	-2.983011	H	-4.295050	-2.215256	2.798775
H	-0.568940	1.081665	-2.222819	H	-4.050479	-4.612174	3.261565
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C	-3.673958	3.487616	-1.243833	H	3.109154	-2.341407	-0.109762
H	-3.659680	3.073985	-2.260780	H	4.393921	-2.132038	-1.313703
H	-3.093939	4.413449	-1.251272	H	2.867673	-3.577768	-2.527593
C	-4.182003	1.947845	0.571121	H	1.456193	-2.795796	-1.791881
H	-4.142965	2.392516	1.575807	H	1.590790	-1.675012	-3.980579
H	-4.058326	0.867395	0.674449	H	3.355241	-1.603148	-3.880191

N	-1.213962	3.392388	1.366248	H	2.875526	0.575078	-3.048859
C	-0.192554	3.165647	2.404127	H	1.321048	0.072468	-2.370957
H	0.689016	2.659751	1.999584	H	4.297812	2.187914	-2.318224
H	-0.602816	2.542939	3.209268	H	5.283234	1.051007	-1.377884
C	-1.705600	4.777675	1.374325	H	3.857904	2.798991	1.533242
H	-2.797022	4.801574	1.294116	H	2.467727	3.382465	0.597878
H	-1.289714	5.355993	0.537136	H	2.030664	-1.614977	2.062901
C	-5.113284	3.694093	-0.766426	H	2.223673	-0.172973	3.081618
H	-5.778452	3.991282	-1.579704	H	5.421045	0.679572	1.359419
H	-5.144618	4.473930	0.002463	H	5.396215	-1.042365	0.918230
C	-5.470879	2.339517	-0.149701	H	6.060818	3.660428	-1.584480
H	-6.327591	2.381846	0.525673	H	6.207524	2.827938	-0.026865
H	-5.690158	1.612267	-0.938878	H	4.819855	4.781632	0.540443
C	0.124509	4.577039	2.902510	H	3.870992	4.583894	-0.943072
H	0.478654	4.580834	3.935279	H	3.603619	-1.729957	4.305354
H	0.900447	5.027578	2.273693	H	4.064437	-2.589990	2.827192
C	-1.199298	5.321871	2.711206	H	6.034174	-1.189914	3.250149
H	-1.087889	6.407780	2.698880	H	5.011835	0.192671	3.684249
H	-1.899141	5.057165	3.510452				
2a (protonated form (in-out))				2a (dication)			
C	0.581828	4.165221	2.373797	C	-0.461799	4.828665	1.488422
C	0.679927	3.878548	0.988317	C	0.169110	4.211225	0.377093
C	0.416786	2.555896	0.533898	C	0.107756	2.799472	0.258716
C	0.064584	1.562232	1.492585	C	-0.557040	2.043466	1.269607
C	-0.023953	1.876889	2.828459	C	-1.158718	2.671743	2.332709
C	0.234011	3.189916	3.274779	C	-1.114860	4.080398	2.435586
C	0.500384	2.267817	-0.869477	C	0.713036	2.168974	-0.868540
C	0.832080	3.282251	-1.741493	C	1.376508	2.910816	-1.815388
C	1.104956	4.592133	-1.287861	C	1.454328	4.315244	-1.682851
C	1.028549	4.883196	0.047401	C	0.859073	4.948308	-0.620427
P	0.108487	0.612732	-1.621414	P	0.451388	0.389636	-0.957465
N	1.141396	-0.695176	-1.664045	N	-0.663952	0.164257	-2.108926
C	2.395022	-0.711319	-2.013774	C	-1.297124	-0.953730	-2.422797
N	3.055680	-1.889279	-1.937829	C	-0.918097	-2.320503	-1.912936
C	2.392894	-3.063906	-1.392007	P	-0.448292	0.257932	1.060057
P	-0.168898	-0.081386	0.779887	N	0.640954	-0.250978	2.143796
N	-1.685861	-0.526048	1.316942	C	1.198135	-1.447464	2.233585
C	-2.247803	-1.637411	0.917486	C	0.704315	-2.673181	1.508626
N	-3.520650	-1.887623	1.294884	N	-1.883758	-0.432543	0.817807
C	-4.279025	-0.896787	2.040140	C	-2.707143	-1.100110	1.601435
N	0.892813	-1.156580	1.483949	C	-2.394856	-1.487203	3.024397
C	2.191408	-1.113420	1.513897	N	-3.882150	-1.482487	1.101294
N	2.844194	-2.189177	2.018387	C	-4.853995	-2.255935	1.870218
C	4.295246	-2.302842	2.008312	C	-4.305797	-1.099457	-0.241030
C	3.051023	0.047557	1.070480	N	1.816214	-0.468352	-0.852386
N	-1.428675	0.094615	-1.925230	C	2.626803	-0.923416	-1.789532
C	-2.591180	0.520193	-1.529667	C	2.349062	-0.833345	-3.268662
N	-3.681916	-0.245667	-1.767889	N	3.755477	-1.521130	-1.409953
C	-5.028195	0.152878	-1.385425	C	4.695234	-2.112678	-2.359148
C	-2.828994	1.826243	-0.810506	C	4.153877	-1.582894	-0.008160
C	3.194012	0.484602	-2.478553	N	-2.325590	-0.843121	-3.260159

C	4.421701	-2.076363	-2.406220	C	-2.690616	0.478002	-3.767717
C	-1.560643	-2.680110	0.066075	C	-3.133403	-1.960692	-3.733483
C	-4.189051	-3.163875	1.086392	N	2.251982	-1.557653	3.038335
C	2.060479	-3.359045	2.385160	C	2.727875	-0.374191	3.752343
C	-3.589792	-1.467533	-2.548822	C	2.975670	-2.797923	3.291102
H	0.881844	3.079879	-2.807935	H	-1.661455	2.097665	3.104169
H	1.367918	5.361438	-2.005352	H	-1.594353	4.565892	3.277906
H	1.229899	5.888324	0.405793	H	-0.419803	5.909661	1.578660
H	-0.294935	1.107648	3.545258	H	1.836619	2.430390	-2.673077
H	0.159924	3.423980	4.331357	H	1.980684	4.891218	-2.435364
H	0.785810	5.177054	2.711277	H	0.910220	6.028810	-0.529452
H	-5.038330	0.643598	-0.412602	H	2.637887	-3.598752	2.639665
H	-5.639749	-0.747465	-1.305429	H	2.836367	-3.105011	4.330898
H	-2.544445	-1.693817	-2.742604	H	3.019464	0.403727	3.043682
H	-4.045731	-2.295692	-1.997817	H	1.942014	0.022212	4.398174
H	4.653447	-1.418402	-3.242498	H	-4.364395	-3.004345	2.491382
H	5.151207	-1.906092	-1.605570	H	-5.464706	-1.601746	2.499561
H	1.919446	-3.657621	-2.181851	H	-4.336692	-1.983248	-0.885307
H	3.135467	-3.683062	-0.882900	H	-5.307775	-0.667957	-0.188592
H	1.627520	-2.751414	-0.682058	H	-3.613472	-0.368226	-0.650313
H	-5.487527	0.815372	-2.128069	H	4.040508	-2.632946	3.111462
H	-4.120267	-1.351287	-3.500140	H	3.587479	-0.659019	4.356753
H	4.768239	-1.363705	2.296063	H	-2.989955	-2.094160	-4.808889
H	2.713421	-4.088814	2.862745	H	-1.840092	0.938454	-4.273461
H	1.263083	-3.077424	3.075554	H	-3.514308	0.361808	-4.470180
H	-4.868706	-3.339796	1.922438	H	5.380490	-1.356635	-2.753729
H	-4.777081	-3.167791	0.161248	H	5.274962	-2.871606	-1.834385
H	-3.479389	-3.989453	1.063080	H	4.175268	-2.597849	-3.183512
H	-3.878574	0.095523	1.844132	H	4.023535	-2.600255	0.373691
H	-5.324290	-0.939734	1.724724	H	5.208121	-1.310479	0.071634
H	-4.227393	-1.087269	3.118238	H	3.552538	-0.890751	0.576064
H	4.594757	-3.056433	2.736408	H	-2.873839	-2.885641	-3.226738
H	1.595234	-3.817128	1.505187	H	-2.999231	1.128895	-2.946531
H	4.187011	0.505474	-2.025517	H	-3.221832	-1.229514	3.688820
H	3.317356	0.453613	-3.565424	H	-2.231045	-2.566973	3.093127
H	2.689361	1.413503	-2.222338	H	-1.495844	-0.983669	3.372991
H	-2.936104	1.636957	0.261926	H	1.448845	-3.017859	0.786357
H	-1.984908	2.496323	-0.956011	H	0.492474	-3.486132	2.206287
H	-3.726889	2.329672	-1.170556	H	-0.215396	-2.449031	0.972103
H	3.490667	0.547873	1.938555	H	-0.745795	-3.014927	-2.738038
H	3.866979	-0.288460	0.427128	H	-0.000066	-2.266071	-1.331305
H	2.464151	0.781316	0.523339	H	-1.709580	-2.725724	-1.276784
H	4.677816	-2.604309	1.025121	H	-4.187544	-1.746432	-3.542334
H	-0.811164	-2.200532	-0.566956	H	3.218466	-0.449797	-3.806242
H	-1.047231	-3.402229	0.707773	H	2.115129	-1.824940	-3.667921
H	-2.256594	-3.215445	-0.579108	H	1.497675	-0.184971	-3.466166
H	4.530121	-3.103461	-2.758180	H	-5.506255	-2.775078	1.168387
H	0.368409	1.105886	-2.939935				
2a (protonated form (in-in))							
C	0.863423	-2.981680	3.018229				
C	-0.132914	-2.966287	2.010707				

C	-0.121021	-1.949237	1.004854
C	1.010004	-1.075170	0.955703
C	1.936771	-1.109447	1.976283
C	1.854969	-2.036734	3.032480
C	-1.281508	-1.871469	0.147422
C	-2.239086	-2.864056	0.186950
C	-2.147484	-3.949033	1.083757
C	-1.144023	-3.964338	2.010271
P	-1.774552	-0.346343	-0.716416
N	-3.366490	-0.553325	-1.009942
C	-4.175508	0.300890	-1.595363
C	-3.767858	1.658457	-2.118484
P	1.442590	-0.113774	-0.574115
N	2.092389	1.272818	0.196314
C	2.026195	2.447816	-0.354634
C	1.452925	2.756351	-1.720534
N	2.708229	-1.134807	-1.034678
C	3.869685	-0.963305	-1.559178
C	4.586095	0.359718	-1.721717
N	4.534607	-2.067735	-2.045063
C	5.967582	-2.049725	-2.290059
C	3.946491	-3.372750	-1.800438
N	-1.380579	1.011919	0.091437
C	-1.542799	1.285932	1.366079
C	-2.049126	0.312064	2.403823
N	-1.234709	2.515883	1.799074
C	-1.275936	2.894473	3.207014
C	-0.901092	3.591064	0.876876
N	-5.452778	-0.074802	-1.734596
C	-5.864947	-1.378481	-1.226666
C	-6.482514	0.704112	-2.408454
N	2.535797	3.500409	0.340305
C	2.984873	3.269678	1.704371
C	2.621004	4.848555	-0.200607
H	2.773807	-0.419393	1.931320
H	2.603435	-2.032646	3.818142
H	0.818706	-3.753958	3.780480
H	-3.117226	-2.769941	-0.440512
H	-2.909955	-4.719805	1.073931
H	-1.102705	-4.741496	2.768000
H	2.844969	4.832971	-1.267461
H	3.436369	5.376586	0.295086
H	3.870231	2.626630	1.728096
H	3.222917	4.228117	2.165753
H	6.269262	-1.139948	-2.808461
H	6.553510	-2.135160	-1.364202
H	4.462373	-4.114616	-2.412767
H	4.023875	-3.667782	-0.744986
H	2.889283	-3.358698	-2.065312
H	1.697078	5.420059	-0.044704
H	2.200901	2.776207	2.285803

H	-6.078353	1.617605	-2.834755				
H	-5.426404	-2.183565	-1.823413				
H	-5.539851	-1.500919	-0.192171				
H	-0.609636	3.746282	3.346572				
H	-2.285046	3.187995	3.514629				
H	-0.921650	2.086575	3.846072				
H	-1.027488	3.242458	-0.144623				
H	-1.563622	4.440911	1.063225				
H	0.134343	3.907511	1.028332				
H	-6.916711	0.111049	-3.217647				
H	-6.951347	-1.442944	-1.278748				
H	5.538007	0.358718	-1.183248				
H	4.799044	0.557153	-2.776484				
H	3.978255	1.165297	-1.323088				
H	0.866734	3.677131	-1.716432				
H	2.258281	2.872007	-2.453548				
H	0.813756	1.933412	-2.039811				
H	-3.859494	1.689633	-3.207475				
H	-4.399191	2.444898	-1.698942				
H	-2.737706	1.882221	-1.847480				
H	-7.274223	0.967172	-1.701305				
H	-1.206103	-0.116935	2.955066				
H	-2.713807	0.801994	3.115924				
H	-2.594710	-0.504442	1.935210				
H	6.225127	-2.892763	-2.934079				
H	-1.086072	-0.230738	-1.924079				
2b (protonated form (<i>in-in</i>))				2b (dication)			
C	0.814142	2.447049	3.512444	C	0.000000	0.000000	0.000000
C	-0.416248	2.014041	2.960676	C	0.000000	0.000000	1.419048
C	-0.450070	1.217642	1.764944	C	1.244495	0.000000	2.098978
C	0.805146	0.956191	1.121363	C	2.455158	0.023790	1.347268
C	1.973634	1.398583	1.710764	C	2.418126	0.015132	-0.026455
C	1.999732	2.129745	2.908558	C	1.177973	0.002055	-0.703761
C	-1.761292	0.763712	1.340987	C	1.260242	-0.021140	3.523052
C	-2.890273	1.174686	2.019824	C	0.086266	-0.023968	4.236794
C	-2.833309	2.013029	3.150302	C	-1.152949	-0.003969	3.558558
C	-1.614244	2.399103	3.622329	C	-1.194205	0.004458	2.186174
P	-2.118286	-0.513698	0.082803	P	2.897475	0.009566	4.282908
N	-1.544199	-1.982523	0.411277	N	3.103553	-1.404137	5.023525
C	-0.594776	-2.409636	1.230467	C	3.768652	-1.735202	6.120131
N	-0.434078	-1.977568	2.516177	N	3.253639	-2.729466	6.885752
C	0.880110	-1.756089	3.100052	C	1.850442	-3.088444	6.753649
P	1.055346	0.149031	-0.554672	P	3.981621	0.044177	2.321001
N	2.036657	1.318443	-1.317841	N	4.628402	1.505172	2.184913
C	1.908391	2.604785	-1.264721	C	5.871875	1.942754	2.039741
N	3.016798	3.395970	-1.471021	N	6.765830	1.403773	1.171784
C	4.324164	2.773555	-1.490523	C	8.201711	1.408817	1.416733
N	2.201763	-0.995646	-0.052775	N	4.966598	-1.185605	2.062356
C	3.193149	-1.494851	-0.714477	C	5.163606	-2.424745	2.488579
N	3.390952	-1.498170	-2.084500	N	6.441603	-2.845601	2.635774
C	4.684253	-1.154247	-2.651051	C	6.839185	-4.236810	2.448257

N	4.207201	-2.130870	-0.015962	N	4.180003	-3.322418	2.743327
C	4.791186	-3.373045	-0.495375	C	2.861094	-3.189643	2.150851
C	4.304298	-1.943566	1.414293	C	4.262800	-4.269098	3.848472
N	-3.739615	-0.568513	-0.097062	N	3.229696	1.305457	5.171518
C	-4.342160	-0.485618	-1.269617	C	2.463415	2.315773	5.566792
N	-3.811220	-0.893943	-2.462895	N	1.560435	2.958032	4.780734
C	-2.918997	-2.036551	-2.580606	C	0.303915	3.474759	5.304515
N	-5.591796	0.040943	-1.315027	N	2.613737	2.754279	6.834875
C	-6.073558	0.839892	-0.200691	C	2.462574	4.156482	7.207070
C	-6.618133	-0.462577	-2.219602	C	3.280679	1.914438	7.817218
N	0.222595	-3.386786	0.791519	N	4.940131	-1.182070	6.521655
C	0.369073	-3.654121	-0.627038	C	5.825338	-0.499644	5.595346
C	0.907458	-4.318652	1.669068	C	5.311841	-1.058030	7.925930
C	-1.565763	-1.672292	3.372739	C	4.089800	-3.720843	7.553295
N	0.745379	3.308326	-1.000560	N	6.264876	3.028722	2.744584
C	-0.541536	2.818361	-1.439587	C	7.160922	4.038288	2.190820
C	0.710854	4.391369	-0.036090	C	5.533721	3.440485	3.932232
C	2.935143	4.664963	-2.176076	C	6.341321	0.715321	-0.036297
C	2.283740	-1.370776	-3.006473	C	7.542512	-1.896280	2.646897
C	-4.067207	-0.184516	-3.707495	C	1.747524	3.133048	3.349952
H	2.912335	1.180885	1.210617	H	0.102172	-0.031828	5.322548
H	2.945279	2.453211	3.330938	H	-2.073096	0.001273	4.131808
H	0.792602	3.038884	4.422610	H	-2.147912	0.014914	1.667712
H	-3.852855	0.801874	1.692704	H	3.336632	0.007826	-0.604081
H	-3.749283	2.313220	3.646569	H	1.165226	-0.003273	-1.787760
H	-1.533635	3.013264	4.514478	H	-0.951180	-0.003969	-0.523093
H	1.893171	4.934735	-2.341229	H	2.374921	4.775567	6.315349
H	3.421082	5.462468	-1.603861	H	1.589549	4.314298	7.846783
H	3.432056	4.588846	-3.151632	H	3.357201	4.467517	7.753034
H	4.357539	1.961441	-0.764934	H	3.080864	0.865162	7.606874
H	5.077281	3.524748	-1.235319	H	2.893485	2.163524	8.807244
H	4.567355	2.358496	-2.478607	H	4.363954	2.080047	7.806949
H	1.718812	4.598058	0.322864	H	0.145297	3.118938	6.321626
H	0.090844	4.104908	0.824069	H	-0.508050	3.094986	4.675857
H	-0.407744	2.051089	-2.203314	H	2.717821	2.746299	3.036878
H	-1.134543	2.402011	-0.615176	H	0.955066	2.627619	2.789126
H	5.437373	-1.109337	-1.865558	H	4.458080	-1.283289	8.563604
H	4.995950	-1.893770	-3.397645	H	6.144645	-1.717584	8.187565
H	2.091535	-0.325562	-3.280147	H	5.693826	0.585676	5.644442
H	1.379064	-1.791235	-2.568398	H	5.634421	-0.840147	4.579145
H	2.517003	-1.938194	-3.913274	H	6.858591	-0.753291	5.844959
H	5.884760	-3.336885	-0.442807	H	4.007408	-3.655236	8.642039
H	4.446026	-4.217556	0.117222	H	3.766890	-4.717914	7.238896
H	4.494417	-3.553190	-1.527467	H	5.132207	-3.595093	7.263580
H	3.959284	-0.945826	1.682491	H	1.262649	-2.209448	6.496444
H	3.702589	-2.675488	1.973002	H	1.696924	-3.850994	5.980657
H	5.348686	-2.064432	1.719009	H	1.505317	-3.485842	7.710705
H	0.296019	5.307319	-0.474572	H	0.271591	4.568991	5.293315
H	4.631812	-0.171717	-3.138870	H	5.618920	-0.024781	8.110601
H	-1.113492	3.644663	-1.877526	H	1.707725	4.202365	3.116484
H	-1.547294	-0.627169	3.696750	H	2.165195	-2.690697	2.834200

H	-2.499381	-1.864424	2.845063	H	2.922019	-2.639397	1.213285
H	-1.526180	-2.312081	4.261925	H	2.478812	-4.190880	1.937430
H	0.876530	-0.771307	3.579645	H	3.367628	-4.144853	4.463366
H	1.625609	-1.734338	2.304363	H	5.133904	-4.053880	4.466975
H	1.138068	-2.509208	3.853608	H	4.311741	-5.304610	3.499674
H	1.972818	-4.080211	1.758895	H	7.128870	-4.708275	3.391536
H	0.813278	-5.322955	1.247732	H	7.696092	-4.260994	1.770214
H	1.431058	-3.775599	-0.859975	H	8.276119	-2.208943	3.394011
H	-0.165524	-4.569172	-0.904429	H	8.029532	-1.865642	1.665692
H	-1.903858	-1.726765	-2.857620	H	5.061091	2.579328	4.401025
H	-2.871101	-2.583358	-1.640184	H	6.237942	3.896832	4.632259
H	-4.685004	-0.771168	-4.396474	H	8.133563	4.040637	2.691499
H	-3.108658	0.021503	-4.194757	H	6.698116	5.019673	2.325356
H	-4.561593	0.764553	-3.503745	H	7.303461	3.874532	1.123599
H	-6.900194	1.459688	-0.553909	H	7.002389	1.012591	-0.854775
H	-6.426517	0.214358	0.627173	H	6.373864	-0.370339	0.086787
H	-5.278899	1.491243	0.161315	H	5.325816	1.018578	-0.290264
H	-6.251729	-1.335900	-2.757392	H	8.403294	1.644076	2.461518
H	-7.490072	-0.765113	-1.632188	H	8.590394	0.409034	1.206637
H	-6.929749	0.299388	-2.940687	H	8.730069	2.121674	0.775860
H	0.450648	-4.315133	2.657445	H	6.026893	-4.802480	1.994498
H	-3.298911	-2.703911	-3.361179	H	4.758915	4.176100	3.684576
H	-0.035862	-2.819717	-1.194295	H	7.177414	-0.900099	2.885864
H	-1.569230	-0.058779	-1.120910				
2b (protonated form (<i>in-out</i>))							
C	-0.674957	-0.791846	4.133817				
C	-1.563046	-1.158174	3.092260				
C	-1.202462	-0.943457	1.720114				
C	-0.009085	-0.199962	1.460061				
C	0.819452	0.131745	2.513225				
C	0.519510	-0.187261	3.848693				
C	-2.095208	-1.493959	0.729034				
C	-3.319428	-2.003099	1.116832				
C	-3.718201	-2.074558	2.466370				
C	-2.826322	-1.711773	3.433849				
P	-1.766989	-1.897583	-1.030507				
N	-2.529319	-0.902911	-2.009304				
C	-2.530211	0.286348	-2.563527				
N	-1.517637	0.763112	-3.325982				
C	-0.469978	-0.140339	-3.766668				
P	0.429077	0.581603	-0.185143				
N	0.641587	2.200824	0.314070				
C	-0.061572	2.878702	1.161678				
N	0.533196	3.904290	1.863148				
C	1.975161	4.027300	1.843261				
N	2.022372	0.010359	-0.237626				
C	3.138458	0.578863	-0.545523				
N	3.336847	1.709012	-1.316860				
C	4.283314	2.738020	-0.926480				
N	4.325385	0.013158	-0.100267				
C	5.473559	-0.112343	-0.984836				

C	4.263885	-1.002654	0.925705
N	-0.270124	-2.407176	-1.396827
C	0.626453	-3.017656	-0.648509
N	1.879899	-3.167971	-1.133556
C	2.716262	-4.300951	-0.768049
N	0.397963	-3.537452	0.603891
C	1.347584	-3.346066	1.684816
C	-0.747579	-4.370051	0.913647
N	-3.655367	1.048079	-2.460392
C	-4.675371	0.685375	-1.489346
C	-4.145602	1.866666	-3.564845
N	-1.399908	2.687441	1.457935
C	-2.297385	2.174417	0.450243
C	-1.881873	2.629585	2.826104
C	-0.177681	5.125279	2.203861
C	2.360049	2.121594	-2.294813
C	-1.198136	2.181735	-3.412722
C	2.332695	-2.401735	-2.278651
H	1.723209	0.694236	2.298243
H	1.206723	0.087233	4.642193
H	-0.969443	-0.989807	5.160133
H	-3.991954	-2.415524	0.369585
H	-4.693508	-2.472932	2.721741
H	-3.070744	-1.830370	4.485324
H	-1.227954	5.036181	1.930445
H	-0.107857	5.335679	3.276779
H	0.251375	5.975426	1.658551
H	2.426517	3.041657	1.734543
H	2.308465	4.488462	2.778148
H	2.318927	4.653584	1.008003
H	-1.069203	2.862155	3.513930
H	-2.243652	1.618481	3.052932
H	-1.917083	2.419254	-0.541356
H	-2.434275	1.087486	0.512393
H	4.851460	2.411530	-0.056178
H	4.982944	2.964493	-1.740064
H	1.637694	2.832561	-1.874315
H	1.823440	1.248474	-2.668964
H	2.876799	2.587957	-3.140150
H	6.393297	0.196798	-0.476769
H	5.595533	-1.156098	-1.307398
H	5.336596	0.505652	-1.870649
H	3.486247	-0.757119	1.648029
H	5.230561	-1.051380	1.436022
H	-2.701695	3.338750	2.992761
H	3.747569	3.660005	-0.666746
H	-3.279192	2.645296	0.569626
H	-1.345758	-3.941143	1.724847
H	-1.377476	-4.499874	0.033797
H	-0.403903	-5.364017	1.224627
H	0.799471	-3.006542	2.570993

H	2.052389	-2.564232	1.406724				
H	1.889338	-4.265586	1.939434				
H	0.268510	-0.298683	-2.976857				
H	-0.897567	-1.107323	-4.031887				
H	-1.215749	2.529915	-4.449800				
H	-0.200403	2.344410	-2.999050				
H	-1.901039	2.771488	-2.828202				
H	-5.215063	1.590320	-1.200120				
H	-5.388298	-0.033326	-1.911273				
H	-4.220258	0.245517	-0.604732				
H	-3.510533	1.746663	-4.441120				
H	-5.154845	1.534420	-3.827676				
H	-4.189456	2.925490	-3.292816				
H	0.009849	0.294286	-4.646186				
H	4.044296	-1.994630	0.506734				
H	3.412302	-2.251915	-2.192107				
H	2.117858	-2.925557	-3.217639				
H	1.849148	-1.430073	-2.275030				
H	3.558515	-4.001466	-0.134984				
H	2.128833	-5.053828	-0.244087				
H	3.115322	-4.750077	-1.681716				
H	-2.575576	-3.036489	-1.149141				
2c (protonated form (in-in))				2c (dication)			
C	-0.770610	0.121256	2.856678	C	0.465363	-0.826381	3.149482
C	-1.811518	-0.251379	1.932353	C	1.491365	-0.761699	2.159998
C	-3.006207	-0.769318	2.395352	C	2.795851	-1.024031	2.500716
C	-3.279542	-0.908624	3.768391	C	3.136767	-1.320118	3.840872
C	-2.365888	-0.440901	4.671640	C	2.171471	-1.338911	4.816657
C	-1.122240	0.093814	4.246208	C	0.809458	-1.093427	4.498948
C	0.576669	0.517201	2.519234	C	-0.902236	-0.632466	2.797003
C	1.391997	1.018985	3.509337	C	-1.876653	-0.645575	3.765779
C	0.989570	1.101257	4.859409	C	-1.529053	-0.867231	5.117489
C	-0.229232	0.606477	5.225320	C	-0.223213	-1.100832	5.472475
H	-0.540325	0.596724	6.265996	H	0.035808	-1.293988	6.508965
H	2.401200	1.310130	3.233152	H	-2.917940	-0.488830	3.499597
H	1.668355	1.507957	5.602462	H	-2.306581	-0.867684	5.873196
H	-3.789342	-1.036955	1.690108	H	3.577283	-1.003288	1.748177
H	-4.223207	-1.332324	4.093882	H	4.171956	-1.521534	4.093070
H	-2.577689	-0.469737	5.736594	H	2.439454	-1.546718	5.847960
P	-1.906342	0.198761	0.165232	P	0.919534	-0.186893	0.533907
N	-2.998415	1.396832	0.095085	N	1.425400	-1.079818	-0.686482
N	-2.155565	-1.069342	-0.779708	N	1.061647	1.404558	0.370397
C	-2.955360	-2.122076	-0.648092	C	2.066198	2.044335	-0.242433
C	-2.694085	2.620728	-0.328955	C	2.329478	-2.053876	-0.770619
N	-2.507886	3.036610	-1.609725	N	3.411653	-1.990544	-1.584138
C	-2.274687	4.414819	-1.617597	C	4.123399	-3.188877	-1.496777
C	-2.313862	4.835853	-0.325828	C	3.454450	-3.987896	-0.625720
N	-2.579458	3.716553	0.464867	N	2.333035	-3.277504	-0.181568
C	-2.558788	3.585115	1.931438	C	1.180086	-3.801098	0.575822
C	-3.510832	4.553389	2.626234	C	1.547980	-4.316578	1.963754
C	-1.127538	3.655373	2.461343	C	0.397704	-4.824112	-0.245846

C	-1.967007	5.205576	-2.844686	C	5.367835	-3.477656	-2.267272
C	-2.115670	6.211277	0.216274	C	3.819181	-5.349138	-0.137283
C	-2.647106	2.119888	-2.753020	C	3.713709	-0.778446	-2.363645
C	-0.518979	-4.745584	-0.768690	C	1.044503	1.924302	-3.755349
C	-1.406358	2.113937	-3.641003	C	3.838835	-1.066340	-3.856481
C	-1.174532	-3.664336	0.087512	C	0.806316	2.416918	-2.332057
C	-1.082508	-3.954296	1.583037	C	0.068373	3.752244	-2.270160
C	-3.948352	2.370000	-3.511228	C	4.904380	-0.018943	-1.786913
N	-2.557335	-3.378556	-0.329585	N	2.035996	2.487965	-1.523961
N	-4.285132	-2.179244	-0.922150	N	3.239139	2.463197	0.298258
C	-4.724362	-3.499559	-0.788440	C	3.961140	3.172165	-0.665467
C	-3.650844	-4.243171	-0.412894	C	3.209062	3.194252	-1.796221
C	-3.573138	-5.709444	-0.149459	C	3.548678	3.761750	-3.132696
C	-6.135671	-3.935159	-0.998926	C	5.352690	3.669512	-0.464727
C	-5.016555	-1.007949	-1.434934	C	3.543462	2.330391	1.735530
C	-5.196137	-1.102576	-2.948285	C	4.857908	1.599013	1.997488
C	-6.316122	-0.743981	-0.680026	C	3.493808	3.684577	2.443367
H	-2.928692	2.569748	2.093183	H	0.523253	-2.941347	0.698135
H	-3.133754	5.578194	2.630422	H	2.197276	-3.614773	2.490002
H	-4.495534	4.540733	2.152470	H	0.627962	-4.429256	2.543431
H	-3.627481	4.241340	3.667224	H	2.036817	-5.292370	1.926155
H	-0.714187	4.665784	2.390730	H	-0.577933	-4.978892	0.221736
H	-0.478630	2.972497	1.907648	H	0.904182	-5.790779	-0.300177
H	-1.107715	3.352134	3.511854	H	0.235509	-4.462452	-1.262800
H	-3.044647	6.627827	0.615105	H	4.093412	-5.333036	0.921099
H	-1.366511	6.231748	1.011690	H	3.007245	-6.067972	-0.265928
H	-1.765475	6.873601	-0.575785	H	4.675769	-5.724072	-0.697739
H	-2.031602	6.271179	-2.623097	H	5.152075	-3.669222	-3.322163
H	-0.955331	5.000908	-3.207553	H	6.085743	-2.657123	-2.212555
H	-0.851623	-5.750292	-0.496062	H	0.082788	1.644851	-4.193216
H	-2.665982	5.000351	-3.657771	H	5.856062	-4.364304	-1.862308
H	-0.503198	2.027767	-3.030814	H	2.992634	-1.661928	-4.209113
H	-1.327481	3.009950	-4.259731	H	4.766318	-1.585668	-4.106145
H	-1.454274	1.251696	-4.311244	H	3.839183	-0.115848	-4.397613
H	0.563759	-4.701653	-0.621122	H	1.688576	1.041734	-3.768519
H	-0.722215	-4.588261	-1.831208	H	1.483723	2.689523	-4.396786
H	-3.961925	3.345954	-4.002445	H	4.733692	0.210478	-0.732744
H	-4.067873	1.604917	-4.282811	H	5.839142	-0.577104	-1.875512
H	-4.802812	2.311497	-2.831499	H	5.022652	0.926288	-2.323297
H	-1.566927	-3.162299	2.158483	H	-0.873415	3.678987	-2.819978
H	-2.720825	1.132342	-2.293754	H	2.823918	-0.163590	-2.213336
H	-1.529988	-4.915378	1.850541	H	-0.160481	4.014841	-1.234140
H	-0.657490	-2.719161	-0.088007	H	0.205072	1.672204	-1.809619
H	-0.028111	-3.979284	1.867699	H	0.654747	4.559913	-2.716285
H	-3.081618	-5.928929	0.800671	H	4.460518	4.354529	-3.060303
H	-3.028831	-6.233259	-0.940251	H	2.762191	4.417327	-3.513641
H	-4.577738	-6.130563	-0.101131	H	3.721713	2.972375	-3.870006
H	-6.793620	-3.573374	-0.203804	H	5.454327	4.280910	0.433448
H	-6.535638	-3.585052	-1.953377	H	6.061590	2.839113	-0.393816
H	-6.187821	-5.024281	-1.005174	H	5.650024	4.285311	-1.313566
H	-4.225430	-1.206231	-3.441068	H	4.954181	0.705402	1.378156

H	-5.674253	-0.190893	-3.316091	H	4.886042	1.289766	3.045397
H	-5.823964	-1.950479	-3.235060	H	5.724436	2.237803	1.815518
H	-4.351906	-0.169056	-1.223113	H	2.722460	1.719783	2.115420
H	-6.158885	-0.798947	0.400481	H	2.594307	4.239209	2.174101
H	-7.113255	-1.437128	-0.955809	H	4.363865	4.301913	2.209323
H	-6.657608	0.265813	-0.921965	H	3.486340	3.519218	3.523781
P	1.350541	0.299442	0.837188	P	-1.225761	-0.501926	1.015843
N	1.241917	-1.396945	0.841579	N	-2.205623	0.640844	0.533977
N	2.976757	0.634772	1.131863	N	-1.706912	-1.953513	0.515694
C	3.630412	1.402790	0.283628	C	-2.701302	-2.065641	-0.378187
C	1.886614	-2.123296	-0.039108	C	-2.323123	1.929214	0.271026
N	1.962829	-2.042149	-1.410947	N	-1.944443	3.001097	1.006926
C	2.794832	-3.060012	-1.896790	C	-2.442811	4.163455	0.407338
C	3.214963	-3.784610	-0.831005	C	-3.106840	3.786363	-0.715229
N	2.635179	-3.221169	0.308604	N	-3.015501	2.394859	-0.801996
C	2.862999	-3.542556	1.721181	C	-3.673990	1.480656	-1.750865
C	4.179700	-2.942672	2.210771	C	-3.340751	1.795448	-3.205342
C	2.721500	-5.031947	2.028469	C	-5.175534	1.394107	-1.488052
C	3.114682	-3.266750	-3.339508	C	-2.210916	5.538267	0.935785
C	4.115179	-4.973809	-0.807900	C	-3.764975	4.643919	-1.742227
C	1.176561	-1.070941	-2.182054	C	-1.278198	2.854259	2.309485
C	1.151720	3.595079	-0.695299	C	-5.414901	-3.341052	1.576881
C	0.272308	-1.731189	-3.219597	C	-2.297029	2.901057	3.443733
C	2.235239	3.465938	0.374624	C	-4.517287	-2.138239	1.296819
C	2.623733	4.810356	0.989028	C	-5.155611	-0.807839	1.687362
C	2.048213	0.038131	-2.769785	C	-0.108044	3.812373	2.491419
N	3.390474	2.698044	-0.105481	N	-4.023980	-2.127218	-0.092125
N	4.776838	1.022834	-0.364801	N	-2.576644	-2.161944	-1.723005
C	5.263576	2.083408	-1.131641	C	-3.845154	-2.232247	-2.299027
C	4.398085	3.116875	-0.985183	C	-4.747823	-2.214118	-1.281185
C	4.471101	4.477555	-1.594818	C	-6.235732	-2.286587	-1.356710
C	6.519422	2.025266	-1.936316	C	-4.094101	-2.316118	-3.767257
C	5.283930	-0.348754	-0.244537	C	-1.258305	-2.160650	-2.376408
C	5.617537	-0.990143	-1.589880	C	-1.087157	-3.316997	-3.357114
C	6.437227	-0.425472	0.752530	C	-0.939303	-0.805892	-2.993338
H	2.052959	-3.006685	2.222126	H	-3.241013	0.508955	-1.508332
H	4.147927	-1.854365	2.105409	H	-3.841296	2.695226	-3.566957
H	4.332847	-3.186586	3.266112	H	-2.263323	1.910036	-3.347618
H	5.034274	-3.328698	1.645584	H	-3.676246	0.960854	-3.826731
H	1.845582	-5.456549	1.529165	H	-5.367910	1.140430	-0.443365
H	2.591662	-5.157571	3.106735	H	-5.603683	0.608978	-2.117377
H	3.601511	-5.608276	1.735243	H	-5.689132	2.330872	-1.719438
H	4.576519	-5.107675	-1.787350	H	-3.178351	4.692463	-2.664548
H	4.921135	-4.860653	-0.077482	H	-4.765543	4.287772	-1.996356
H	3.572776	-5.893630	-0.569781	H	-3.866122	5.661230	-1.363318
H	2.298501	-3.757785	-3.878131	H	-2.472648	5.618330	1.993699
H	3.333666	-2.325723	-3.848568	H	-1.169227	5.849247	0.817805
H	1.491988	4.177575	-1.556202	H	-6.413341	-3.222565	1.151517
H	3.998893	-3.898922	-3.435017	H	-2.832468	6.249114	0.390680
H	-0.441141	-0.986448	-3.582259	H	-2.760605	3.888181	3.526256
H	-0.298753	-2.544594	-2.766794	H	-1.800430	2.674774	4.390967

H	0.823938	-2.113393	-4.081106	H	-3.084152	2.159481	3.282646
H	0.277924	4.102379	-0.275406	H	-5.528250	-3.446222	2.658655
H	0.845471	2.601896	-1.032681	H	-4.969998	-4.260153	1.187797
H	2.659490	0.505993	-1.994359	H	0.486212	3.853880	1.576246
H	2.709473	-0.333453	-3.557554	H	-0.420764	4.820680	2.767296
H	1.411751	0.809038	-3.212893	H	0.527634	3.430104	3.294115
H	3.475680	4.700377	1.664827	H	-6.088476	-0.628239	1.146319
H	0.518232	-0.623572	-1.438416	H	-0.847400	1.855884	2.278951
H	2.865788	5.561895	0.234898	H	-5.392126	-0.822734	2.755143
H	1.835239	2.848899	1.182801	H	-3.603248	-2.264254	1.881849
H	1.774923	5.187198	1.566657	H	-4.466788	0.017508	1.489622
H	3.513317	4.787670	-2.019426	H	-6.563535	-2.060417	-2.372225
H	5.199116	4.477521	-2.407162	H	-6.713092	-1.565085	-0.690723
H	4.778820	5.238626	-0.871521	H	-6.608000	-3.283162	-1.104103
H	6.819467	3.032130	-2.229618	H	-3.475311	-1.610092	-4.325412
H	7.344197	1.593971	-1.363103	H	-3.899938	-3.318919	-4.157723
H	6.399011	1.432992	-2.848024	H	-5.136594	-2.074287	-3.978013
H	6.576809	-0.654803	-1.990353	H	-0.021076	-3.434174	-3.571013
H	4.835210	-0.785453	-2.325083	H	-1.594153	-3.137914	-4.307258
H	5.671114	-2.073624	-1.453372	H	-1.457520	-4.253621	-2.932568
H	4.433924	-0.887187	0.179504	H	-0.564467	-2.304823	-1.546918
H	6.129694	-0.022309	1.720963	H	0.104994	-0.799158	-3.312787
H	7.310168	0.134303	0.403031	H	-1.069684	-0.013271	-2.251663
H	6.737700	-1.467793	0.892794	H	-1.570214	-0.583575	-3.858278
H	-0.657352	0.716285	-0.205367				
2c (protonated form (in-out))							
N	-3.807765	1.115680	0.918219				
C	-3.586794	-0.143422	0.452581				
N	-4.797706	-0.624445	0.042694				
C	-5.784223	0.340035	0.283274				
C	-5.167545	1.417072	0.828805				
N	-2.380164	-0.684187	0.366379				
P	-1.828221	-2.138758	0.767857				
N	-1.189089	-3.067137	-0.368024				
C	-0.062305	-3.050826	-1.069140				
N	1.199112	-3.289961	-0.615584				
C	2.089815	-3.279129	-1.694563				
C	1.354894	-3.072695	-2.814563				
N	0.020739	-2.925488	-2.419210				
C	1.430053	-3.904360	0.705371				
C	3.571046	-3.371056	-1.542253				
C	1.766698	-3.007968	-4.246243				
C	-1.088504	-2.996818	-3.387766				
C	-4.975371	-1.948803	-0.564860				
C	-7.228350	0.170688	-0.052700				
C	-5.767971	2.713870	1.256199				
C	-2.734887	1.912019	1.533679				
C	-0.937214	-2.043955	2.366383				
C	-0.249747	-0.915361	2.939114				
C	-0.054777	-0.941567	4.362037				
C	-0.342978	-2.112355	5.111491				

C	-0.864290	-3.222215	4.509790
C	-1.205995	-3.153811	3.145083
C	0.430503	0.203395	5.041374
C	0.733268	1.341598	4.344885
C	0.662201	1.323551	2.940510
C	0.234349	0.225410	2.224832
P	0.725800	0.221358	0.400026
N	2.361283	0.099209	0.798261
C	3.515553	0.085035	0.232305
N	3.917559	0.208731	-1.091667
C	5.326640	0.229875	-1.151958
C	5.788872	0.062591	0.104657
N	4.686870	-0.058290	0.963434
C	2.990741	0.667852	-2.127087
C	6.106737	0.329310	-2.419759
C	7.190764	-0.057429	0.599683
C	4.775417	0.246566	2.401715
N	0.558955	1.873828	0.138674
C	0.057063	2.724163	-0.693712
N	-0.880131	2.631480	-1.700810
C	-1.086430	3.902159	-2.270335
C	-0.300750	4.780273	-1.605721
N	0.420168	4.059440	-0.651270
C	-2.038734	4.180406	-3.385690
C	-1.420918	1.352665	-2.163947
C	1.429039	4.530533	0.299035
C	-0.187195	6.256951	-1.792458
H	0.550753	0.156236	6.119870
H	1.003387	2.184742	2.375187
H	1.081631	2.231817	4.859555
H	-1.734176	-3.999867	2.711702
H	-1.077172	-4.121375	5.077171
H	-0.145964	-2.103104	6.179715
H	-5.461583	2.992095	2.267476
H	-5.494137	3.530403	0.582686
H	-6.855453	2.633854	1.253116
H	-7.816779	0.926802	0.468416
H	-7.415406	0.288622	-1.123877
H	-7.611592	-0.804790	0.252395
H	3.885285	-4.281379	-1.026265
H	3.959256	-2.511056	-0.987655
H	4.043102	-3.372866	-2.526014
H	1.301678	-3.804196	-4.834854
H	1.501075	-2.051976	-4.706322
H	2.846782	-3.129690	-4.331963
H	7.889871	-0.075121	-0.237276
H	7.472149	0.780796	1.246160
H	7.332412	-0.980671	1.171155
H	5.928006	-0.523012	-3.082173
H	5.874343	1.241661	-2.977339
H	7.173000	0.354233	-2.190712

H	-1.873360	3.521952	-4.243066
H	-1.899390	5.203737	-3.736565
H	-3.083288	4.072769	-3.078741
H	-1.008606	6.618811	-2.412116
H	-0.242071	6.788353	-0.838454
H	0.749516	6.542358	-2.280153
C	-2.777308	1.773990	3.052996
H	-1.820661	1.440107	1.173597
C	-2.719593	3.366107	1.068473
C	-5.654614	-1.881502	-1.931865
H	-3.957097	-2.294608	-0.739648
C	-5.653664	-2.932678	0.387135
C	2.508795	-3.209100	1.519925
H	0.487460	-3.759412	1.226498
C	1.644921	-5.410137	0.556006
H	-0.708981	-2.489391	-4.277695
C	-1.377674	-4.460033	-3.727415
C	-2.360507	-2.283440	-2.942347
C	-2.932339	1.387134	-2.407142
C	-0.646987	0.862016	-3.388465
H	-1.246812	0.658144	-1.337202
C	0.794639	5.157520	1.540336
H	1.920037	3.605632	0.612710
C	2.483836	5.435935	-0.337692
C	3.210754	-0.003769	-3.479627
H	2.010326	0.347767	-1.767699
C	2.992849	2.192173	-2.227196
H	5.830076	0.105156	2.650027
C	4.417234	1.711853	2.659393
C	3.976999	-0.707447	3.285373
H	-2.904149	-2.937139	1.187792
H	-5.595143	-3.939730	-0.034209
H	-5.161864	-2.937632	1.363059
H	-6.709220	-2.694058	0.537750
H	-5.509897	-2.836798	-2.442843
H	-6.729308	-1.709416	-1.855175
H	-5.214540	-1.094562	-2.549856
H	-3.315857	0.364849	-2.382896
H	-3.449762	1.952103	-1.628281
H	-3.192624	1.807979	-3.379822
H	-1.059669	-0.079209	-3.757630
H	-0.690911	1.590437	-4.203433
H	0.401057	0.697236	-3.132252
H	1.575807	5.477479	2.236239
H	0.187355	6.031759	1.286577
H	0.160217	4.431208	2.055431
H	3.356204	5.475671	0.320336
H	2.805533	5.045296	-1.306779
H	2.129764	6.460195	-0.473818
H	-1.941917	2.322954	3.493916
H	-3.709389	2.170290	3.467262

H	-2.679200	0.724351	3.343229				
H	-1.731284	3.779061	1.279538				
H	-2.881380	3.447056	-0.009095				
H	-3.454495	3.984740	1.586997				
H	-2.915706	-1.959722	-3.826984				
H	-2.991258	-2.963260	-2.371140				
H	-2.148268	-1.418682	-2.313996				
H	-2.162388	-4.514744	-4.486614				
H	-0.492435	-4.974599	-4.108716				
H	-1.725152	-4.984380	-2.832255				
H	1.691154	-5.866308	1.548557				
H	0.817371	-5.865685	0.005330				
H	2.578035	-5.643677	0.036504				
H	2.434958	-3.548774	2.557250				
H	3.516626	-3.441022	1.165627				
H	2.369758	-2.126669	1.496390				
H	2.191148	2.532682	-2.890573				
H	2.827549	2.626431	-1.240023				
H	3.944885	2.560084	-2.622601				
H	2.310867	0.113954	-4.089228				
H	4.036760	0.440337	-4.037043				
H	3.404398	-1.069550	-3.353399				
H	4.210146	-0.494827	4.333514				
H	2.905623	-0.579959	3.126500				
H	4.249594	-1.745284	3.078398				
H	4.569055	1.956661	3.714715				
H	5.046411	2.374065	2.056286				
H	3.369332	1.887062	2.406294				
2d (protonated form (in-out))				2d (dication)			
N	4.011284	-1.287490	0.772416	C	-2.311910	-1.960375	-2.054500
C	2.646709	-1.353684	0.460347	C	-2.530540	-0.605417	-1.692083
C	2.289190	-2.416099	-0.453316	N	-3.815372	-0.259971	-1.336008
C	3.218892	-3.262365	-0.972928	C	-4.832817	-1.164017	-1.340564
C	4.588182	-3.134134	-0.623212	C	-4.633608	-2.471435	-1.675300
C	4.928270	-2.147665	0.248422	C	-3.334782	-2.871476	-2.040724
N	1.866782	-0.475697	1.020412	N	-1.627702	0.373799	-1.700285
P	0.253610	-0.270066	0.538934	P	-0.084824	0.333229	-1.284650
N	-0.483506	-1.732822	1.015221	C	0.668424	1.863013	-1.879971
C	-1.764099	-1.940571	0.985444	C	0.913224	2.848709	-0.876227
N	-2.208784	-3.264759	1.126237	C	1.439223	4.109173	-1.258205
C	-3.529197	-3.598027	1.145065	C	1.740471	4.335147	-2.626985
C	-4.518988	-2.674969	1.008682	C	1.519855	3.362575	-3.569759
C	-4.136729	-1.317874	0.851509	C	0.969917	2.115452	-3.196866
C	-2.822427	-0.966382	0.837799	C	1.638540	5.095644	-0.257750
C	-1.203244	-4.318590	1.304976	C	1.326671	4.844737	1.055729
C	-0.730181	-4.417115	2.749583	C	0.820984	3.584189	1.443175
C	4.457452	-0.270191	1.729984	C	0.629709	2.600676	0.500830
C	4.278361	-0.728583	3.171357	P	0.090614	0.920443	0.863864
C	-0.266941	0.889273	1.889694	N	-1.345479	1.014058	1.596101
C	-0.999100	2.098971	1.654955	C	-2.166741	-0.024849	1.736609
C	-1.527978	2.776023	2.804774	C	-1.910807	-1.381564	1.389229

C	-1.259200	2.296732	4.111075	C	-2.872602	-2.346230	1.526955
C	-0.502579	1.173059	4.304543	C	-4.138139	-2.013245	2.045066
C	-0.028451	0.470953	3.182945	C	-4.363314	-0.716128	2.401183
C	-2.333856	3.936914	2.664811	N	-3.416250	0.249719	2.248360
C	-2.609827	4.454738	1.433871	C	-3.732224	1.627220	2.677261
C	-2.043170	3.845587	0.297125	C	-3.196184	1.915302	4.071979
C	-1.261526	2.707791	0.366507	C	-4.111916	1.139000	-0.967506
P	-0.567080	2.277492	-1.274209	C	-4.392095	1.995254	-2.193174
N	-1.249210	1.044903	-2.065718	N	1.113507	-0.092540	1.568913
C	-2.501684	0.633771	-2.096417	C	2.426172	-0.141944	1.740682
N	-2.710630	-0.685373	-2.458339	C	3.348425	0.937957	1.681662
C	-3.954431	-1.210844	-2.612820	C	4.685076	0.740040	1.903454
C	-5.081690	-0.480697	-2.378961	C	5.174647	-0.546883	2.196425
C	-4.925585	0.854306	-1.956304	C	4.281073	-1.575275	2.249688
C	-3.675327	1.393150	-1.814149	N	2.952454	-1.385925	2.022308
C	-1.542315	-1.559036	-2.673368	C	2.046100	-2.548225	2.097234
C	-1.045588	-1.498646	-4.110459	C	1.321660	-2.630400	3.432204
N	1.037631	2.305582	-1.173007	N	0.676332	-1.058883	-1.554420
C	1.976415	1.512188	-1.649816	C	1.956222	-1.392432	-1.421196
N	3.263154	1.745505	-1.205750	N	2.230008	-2.740490	-1.320643
C	4.324973	1.012374	-1.642060	C	3.500061	-3.216484	-1.199107
C	4.181898	-0.007991	-2.532453	C	4.580255	-2.386001	-1.153098
C	2.883019	-0.297546	-2.999486	C	4.352512	-1.000794	-1.254435
C	1.813430	0.438632	-2.573832	C	3.077518	-0.519048	-1.388876
H	0.807085	0.236843	-2.911564	C	1.120649	-3.711922	-1.384363
H	-2.724076	4.406248	3.563083	C	0.766980	-4.058990	-2.823340
H	-2.220366	4.322782	-0.662735	H	-0.926607	-1.633258	1.012991
H	-3.225608	5.339647	1.320695	H	2.040478	6.061095	-0.549312
H	0.533979	-0.446685	3.329386	H	0.597108	3.393439	2.488013
H	-0.290611	0.811701	5.305430	H	1.475798	5.611639	1.807235
H	-1.669156	2.842740	4.955559	H	0.784599	1.362464	-3.956407
C	3.496689	2.823120	-0.230083	H	1.757358	3.548996	-4.610914
H	2.728402	-1.112653	-3.698462	H	2.150493	5.296907	-2.918970
H	5.045099	-0.579330	-2.844278	H	-2.653972	-3.367322	1.234926
H	-5.798833	1.463269	-1.748552	H	-4.919007	-2.750735	2.167871
H	-6.056047	-0.932072	-2.505529	H	5.366557	1.582036	1.853898
H	-3.553831	2.422577	-1.504757	H	6.224226	-0.733887	2.376439
H	-3.985469	-2.248774	-2.919457	H	2.963968	1.924513	1.462359
H	-0.774865	-1.231105	-1.971091	H	4.575344	-2.593578	2.468539
H	-1.848254	-2.571201	-2.402207	H	1.334034	-2.451507	1.277731
H	-0.785023	-0.473622	-4.385396	H	2.654477	-3.436464	1.920729
H	-1.806773	-1.862025	-4.806246	H	0.699449	-1.746630	3.585806
H	-0.155610	-2.124261	-4.216106	H	2.033812	-2.717229	4.256627
H	1.240113	-2.522288	-0.697217	H	0.677780	-3.513011	3.436470
H	3.863752	0.624624	1.544825	H	-1.307438	-2.234047	-2.343895
H	5.505114	-0.050422	1.512803	H	-3.247288	1.515617	-0.421070
H	4.858691	-1.634545	3.368029	H	-4.971233	1.115347	-0.295137
H	3.223530	-0.931196	3.369654	H	-5.250138	1.610686	-2.750664
H	4.617104	0.054155	3.855027	H	-3.520677	2.018019	-2.850672
H	5.949278	-1.987979	0.574366	H	-4.615242	3.016675	-1.876630
H	5.346861	-3.794592	-1.020621	H	-5.802008	-0.775821	-1.054713

H	2.909444	-4.043519	-1.660420	H	-5.463913	-3.163954	-1.659018
H	-4.896658	-0.551055	0.741049	H	-3.140520	-3.900949	-2.321507
H	-5.555899	-2.981605	1.023687	H	5.186507	-0.308694	-1.224912
H	-2.537604	0.072200	0.732009	H	5.574248	-2.796983	-1.044070
H	-3.736516	-4.653829	1.274026	H	2.900409	0.544197	-1.482067
H	-1.652117	-5.257682	0.974863	H	3.587991	-4.293456	-1.136433
H	-0.366872	-4.081966	0.646192	H	1.437091	-4.595449	-0.828585
H	-0.282658	-3.471373	3.061912	H	0.269915	-3.268435	-0.867464
H	0.021326	-5.205719	2.840719	H	0.505049	-3.159682	-3.386113
H	-1.563344	-4.655545	3.416875	H	-0.088429	-4.738676	-2.834536
H	-0.890650	3.465577	-1.957047	H	1.606087	-4.549531	-3.323055
H	5.284828	1.294345	-1.227815	H	-5.304694	-0.381618	2.817510
H	4.420823	2.580863	0.297409	H	-4.817391	1.729549	2.641326
C	3.596541	4.187691	-0.896586	H	-3.295550	2.304246	1.943955
H	2.672412	2.790559	0.482889	H	-3.458995	2.937085	4.355245
H	3.777115	4.951527	-0.136310	H	-3.630422	1.230719	4.805206
H	4.423452	4.211137	-1.611603	H	-2.108726	1.818509	4.092755
H	2.667995	4.428349	-1.417559				
2d (protonated form (in-in))							
C	-3.380430	-3.273891	-0.218505				
C	-2.044546	-3.206876	-0.708582				
N	-1.427661	-4.412432	-0.996756				
C	-2.064705	-5.600533	-0.822444				
C	-3.340560	-5.675731	-0.343978				
C	-4.009217	-4.475770	-0.037309				
N	-1.329122	-2.120120	-0.948297				
P	-1.550755	-0.628177	-0.377716				
N	-3.069674	-0.046238	-0.588911				
C	-3.393815	1.208962	-0.317723				
N	-4.685052	1.594826	-0.637836				
C	-5.129864	2.860341	-0.418782				
C	-4.339166	3.825080	0.135276				
C	-3.022140	3.480356	0.492194				
C	-2.564939	2.209412	0.275721				
C	-5.555335	0.556500	-1.234906				
C	-6.962638	1.008959	-1.574270				
C	-0.033137	-4.342213	-1.492696				
C	0.634802	-5.681770	-1.737256				
C	-1.138486	-0.571696	1.407421				
C	0.156588	-0.461477	2.044644				
C	0.162461	-0.632257	3.472830				
C	-1.035163	-0.864187	4.197698				
C	-2.241559	-0.928062	3.565341				
C	-2.275799	-0.781739	2.168608				
C	1.369393	-0.574757	4.215894				
C	2.556250	-0.340094	3.587860				
C	2.561534	-0.136096	2.195743				
C	1.424889	-0.173044	1.411753				
P	1.706434	0.027192	-0.443570				
N	3.358889	0.412461	-0.534219				
C	4.264722	-0.526232	-0.613424				

N	5.566415	-0.125558	-0.936177
C	6.593340	-1.013583	-1.024839
C	6.425493	-2.349238	-0.815725
C	5.131349	-2.814055	-0.483124
C	4.094223	-1.936838	-0.376251
C	5.760873	1.318649	-1.163676
C	7.179003	1.737471	-1.505510
N	0.954993	1.489188	-0.874000
C	1.088376	2.661588	-0.312932
N	0.327470	3.700321	-0.866509
C	0.310302	4.950296	-0.325960
C	1.051663	5.281484	0.767082
C	1.892033	4.289920	1.325608
C	1.919730	3.033005	0.799571
C	-0.433027	3.376549	-2.090210
C	-1.313156	4.490933	-2.623889
H	1.322920	-0.721752	5.290708
H	3.508808	0.090878	1.719663
H	3.485993	-0.294733	4.145215
H	-3.240341	-0.830558	1.675468
H	-3.160450	-1.092339	4.116578
H	-0.967923	-0.983169	5.275058
H	2.575241	2.273678	1.199352
H	-1.036902	2.496660	-1.866871
H	0.295286	3.061907	-2.842569
H	-1.825742	4.108721	-3.509460
H	-0.743340	5.372585	-2.929042
H	-2.080806	4.790914	-1.904507
H	-0.326374	5.672779	-0.815410
H	1.003432	6.285315	1.166744
H	2.525479	4.532690	2.172865
H	4.965250	-3.871073	-0.300964
H	7.271915	-3.017533	-0.896846
H	3.104575	-2.279131	-0.097813
H	7.559901	-0.599903	-1.272867
H	5.071146	1.609951	-1.959680
H	5.414239	1.830817	-0.262310
H	7.886296	1.510971	-0.702960
H	7.178366	2.820580	-1.646648
H	7.535724	1.285011	-2.434866
H	-3.887872	-2.336562	-0.029648
H	0.527546	-3.760520	-0.758196
H	-0.053213	-3.746793	-2.408017
H	1.652597	-5.479424	-2.077895
H	0.137391	-6.263487	-2.517775
H	0.705563	-6.284217	-0.827746
H	-1.503226	-6.485756	-1.080668
H	-3.809443	-6.641985	-0.217545
H	-5.027955	-4.500127	0.334359
H	-2.364006	4.218476	0.939351
H	-4.734562	4.819312	0.291119

H	-1.552622	1.942205	0.554099				
H	-6.150057	3.062988	-0.708108				
H	-5.040565	0.191330	-2.125945				
H	-5.579040	-0.274833	-0.526622				
H	-7.522262	1.331947	-0.692469				
H	-7.486885	0.150410	-1.999287				
H	-6.976494	1.805312	-2.322964				
H	-0.662628	0.189931	-1.074177				
2e (protonated form (in-in))				2e (dication)			
C	1.192617	-0.359836	4.611881	C	1.035480	0.849697	2.152163
C	0.240470	-0.981822	3.758435	C	0.204894	-0.046174	2.886166
C	0.179246	-0.644158	2.368769	C	0.281086	-0.080366	4.300679
C	1.266406	0.158634	1.860283	C	1.140044	0.841714	4.953147
C	2.157771	0.752401	2.728118	C	1.898969	1.728901	4.230046
C	2.093869	0.542266	4.121739	C	1.861922	1.723811	2.816596
C	-0.665350	-1.925782	4.308098	C	-0.660392	-0.950240	2.206201
C	-1.641853	-2.477244	3.526294	C	-1.338146	-1.920351	2.901422
C	-1.809128	-2.016881	2.203838	C	-1.235166	-1.979854	4.311640
C	-0.964218	-1.096698	1.620159	C	-0.471322	-1.064967	4.994881
P	-1.419054	-0.448067	-0.082319	P	-0.844794	-0.608046	0.441476
N	-3.027914	-0.942639	-0.141941	N	-2.022667	0.416646	0.152262
P	-3.794185	-1.326420	-1.458983	P	-3.409631	1.000636	0.637465
N	-3.350032	-2.821865	-2.066326	N	-4.097793	0.449997	2.046781
C	-3.041367	-3.918254	-1.162953	C	-3.641534	0.971761	3.332786
P	1.773128	0.197276	0.110688	P	1.013988	0.605878	0.351510
N	2.937572	1.315685	-0.005344	N	2.263058	-0.232935	-0.186703
P	3.142315	2.170834	-1.330859	P	3.164399	-1.390469	0.430780
N	4.479130	1.587692	-2.149550	N	3.623906	-2.322001	-0.878361
C	5.610036	1.099896	-1.364745	C	3.848627	-1.667579	-2.164581
N	2.124934	-1.264431	-0.433868	N	0.733197	1.962922	-0.403978
P	2.844278	-2.593570	0.012943	P	1.311425	2.978295	-1.464314
N	3.840936	-2.612676	1.348688	N	0.068091	3.336336	-2.507511
C	5.168695	-2.019995	1.247968	C	0.229007	4.416851	-3.475472
N	1.722934	-3.755332	0.393117	N	1.940671	4.280587	-0.630769
C	0.431604	-3.768912	-0.283260	C	2.618493	5.372605	-1.326057
N	3.783175	-3.046945	-1.286091	N	2.562218	2.551093	-2.461868
C	4.442601	-4.344170	-1.300723	C	3.914565	2.390947	-1.935664
C	2.030545	-5.004499	1.078434	C	1.311165	4.707955	0.614947
N	-1.377989	1.219311	0.150907	N	-0.780845	-1.990194	-0.351122
P	-2.201534	2.209306	1.048621	P	-1.250417	-2.556243	-1.761916
N	-1.331162	3.645178	1.075145	N	-2.783525	-3.166496	-1.700208
C	-1.934886	4.874530	1.559730	C	-3.286683	-4.185071	-2.615353
N	-2.567441	1.854835	2.645188	N	-1.156820	-1.374099	-2.923675
C	-3.499528	0.780481	2.964734	C	-1.981980	-1.405706	-4.123679
N	-3.728893	2.518064	0.432941	N	-0.357230	-3.865075	-2.258793
C	-4.826707	3.114461	1.176781	C	0.873800	-3.693258	-3.020171
C	-1.670771	2.202249	3.734596	C	-0.018812	-0.466778	-3.002920
N	-5.415529	-1.360499	-1.068527	N	-3.216610	2.643193	0.815686
C	-5.993955	-0.319120	-0.233298	C	-4.375615	3.484169	1.091979
N	-3.631813	-0.324061	-2.793139	N	-4.541271	0.625674	-0.515726
C	-2.335337	-0.147999	-3.427320	C	-4.132943	0.549560	-1.915979

C	-6.379213	-2.190579	-1.768060	C	-1.949029	3.264418	1.170598
C	-4.726869	0.323813	-3.487110	C	-5.977398	0.815664	-0.339953
C	-3.549206	-3.237381	-3.445571	C	-4.739948	-0.856051	2.155481
N	1.962672	2.161045	-2.505245	N	2.522285	-2.483177	1.491375
C	1.761226	0.987617	-3.354287	C	1.718973	-3.615952	1.045295
N	3.249664	3.767235	-0.876479	N	4.407759	-0.698222	1.290758
C	3.638811	4.774731	-1.856196	C	4.789170	0.699500	1.148914
C	0.755126	2.977032	-2.368493	C	2.582174	-2.336728	2.942523
C	3.483223	4.158569	0.507109	C	5.459526	-1.522225	1.879625
C	4.873357	2.120244	-3.450835	C	4.487270	-3.483838	-0.675577
C	4.328689	-2.092441	-2.239886	C	2.354577	1.852392	-3.724107
C	3.304270	-2.588620	2.707144	C	-1.322600	3.007531	-2.217594
C	-3.900442	2.590185	-1.008546	C	-0.411537	-5.107155	-1.491578
C	0.121224	3.661639	1.069613	C	-3.761304	-2.704354	-0.730699
H	-0.567604	-2.192774	5.356363	H	1.198506	0.827780	6.037072
H	1.178178	-0.609837	5.668918	H	-0.415318	-1.099657	6.078450
H	-2.682375	-2.326920	1.639568	H	2.502842	2.403861	2.263988
H	2.959505	1.355821	2.316357	H	-1.958067	-2.638304	2.372524
H	-3.143558	1.980301	-1.500575	H	3.978889	1.267413	0.698416
H	5.566469	-2.128324	0.238227	H	-5.079797	-1.201422	1.180358
H	-3.878386	0.317234	2.051492	H	2.977512	-1.359405	3.219053
H	0.205676	-2.783197	-0.691208	H	-1.119824	2.625502	0.876963
H	-4.885520	2.193627	-1.277555	H	5.006800	1.118504	2.137212
H	5.153783	-0.952346	1.507959	H	-4.059607	-1.603159	2.580165
H	-2.994684	0.000328	3.543917	H	1.575994	-2.436386	3.360249
H	0.413790	-4.514877	-1.089252	H	-1.851263	4.211323	0.628457
H	-4.343292	1.163566	3.553561	H	3.216545	-3.115950	3.381294
H	-0.348556	-4.020180	0.442910	H	-1.884989	3.480977	2.246306
H	-4.585344	3.170311	2.237757	H	5.134743	-2.557473	1.983376
H	2.240377	-2.826044	2.705848	H	-3.201199	1.961201	3.217063
H	-5.049665	4.127873	0.814504	H	6.367723	-1.501062	1.265330
H	3.829810	-3.326216	3.323765	H	-4.496849	1.055834	4.010113
H	-5.734365	2.509539	1.055422	H	5.703995	-1.143406	2.877424
H	3.430367	-1.600079	3.159325	H	-2.896082	0.310392	3.790626
H	-2.259290	2.471143	4.619469	H	2.160735	-4.554609	1.400229
H	1.313803	-5.161584	1.892598	H	-4.496698	3.671219	2.167311
H	-1.009270	1.368042	4.000410	H	0.697418	-3.529930	1.427174
H	1.959331	-5.857108	0.390816	H	-4.246255	4.445923	0.586674
H	-1.052927	3.059906	3.470805	H	1.670135	-3.630841	-0.041242
H	3.034045	-4.979071	1.502396	H	-5.292021	3.031828	0.716960
H	-3.010150	4.873478	1.384918	H	4.278803	-3.958642	0.283564
H	3.897456	-5.068116	-0.695867	H	-6.228168	0.925405	0.715193
H	-1.509513	5.723807	1.014186	H	5.550922	-3.215885	-0.713521
H	5.474166	-4.284644	-0.926827	H	-6.507366	-0.059692	-0.730985
H	-1.758512	5.039969	2.632945	H	4.285293	-4.214274	-1.464772
H	4.471050	-4.722373	-2.327390	H	-6.330955	1.701308	-0.882537
H	0.544587	3.778721	2.078872	H	3.768449	-2.414514	-2.959818
H	4.130447	-2.431124	-3.263190	H	-4.260233	1.513399	-2.425563
H	0.477017	4.499383	0.458266	H	4.844011	-1.206528	-2.224508
H	5.416409	-1.993200	-2.119137	H	-4.754751	-0.193842	-2.425197
H	-4.502094	1.387540	-3.633687	H	4.133190	1.333779	-1.746097

H	4.551709	4.301977	0.714784	H	1.735388	-3.493836	-2.368428
H	-5.649088	0.252476	-2.912006	H	4.029521	2.947182	-1.005609
H	3.088985	3.396927	1.177538	H	0.773551	-2.876720	-3.735483
H	-4.897965	-0.125363	-4.476140	H	4.634828	2.778429	-2.663241
H	2.963915	5.102808	0.702192	H	1.067689	-4.609508	-3.584702
H	-2.047781	0.911911	-3.434402	H	2.563470	0.780882	-3.621518
H	4.721703	4.954145	-1.851303	H	0.487022	-5.241158	-0.879356
H	-2.355363	-0.506774	-4.465400	H	3.033687	2.262244	-4.478538
H	3.130783	5.715935	-1.623527	H	-0.492552	-5.956728	-2.177527
H	-1.566662	-0.701047	-2.884369	H	1.329953	1.979699	-4.069340
H	3.334996	4.470561	-2.859107	H	-1.280426	-5.111384	-0.832134
H	-3.883216	-2.398214	-4.055483	H	1.279644	4.550780	-3.737502
H	4.000540	2.471802	-4.001381	H	-2.522701	-4.458564	-3.342118
H	-2.609717	-3.619077	-3.863077	H	-0.314566	4.162520	-4.390690
H	5.588664	2.947316	-3.354950	H	-3.576588	-5.082836	-2.056973
H	-4.300179	-4.036031	-3.518323	H	-0.163773	5.366060	-3.089794
H	5.345783	1.321502	-4.031503	H	-4.167208	-3.811388	-3.150547
H	-2.185047	-4.483762	-1.548372	H	-1.814502	2.691243	-3.144791
H	6.294165	1.912581	-1.085014	H	-4.070828	-3.528407	-0.077103
H	-7.105121	-2.586543	-1.049386	H	1.924250	6.182070	-1.585503
H	0.405969	3.253696	-3.368309	H	-2.205946	-0.376696	-4.422253
H	-3.888807	-4.610193	-1.058373	H	-1.865056	3.874643	-1.819035
H	6.167180	0.371705	-1.961696	H	-4.648137	-2.305525	-1.236426
H	-6.933199	-1.634670	-2.538137	H	3.395430	5.780830	-0.672318
H	-0.044796	2.433918	-1.845554	H	-1.477358	-1.909207	-4.958103
H	-2.778995	-3.526207	-0.180798	H	-1.378822	2.195416	-1.493448
H	5.248813	0.608142	-0.462099	H	-3.339751	-1.910746	-0.120013
H	-6.603981	-0.768611	0.559327	H	0.517318	5.445774	0.436683
H	1.523007	1.313914	-4.371889	H	-0.355454	0.573106	-2.937506
H	-6.640196	0.353789	-0.816369	H	2.069303	5.166739	1.257104
H	0.932654	0.368898	-2.985040	H	0.513425	-0.598715	-3.952827
H	-5.194490	0.265059	0.225077	H	0.887831	3.851645	1.137723
H	2.662807	0.376846	-3.386699	H	0.693443	-0.656525	-2.197126
H	-5.882888	-3.036945	-2.242945	H	3.095031	5.011670	-2.237436
H	0.977681	3.886878	-1.812894	H	-2.928148	-1.907420	-3.921732
H	-2.330829	-3.209770	3.935124	H	2.552513	2.427137	4.740960
H	2.799967	1.039964	4.777345	H	-1.780231	-2.745213	4.852689
H	0.497847	2.735911	0.640212	H	3.088945	-0.904259	-2.322841
H	3.870739	-1.114633	-2.094793	H	-3.091205	0.235899	-1.988831
H	-3.836827	3.625437	-1.373843	H	5.681930	0.806445	0.519731
H	5.846342	-2.532590	1.937523	H	-5.611502	-0.771714	2.812313
H	0.688094	0.623064	-0.645153				
2e(protonated form (in-out))							
C	1.212621	0.767439	4.718428				
C	0.570729	-0.328558	4.084293				
C	0.348383	-0.311251	2.670372				
C	0.988771	0.720908	1.905594				
C	1.599122	1.761915	2.570825				
C	1.675725	1.820421	3.978135				
C	0.143787	-1.431585	4.869596				
C	-0.542884	-2.468131	4.304489				

C	-0.934407	-2.367269	2.953820
C	-0.540814	-1.319184	2.143857
P	-1.570149	-1.212833	0.636518
H	-2.604713	-2.082774	1.048109
P	1.099990	0.629669	0.036289
N	1.828697	2.135491	-0.259099
P	1.301361	3.110639	-1.371709
N	1.061121	2.589831	-2.956210
C	2.237468	2.152104	-3.700176
N	2.292276	-0.519527	-0.147659
P	3.582190	-1.160122	0.426751
N	3.262880	-2.761388	0.826652
C	2.067673	-3.430280	0.339813
N	4.812598	-1.001550	-0.719425
C	6.143056	-1.546534	-0.494293
N	4.373094	-0.619572	1.801047
C	5.042414	0.673562	1.779315
C	4.457699	-0.921368	-2.126786
N	-2.213521	0.250090	0.491236
P	-3.614684	0.836713	0.934843
N	-4.738195	-0.199630	1.607037
C	-5.364188	-1.252858	0.813678
N	-0.859257	-1.879813	-0.618036
P	-1.248307	-2.516862	-2.005950
N	-0.960170	-4.148900	-1.898301
C	-1.023198	-4.886844	-0.646286
N	-4.401628	1.433743	-0.401958
C	-5.837006	1.671719	-0.491369
N	-3.350631	2.062656	2.023646
C	-4.441596	2.947818	2.408789
C	-3.618879	2.217242	-1.350598
N	-2.800492	-2.292718	-2.571339
C	-3.269055	-0.927838	-2.801668
N	-0.317628	-1.869297	-3.219616
C	1.122441	-1.796213	-2.994885
C	-3.859516	-3.235407	-2.236589
C	-0.691216	-1.862763	-4.628655
C	-0.925671	-4.983794	-3.090324
N	-0.219780	3.752096	-1.022246
C	-0.853167	4.725608	-1.903484
N	2.489176	4.280647	-1.578787
C	3.354538	4.634044	-0.461986
C	-0.627887	3.910648	0.367311
C	2.310912	5.363284	-2.535756
C	-0.124477	1.803085	-3.290247
C	3.963638	-1.026602	3.137973
C	4.324122	-3.673974	1.219838
C	-2.205050	2.098760	2.919783
C	-4.666781	-0.512480	3.030871
H	0.370758	-1.430528	5.931795
H	1.326526	0.748371	5.798432

H	-1.614370	-3.122576	2.569016
H	2.051659	2.544470	1.967439
H	-2.557230	1.990799	-1.238629
H	5.331738	0.930777	0.760090
H	-5.302019	-1.020182	-0.249945
H	1.292647	-2.700307	0.108481
H	-3.924095	1.972741	-2.373829
H	4.390388	1.465589	2.172536
H	-4.886366	-2.225754	0.988758
H	2.270447	-4.027188	-0.562911
H	-6.421850	-1.336987	1.084473
H	1.691918	-4.110741	1.114579
H	-6.359965	1.198092	0.338819
H	3.320545	-1.904645	3.087927
H	-6.058467	2.746649	-0.477464
H	4.849090	-1.272127	3.737726
H	-6.219466	1.256523	-1.430486
H	3.415970	-0.223470	3.641456
H	-5.671591	-0.744721	3.395813
H	3.942439	-4.375362	1.971057
H	-4.017103	-1.376118	3.228454
H	4.701577	-4.259484	0.369367
H	-4.290174	0.340671	3.594730
H	5.157479	-3.129388	1.665418
H	-5.225851	2.954707	1.652623
H	6.392135	-1.513541	0.566972
H	-4.058833	3.968597	2.506513
H	6.877372	-0.938306	-1.034417
H	-4.888149	2.652301	3.367403
H	6.237086	-2.583614	-0.847691
H	-2.455553	1.727577	3.923014
H	4.376186	-1.914076	-2.595999
H	-1.855956	3.132434	3.013850
H	5.227333	-0.355423	-2.663641
H	-4.362591	-2.977897	-1.295987
H	-0.392127	4.914692	0.749447
H	-3.460690	-4.246033	-2.150103
H	-0.130508	3.172590	0.994292
H	-4.606465	-3.230883	-3.036289
H	-1.709866	3.753812	0.451506
H	-3.790419	-0.522702	-1.925976
H	-0.608063	5.757734	-1.616965
H	-3.950618	-0.916323	-3.658406
H	-1.941299	4.610533	-1.848702
H	-2.425360	-0.271788	-3.024306
H	-0.545561	4.566770	-2.937175
H	-1.749221	-2.092282	-4.749432
H	1.714691	5.026116	-3.384294
H	-0.493583	-0.871034	-5.051262
H	1.825305	6.241243	-2.086623
H	-0.104678	-2.597046	-5.196441

H	3.291699	5.674688	-2.911689				
H	1.531093	-0.992942	-3.616484				
H	2.933220	5.450170	0.143631				
H	-0.066775	-5.661219	-3.039485				
H	-0.287021	1.855329	-4.372226				
H	1.621715	-2.733828	-3.278923				
H	4.323692	4.966504	-0.850544				
H	-1.836407	-5.589102	-3.188613				
H	-0.021574	0.748113	-3.000996				
H	1.343528	-1.559077	-1.951623				
H	3.504282	3.760608	0.171240				
H	-0.200708	-5.609394	-0.612416				
H	2.051127	2.270905	-4.772567				
H	-1.969282	-5.434766	-0.541746				
H	2.473025	1.096220	-3.508625				
H	-0.910194	-4.203314	0.194264				
H	3.103082	2.755189	-3.426111				
H	-0.823336	-4.374831	-3.988162				
H	-1.003886	2.206779	-2.791304				
H	-0.856861	-3.321394	4.895366				
H	2.148988	2.669796	4.461032				
H	-1.395010	1.500635	2.510288				
H	3.504372	-0.405426	-2.227365				
H	-3.775201	3.292226	-1.189839				
H	5.946325	0.630717	2.397989				
2f (protonated form (in-in))				2f (dication)			
C	-3.172299	5.159154	-1.547180	C	1.453572	3.112629	-1.946813
N	-3.090908	4.031926	-0.606263	N	0.013327	3.096853	-2.251190
C	-2.959250	4.490820	0.782018	C	-0.267457	3.747476	-3.546769
C	-2.447653	5.920099	0.617258	C	1.095750	4.289872	-3.987577
C	-3.184615	6.395264	-0.638279	C	2.087573	3.336596	-3.315842
P	-2.804140	2.501581	-1.148970	P	-1.079218	2.988167	-1.014363
N	-4.141508	2.107874	-2.059400	N	-1.132014	4.425962	-0.209859
C	-4.167812	0.810204	-2.775275	C	-1.382027	4.560995	1.231805
C	-5.579108	0.264125	-2.541381	C	-0.951682	5.998321	1.527226
C	-6.411073	1.520203	-2.280658	C	-1.279803	6.734569	0.226831
C	-5.462469	2.383846	-1.455290	C	-0.885807	5.725772	-0.853605
N	-2.547247	1.615102	0.140526	N	-0.607746	1.889570	0.012594
P	-1.619888	0.298911	0.270228	P	-0.850313	0.469830	0.659277
C	-1.125001	0.252905	2.040034	N	-2.036011	-0.426421	0.080731
C	-0.088333	-0.562543	2.634320	P	-3.458985	-0.950530	0.537018
C	-0.175116	-0.776750	4.048213	N	-3.335784	-2.360573	1.382493
C	-1.116595	-0.063047	4.836283	C	-2.289532	-2.602776	2.390908
C	-1.978979	0.823590	4.258823	C	-2.773378	-3.858036	3.122060
C	-2.003017	0.939556	2.854621	C	-3.619913	-4.583542	2.073622
C	0.693676	-1.697439	4.693190	C	-4.334825	-3.438456	1.356807
C	1.655318	-2.357509	3.981762	P	0.966574	-0.807154	0.659112
C	1.840208	-2.045770	2.618483	N	2.184508	0.083744	0.183369
C	1.033264	-1.153438	1.949012	P	3.612334	0.652854	0.549435
P	1.434716	-0.747444	0.183778	N	4.425038	-0.003976	1.831702
N	2.967486	-1.433524	0.038954	C	4.308281	0.524285	3.200518

P	3.467526	-2.027495	-1.332464	C	5.332817	-0.309446	3.964549
N	3.167914	-1.135374	-2.712983	C	5.203633	-1.692442	3.318132
C	1.786306	-0.791028	-3.095386	C	4.923642	-1.391339	1.838011
C	1.871980	-0.517131	-4.599123	N	0.723694	-2.212208	-0.045638
C	3.311886	-0.035886	-4.783459	P	1.028161	-2.837531	-1.473253
C	4.099419	-0.937440	-3.832561	N	-0.180300	-3.928958	-1.729849
N	-2.248684	-1.111486	-0.179906	C	-0.227976	-4.803408	-2.912399
P	-3.343686	-2.109528	0.378605	C	-0.964889	-6.041901	-2.404065
N	-4.406409	-2.493844	-0.836031	C	-1.948276	-5.452044	-1.389938
C	-3.877228	-2.904562	-2.149823	C	-1.130990	-4.362711	-0.689059
C	-5.100274	-3.466373	-2.875849	N	2.453736	-3.678857	-1.619625
C	-5.940472	-4.058885	-1.742220	C	3.729228	-2.933898	-1.514962
C	-5.755828	-3.047255	-0.609587	C	4.719625	-3.944558	-0.932570
N	-2.593312	-3.490347	0.887431	C	3.832082	-4.853801	-0.082429
C	-3.212560	-4.816840	0.907527	C	2.577996	-4.990767	-0.943876
C	-2.006562	-5.749086	0.803902	N	1.159650	-1.694318	-2.660425
C	-0.953875	-5.027058	1.649248	C	0.275037	-0.508071	-2.641337
C	-1.206106	-3.537179	1.376017	C	0.155984	-0.100614	-4.110991
N	-4.319449	-1.602172	1.611592	C	1.442447	-0.641019	-4.737507
C	-4.090437	-1.977196	3.019854	C	1.622725	-1.982061	-4.030981
C	-5.036027	-1.053687	3.805585	C	0.914828	-1.082051	2.447149
C	-6.065302	-0.583772	2.772184	C	0.036954	-0.222048	3.165400
C	-5.229455	-0.456661	1.502078	C	0.010484	-0.273948	4.582423
N	-1.561535	2.479626	-2.254156	C	0.839539	-1.218894	5.242077
C	-1.732339	2.588931	-3.718726	C	1.627114	-2.084734	4.524728
C	-0.581859	3.488669	-4.166295	C	1.666745	-2.016722	3.113004
C	0.517858	3.165277	-3.155997	C	-0.870702	0.595672	5.276228
C	-0.243650	3.018545	-1.838614	C	-1.692637	1.454329	4.589729
N	1.600218	0.921851	0.277031	C	-1.695399	1.470696	3.176166
P	2.725036	1.841735	0.872583	C	-0.856939	0.643108	2.470503
N	1.977921	3.307265	1.163797	N	-2.535714	2.758389	-1.748034
C	2.729763	4.537441	1.419463	C	-2.792950	1.595037	-2.612901
C	1.634225	5.556130	1.736040	C	-4.284234	1.703881	-2.932315
C	0.606429	4.708631	2.489049	C	-4.555278	3.209474	-2.862077
C	0.616605	3.383657	1.722221	C	-3.680746	3.681347	-1.697934
N	3.542541	1.475810	2.286099	N	4.608798	0.391448	-0.734654
C	2.873446	1.634379	3.584202	C	4.094229	0.505135	-2.112881
C	3.914550	1.115822	4.572757	C	5.336611	0.281701	-2.969696
C	4.544638	-0.055760	3.814024	C	6.439819	0.928375	-2.128186
C	4.568295	0.414642	2.353574	C	6.081360	0.491194	-0.706882
N	3.990147	2.073456	-0.183069	N	3.438200	2.262921	0.856170
C	3.703292	2.143537	-1.625749	C	4.536434	3.229577	0.731859
C	5.019585	2.622487	-2.239410	C	3.858471	4.560150	1.061034
C	5.617234	3.497364	-1.134571	C	2.824043	4.161040	2.116506
C	5.282248	2.702594	0.127410	C	2.294410	2.818539	1.607865
N	2.830949	-3.536560	-1.612230	N	-4.358545	-1.219114	-0.820562
C	2.815779	-4.175279	-2.934364	C	-3.810679	-1.931682	-1.986256
C	1.978516	-5.448822	-2.726173	C	-5.016182	-2.061819	-2.914698
C	1.134723	-5.137052	-1.484787	C	-6.181950	-2.232883	-1.937571
C	2.107080	-4.337150	-0.622267	C	-5.834757	-1.269557	-0.799442
N	5.140307	-2.166917	-1.364354	N	-4.321101	0.110274	1.458062

C	5.892768	-0.945881	-0.981536	C	-4.923751	-0.185587	2.768316
C	6.851196	-1.374762	0.151052	C	-5.413415	1.185209	3.241800
C	6.294087	-2.718277	0.631140	C	-5.752638	1.915230	1.939066
C	5.746792	-3.313178	-0.665177	C	-4.648011	1.460042	0.985087
H	6.047381	1.932438	0.297615	H	6.518099	-0.490728	-0.490595
H	2.676475	-2.475294	2.074126	H	2.292344	-2.708763	2.557535
H	-2.748606	1.576051	2.391078	H	-2.373401	2.137689	2.654600
H	2.311083	-3.073100	4.468468	H	2.230758	-2.824131	5.040002
H	-2.673653	1.400869	4.859809	H	-2.359075	2.117584	5.130582
H	0.573611	-1.862723	5.759932	H	0.823932	-1.262999	6.326665
H	-1.122818	-0.226803	5.910120	H	-0.890996	0.566694	6.361280
H	3.468012	0.820332	5.525178	H	5.135550	-0.322018	5.038152
H	4.660759	1.893387	4.768307	H	6.335153	0.098177	3.800775
H	2.609664	2.682241	3.757809	H	4.527751	1.594178	3.220359
H	1.954921	1.033591	3.647663	H	3.300608	0.367767	3.610710
H	5.542186	-0.314696	4.177048	H	6.095774	-2.308392	3.443430
H	3.907431	-0.938052	3.910470	H	4.361389	-2.229835	3.760842
H	4.346749	-0.396377	1.650856	H	4.191805	-2.086893	1.410880
H	5.547089	0.839388	2.101308	H	5.836674	-1.463519	1.239534
H	3.414700	4.428950	2.275497	H	5.346656	3.019230	1.445410
H	0.942296	4.549519	3.519922	H	3.314081	4.030885	3.087315
H	-0.387587	5.160611	2.527507	H	2.025879	4.895920	2.238442
H	3.326040	4.819020	0.545633	H	4.956035	3.207954	-0.278485
H	1.200819	5.935905	0.803775	H	3.358477	4.952644	0.169279
H	2.006912	6.405691	2.312067	H	4.569270	5.309965	1.413011
H	-0.125547	3.380068	0.915388	H	1.431594	2.935770	0.946265
H	5.227777	3.318683	1.027703	H	6.430469	1.190665	0.056076
H	0.389508	2.530170	2.365314	H	1.990599	2.162443	2.430976
H	6.690094	3.669701	-1.245920	H	7.446425	0.615514	-2.411792
H	5.113823	4.470728	-1.113024	H	6.382614	2.019220	-2.212645
H	4.866262	3.152802	-3.181995	H	5.232406	0.721742	-3.963459
H	2.901281	2.865098	-1.824951	H	3.694107	1.508921	-2.291793
H	5.676473	1.767251	-2.433866	H	5.531013	-0.790025	-3.086469
H	3.392602	1.166280	-1.999319	H	3.295118	-0.220354	-2.284867
H	1.446208	0.094895	-2.542895	H	0.742463	0.286811	-2.050110
H	1.094154	-1.606228	-2.857580	H	-0.697875	-0.738487	-2.195571
H	1.712738	-1.443718	-5.161093	H	-0.715123	-0.580644	-4.568613
H	1.124612	0.209399	-4.928022	H	0.046366	0.979554	-4.217117
H	3.667216	-0.112372	-5.813231	H	1.383417	-0.751086	-5.821822
H	3.403831	1.009307	-4.467084	H	2.286821	0.017805	-4.505625
H	4.356920	-1.888484	-4.318173	H	1.006910	-2.752540	-4.511998
H	5.027128	-0.468273	-3.498462	H	2.658520	-2.326059	-4.029898
H	1.618263	-3.693584	0.110360	H	-1.739146	-3.525384	-0.339559
H	6.451053	-0.559706	-1.841577	H	4.047746	-2.564975	-2.493641
H	5.198410	-0.169050	-0.644178	H	3.621506	-2.066936	-0.853399
H	6.902725	-0.626036	0.944457	H	5.513011	-3.453238	-0.365028
H	7.863155	-1.510951	-0.243301	H	5.187084	-4.522520	-1.735978
H	5.016177	-4.110246	-0.517673	H	1.687861	-5.225776	-0.356139
H	6.563759	-3.717898	-1.276341	H	2.701034	-5.779340	-1.695618
H	7.049116	-3.349629	1.106064	H	4.290156	-5.818173	0.145613
H	5.469952	-2.561460	1.335024	H	3.578706	-4.362094	0.863918

H	3.828848	-4.405125	-3.284791	H	0.778368	-5.027828	-3.278247
H	0.765345	-6.034979	-0.983329	H	-2.333963	-6.192057	-0.685580
H	2.353247	-3.507558	-3.671179	H	-0.788142	-4.320825	-3.723462
H	0.276114	-4.508330	-1.747611	H	-2.802111	-5.009892	-1.915179
H	1.380897	-5.694603	-3.606271	H	-1.452402	-6.595913	-3.208414
H	2.636492	-6.298657	-2.518403	H	-0.260073	-6.712086	-1.900664
H	2.784723	-5.012789	-0.078163	H	-0.600857	-4.771731	0.180669
H	-4.677841	0.493233	1.475450	H	-3.769570	2.118454	1.036156
H	-5.828897	-0.522770	0.590004	H	-4.977603	1.442463	-0.057422
H	-6.550001	0.354781	3.048851	H	-5.782675	3.001020	2.047477
H	-6.839767	-1.343927	2.626709	H	-6.724296	1.580301	1.562405
H	-5.487577	-1.564767	4.658107	H	-6.262952	1.102872	3.921946
H	-4.476896	-0.194699	4.185909	H	-4.607504	1.706100	3.767928
H	-3.048394	-1.823677	3.322451	H	-4.192290	-0.621571	3.454084
H	-4.337080	-3.033627	3.168534	H	-5.761787	-0.886550	2.666594
H	-6.505712	-2.248727	-0.685260	H	-6.248596	-0.270842	-0.986446
H	-6.991508	-4.190208	-2.007044	H	-7.154642	-2.010469	-2.379890
H	-5.848513	-3.492782	0.383733	H	-6.221331	-1.612261	0.164417
H	-1.075777	-2.942514	2.283976	H	-2.184961	-1.756220	3.076522
H	-0.533689	-3.129795	0.614978	H	-1.324659	-2.762149	1.895411
H	-5.542362	-5.036765	-1.450113	H	-6.206645	-3.261599	-1.562453
H	0.070021	-5.317618	1.402823	H	-1.941443	-4.457751	3.495905
H	-1.116194	-5.245224	2.709432	H	-3.399071	-3.573632	3.974130
H	-2.224695	-6.759003	1.157150	H	-4.321170	-5.299702	2.505558
H	-1.682966	-5.808351	-0.240713	H	-2.974766	-5.117950	1.369718
H	-3.906461	-4.935610	0.073022	H	-4.607933	-3.691645	0.328509
H	-3.766471	-4.992671	1.841074	H	-5.249286	-3.155472	1.896106
H	-3.103655	-3.676808	-2.032123	H	-3.433683	-2.922017	-1.700221
H	-4.824078	-4.198031	-3.637486	H	-4.909714	-2.896481	-3.610053
H	-5.649675	-2.656491	-3.365580	H	-5.140412	-1.143118	-3.496620
H	-3.427473	-2.056298	-2.670399	H	-2.983062	-1.374847	-2.431431
H	-0.290200	3.297575	-5.201200	H	1.191848	4.323429	-5.074318
H	1.003857	2.217423	-3.413850	H	2.135356	2.389761	-3.866387
H	-0.871227	4.541999	-4.082900	H	1.237142	5.304541	-3.600732
H	-2.713129	2.996423	-3.972951	H	-1.020253	4.535565	-3.463757
H	-1.644915	1.595680	-4.175740	H	-0.646570	3.010894	-4.264763
H	-2.297963	5.166528	-2.211371	H	0.171908	5.826137	-1.129590
H	-2.718316	7.258847	-1.116069	H	-0.749057	7.682058	0.117945
H	-4.215498	6.662512	-0.384989	H	-2.354828	6.934371	0.170184
H	-1.366049	5.905720	0.437251	H	0.126678	6.033397	1.713110
H	-2.643129	6.540987	1.494187	H	-1.462292	6.411517	2.398883
H	-2.283435	3.842252	1.341074	H	-0.805515	3.820257	1.791480
H	-3.934903	4.480735	1.286056	H	-2.447161	4.417357	1.462311
H	-0.369402	4.000061	-1.356337	H	1.706223	3.941271	-1.268473
H	1.289444	3.935831	-3.098084	H	3.098724	3.743203	-3.245110
H	-5.492383	2.078806	-0.399534	H	-4.213118	3.599506	-0.742817
H	-3.402350	0.127265	-2.389976	H	-2.547176	0.671609	-2.083793
H	-7.345123	1.317078	-1.752732	H	-5.608618	3.450819	-2.707129
H	-5.574472	-0.383861	-1.660639	H	-4.864517	1.168785	-2.174809
H	-5.938099	-0.321031	-3.390797	H	-4.526308	1.271915	-3.905575
H	-6.650284	2.023073	-3.223373	H	-4.225427	3.691138	-3.788166

H	-3.976245	0.973906	-3.840603	H	-2.191306	1.649793	-3.528177
H	-5.693039	3.450429	-1.509615	H	-3.367071	4.721096	-1.814974
H	-4.067320	5.092501	-2.174971	H	-1.482771	5.855009	-1.762165
H	0.270034	2.355876	-1.134587	H	1.748687	2.183453	-1.454577
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2f protonated (in-out)							
C	4.088799	-4.362808	-0.639347				
N	3.796977	-3.141408	-1.410709				
C	4.924169	-2.193454	-1.230349				
C	5.868363	-2.857195	-0.207498				
C	4.985500	-3.886745	0.501247				
P	2.250085	-2.493707	-1.283843				
N	1.193053	-3.767869	-1.465401				
C	1.108510	-4.544582	-2.707132				
C	0.325066	-5.795187	-2.302236				
C	-0.561388	-5.290767	-1.161622				
C	0.358575	-4.334724	-0.400542				
N	2.023796	-1.733736	0.064967				
P	0.863801	-0.536004	0.383792				
N	1.634905	0.951103	0.298316				
P	3.061412	1.523521	0.576096				
N	4.131220	1.280813	-0.685713				
C	3.618113	1.454352	-2.054937				
C	4.877190	1.476848	-2.918573				
C	5.898821	2.153168	-2.001787				
C	5.582768	1.523986	-0.644593				
C	0.790645	-0.741409	2.253729				
C	0.069869	0.172077	3.099136				
C	0.399398	0.191435	4.492073				
C	1.214048	-0.830144	5.047569				
C	1.726161	-1.810804	4.244982				
C	1.553612	-1.722817	2.847050				
C	-0.075943	1.231452	5.335934				
C	-0.913059	2.197450	4.856134				
C	-1.406739	2.069676	3.541200				
C	-0.966713	1.085439	2.678958				
P	-2.111904	0.834884	1.280486				
N	-2.420958	-0.718278	1.270890				
P	-3.368744	-1.862738	0.779195				
N	-4.984982	-1.793812	1.210613				
C	-5.324348	-1.951707	2.633003				
C	-5.474611	-0.518053	3.148401				
C	-6.110761	0.220956	1.956267				
C	-5.781680	-0.652811	0.718068				
N	-1.705823	1.558753	-0.070265				
P	-2.163072	2.556059	-1.191591				
N	-1.170962	2.419690	-2.507031				
C	-1.559239	2.666123	-3.908376				
C	-0.346895	3.377065	-4.511860				
C	0.824385	2.808861	-3.707500				
C	0.261049	2.724761	-2.290810				

N	-2.095251	4.107562	-0.630984
C	-2.199840	5.258531	-1.540210
C	-2.298684	6.457901	-0.591753
C	-1.545389	5.981560	0.653321
C	-1.974285	4.520040	0.770190
N	-3.697918	2.377413	-1.823422
C	-4.105064	1.113201	-2.460832
C	-5.638076	1.229963	-2.623420
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C	-4.840269	2.879870	-1.048609
N	2.139762	-1.613967	-2.705739
C	0.839920	-1.019043	-3.055959
C	0.840722	-0.973151	-4.585724
C	2.328212	-0.868062	-4.925358
C	2.976324	-1.797868	-3.899603
N	-3.467467	-1.961109	-0.865682
C	-2.231955	-1.841282	-1.660749
C	-2.661353	-2.268120	-3.066726
C	-3.798711	-3.260321	-2.808901
C	-4.534267	-2.642694	-1.620310
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C	-2.541099	-5.504999	2.075513
C	-2.192230	-4.614900	3.270806
C	-1.865007	-3.273977	2.615833
N	2.838214	3.164324	0.790092
C	3.946899	4.115001	0.890081
C	3.258230	5.440323	1.233768
C	2.036615	4.991729	2.040161
C	1.584043	3.734793	1.297263
N	4.011160	1.057350	1.876729
C	3.632621	1.471967	3.231799
C	4.706543	0.816579	4.094950
C	4.922377	-0.537451	3.407877
C	4.666548	-0.263008	1.915554
H	6.120543	0.570657	-0.544900
H	2.084876	-2.408484	2.193182
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H	2.322932	-2.614072	4.667400
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H	1.412737	-0.815669	6.115337
H	0.240182	1.238229	6.375331
H	4.395615	0.718765	5.138037
H	5.622579	1.415838	4.062969
H	3.627764	2.563045	3.312440
H	2.637821	1.102692	3.511717
H	5.921055	-0.945084	3.582271
H	4.194711	-1.259706	3.782875
H	4.036553	-1.035405	1.458411
H	5.607713	-0.216383	1.358906
H	4.655518	3.824008	1.680433

H	2.334919	4.734492	3.062837
H	1.252733	5.751017	2.098599
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H	2.934110	5.941270	0.315099
H	3.916577	6.120871	1.777920
H	0.912528	3.989321	0.464863
H	5.866280	2.152073	0.202978
H	1.053375	3.025315	1.936802
H	6.935792	1.990688	-2.304434
H	5.715714	3.233507	-1.971301
H	4.720712	2.000515	-3.864591
H	3.082823	2.409118	-2.145511
H	5.197803	0.453108	-3.143246
H	2.934815	0.643225	-2.313313
H	0.737803	-0.019696	-2.616441
H	0.024725	-1.630598	-2.665878
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H	0.241160	-0.147666	-4.977667
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H	2.963130	-2.837198	-4.254385
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H	6.311968	-2.128363	0.473932
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H	5.555525	-4.696264	0.963877
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H	-0.948428	-6.094358	-0.531936
H	0.575964	-3.975730	-3.482741
H	-1.414132	-4.736762	-1.569072
H	-0.239027	-6.222035	-3.134023
H	1.013365	-6.560213	-1.927581
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H	-6.080682	-0.458395	4.054874
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H	-4.563957	-2.533961	3.156686
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H	-4.452106	-3.401317	-3.672179
H	-5.054140	-3.379975	-1.005523
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H	-3.230792	-4.826306	0.103777				
H	-4.406516	-4.589964	1.412824				
H	-1.454090	-2.506975	-1.269525				
H	-1.834396	-2.703656	-3.632965				
H	-3.034463	-1.405223	-3.627908				
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H	1.088801	1.810247	-4.070574				
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H	-1.306386	5.324479	-2.175306				
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H	-0.464758	6.034310	0.479531				
H	-1.779746	6.558180	1.550202				
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H	1.719637	3.432111	-3.757783				
H	-4.950482	2.347375	-0.089988				
H	-3.849462	0.254028	-1.828496				
H	-6.963295	2.529317	-1.429724				
H	-6.135614	0.397937	-2.118319				
H	-5.934678	1.193897	-3.673196				
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H	-3.593358	0.992831	-3.418162				
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H	-3.072923	5.172774	-2.196583				
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3a (protonated form)				3a (dication)			
C	-0.227989	-0.110178	0.136062	C	-0.062294	-0.351578	0.120276
C	-0.080576	-0.273704	1.539020	C	0.040103	-0.094854	1.511924
C	1.145602	0.092413	2.166928	C	1.237237	0.467293	2.039025
C	2.196287	0.611811	1.339692	C	2.267260	0.807807	1.098051
C	2.014977	0.747955	-0.018565	C	2.142743	0.521725	-0.254728
C	0.792971	0.388769	-0.626936	C	0.969809	-0.076333	-0.741952
C	-1.140276	-0.797139	2.324999	C	-1.025704	-0.413492	2.392167
C	-0.997996	-0.956892	3.678393	C	-0.906330	-0.202939	3.741116
C	0.215658	-0.595276	4.304584	C	0.301636	0.301677	4.269114
P	3.779546	1.113790	2.054776	P	3.641860	1.804621	1.545146
N	3.590505	2.112281	3.329519	N	3.547451	2.889005	2.640092
C	2.983087	3.282735	3.304635	C	2.531625	3.537074	3.245797
N	2.824936	3.938406	4.456735	N	2.586735	3.699247	4.542459
C	3.362606	3.407984	5.704276	C	3.715030	3.212803	5.339548

N	4.680461	1.596502	0.792693	N	4.903519	1.556073	0.693780
C	5.908319	2.074127	0.828591	C	6.153604	2.063737	0.721624
N	6.452305	2.419711	-0.340106	N	6.722975	2.299907	-0.431721
C	7.800028	2.948037	-0.507729	C	8.074698	2.844339	-0.568839
C	6.725603	2.249397	2.085808	C	6.875823	2.281992	2.017250
C	2.439588	3.930169	2.054005	C	1.384384	4.086113	2.454231
C	2.091155	5.197017	4.557261	C	1.517178	4.371739	5.288022
C	5.661239	2.273716	-1.558418	C	6.003235	2.043020	-1.684325
H	0.323715	-0.720552	5.376922	H	0.410165	0.425563	5.340993
H	-1.812714	-1.358228	4.271597	H	-1.726035	-0.444539	4.408034
H	-2.067971	-1.069769	1.830667	H	-1.935378	-0.834114	1.976027
H	2.826669	1.139239	-0.621637	H	2.936132	0.785108	-0.944647
H	0.673897	0.509257	-1.697930	H	0.880288	-0.289546	-1.800000
H	-1.171186	-0.391495	-0.323147	H	-0.983256	-0.784409	-0.257764
H	8.346575	2.955008	0.430619	H	8.451641	3.214154	0.379701
H	5.401614	1.225501	-1.724091	H	5.514437	1.070593	-1.633568
H	4.737117	2.851216	-1.483533	H	5.254604	2.820220	-1.849688
H	1.739463	5.304052	5.583132	H	1.546498	4.009751	6.313989
H	2.732077	6.050640	4.316024	H	1.680148	5.451722	5.280213
H	1.219049	5.201324	3.904379	H	0.542852	4.135590	4.865448
H	4.156093	2.697273	5.487315	H	4.582441	3.065424	4.701136
H	3.759688	4.235072	6.295576	H	3.936792	3.957305	6.103658
H	2.575707	2.905510	6.275200	H	3.442835	2.270010	5.820181
H	8.347278	2.325216	-1.219509	H	8.736978	2.065548	-0.952366
H	6.249687	2.639035	-2.398974	H	6.724605	2.049500	-2.498734
H	7.608571	1.605746	2.060827	H	7.860016	1.811216	1.998333
H	7.058100	3.284604	2.191300	H	7.002476	3.353388	2.197707
H	6.138508	2.000106	2.968003	H	6.302586	1.857095	2.838162
H	7.752808	3.969379	-0.895243	H	8.038255	3.671357	-1.278355
H	1.363779	3.741934	1.978878	H	0.509314	3.442300	2.596025
H	2.599561	5.008833	2.055777	H	1.125518	5.094918	2.777334
H	2.922248	3.516631	1.169328	H	1.635238	4.107317	1.395715
H	4.327450	-0.030743	2.649977	C	1.352063	0.617260	3.443244
C	1.258000	-0.083407	3.573560	H	2.286213	0.945380	3.884809
H	2.169469	0.205714	4.085261				
3a (neutral)							
C	-0.527439	0.712965	0.552724				
C	-0.037910	-0.040811	1.653012				
C	1.313823	0.127273	2.077265				
C	2.127065	1.042900	1.351006				
C	1.628823	1.750278	0.285966				
C	0.283771	1.590499	-0.117857				
C	1.797416	-0.631441	3.198785				
C	0.947877	-1.531770	3.802562				
C	-0.390534	-1.699246	3.377070				
C	-0.876995	-0.965035	2.330526				
P	3.580883	-0.520010	3.716489				
N	3.627374	-1.461197	5.137855				
C	3.125079	-1.162507	6.301230				
N	3.424250	-1.977348	7.350137				
C	4.196076	-3.182650	7.093610				

H	3.155179	1.194790	1.656312				
N	3.616857	1.151402	4.105466				
C	4.577201	1.743911	4.730325				
N	4.580849	3.118952	4.767532				
C	5.244722	3.852133	5.833679				
C	5.728196	1.050413	5.428407				
C	2.226725	0.015600	6.611876				
C	2.754603	-1.874393	8.637624				
C	3.454746	3.808808	4.162283				
H	1.308533	-2.129864	4.632634				
H	-1.027683	-2.412180	3.891075				
H	-1.904470	-1.082847	1.997701				
H	2.272428	2.439852	-0.251265				
H	-0.100320	2.159666	-0.958359				
H	-1.561744	0.576002	0.249074				
H	6.192854	3.391430	6.105256				
H	4.619737	3.918036	6.735397				
H	3.233375	3.374286	3.187779				
H	2.548315	3.732221	4.778755				
H	2.642640	-0.833920	8.941959				
H	1.763821	-2.346050	8.628214				
H	4.540740	-3.592483	8.043789				
H	3.600191	-3.942473	6.573592				
H	5.053933	-2.942640	6.465165				
H	5.456384	4.867345	5.490306				
H	3.711683	4.863514	4.042767				
H	1.298933	-0.326616	7.078154				
H	2.716885	0.707787	7.304079				
H	1.985301	0.559526	5.703398				
H	6.680520	1.536725	5.206006				
H	5.585738	1.061784	6.513924				
H	5.785287	0.008227	5.115878				
H	3.363837	-2.374063	9.391827				
3b (protonated form)				3b (dication)			
C	2.282302	-3.293426	-0.367967	C	2.811620	-3.254930	-0.064813
C	2.693626	-2.248340	0.501918	C	3.108080	-1.972862	0.466505
C	1.784247	-1.198794	0.819240	C	2.049496	-1.059882	0.733118
C	0.485713	-1.218221	0.211972	C	0.722813	-1.471313	0.372079
C	0.126526	-2.252083	-0.621739	C	0.465217	-2.745265	-0.113276
C	1.025676	-3.302861	-0.910058	C	1.521414	-3.648177	-0.319239
C	2.220698	-0.180958	1.709004	C	2.358648	0.166917	1.368426
C	3.492596	-0.186834	2.223176	C	3.659009	0.501433	1.653386
C	4.398895	-1.217016	1.886784	C	4.715833	-0.378158	1.332551
C	4.001840	-2.228846	1.051914	C	4.442743	-1.595859	0.765756
H	1.542693	0.615110	1.994297	H	1.564065	0.840474	1.668210
P	-0.671345	0.164520	0.423412	P	-0.606000	-0.325385	0.234939
N	-2.032066	-0.237923	-0.355913	N	-1.993631	-0.913251	0.528826
C	-3.267996	-0.086531	0.097146	C	-3.264602	-0.457611	0.312112
N	-4.205425	-0.978486	-0.300136	N	-3.904152	-0.888919	-0.776700
C	-5.588596	-0.596154	-0.561176	C	-4.971607	-0.123014	-1.422590
N	0.018694	1.584837	0.039886	N	-0.404431	1.153266	-0.202815

C	1.101247	1.729923	-0.712931	C	0.699480	1.763644	-0.726135
N	1.970019	2.717333	-0.409860	N	1.016691	2.960104	-0.237212
C	2.831511	3.344146	-1.403423	C	1.732765	3.973618	-1.012415
N	1.398689	0.950807	-1.795083	N	1.407127	1.205652	-1.722760
C	0.371004	0.470461	-2.703169	C	0.822277	0.229658	-2.637760
C	2.744421	0.458711	-2.048259	C	2.852690	1.383021	-1.861367
N	-3.675136	0.910908	0.931136	N	-3.845069	0.321402	1.224534
C	-4.705367	0.712954	1.941473	C	-5.284920	0.281100	1.493821
C	-3.069897	2.234367	0.916275	C	-3.026740	1.030899	2.208823
C	-3.791756	-2.258833	-0.852065	C	-3.372923	-2.007674	-1.553556
C	1.937189	3.385134	0.880997	C	0.443050	3.438339	1.019058
H	3.802858	0.604500	2.897453	H	3.873254	1.446135	2.140820
H	5.402686	-1.207771	2.297641	H	5.737839	-0.096142	1.558364
H	4.685132	-3.033059	0.795796	H	5.242042	-2.296379	0.546969
H	-0.854365	-2.239090	-1.083316	H	-0.545911	-3.040243	-0.368078
H	0.715950	-4.104029	-1.571834	H	1.309078	-4.637289	-0.705798
H	2.987259	-4.086969	-0.597596	H	3.634218	-3.936409	-0.258033
H	0.303390	-0.621859	-2.682703	H	1.126096	-0.789589	-2.378697
H	-0.597616	0.887092	-2.429978	H	-0.263968	0.309980	-2.642672
H	0.617910	0.785193	-3.722666	H	1.183011	0.451188	-3.643885
H	2.697901	-0.630932	-2.151981	H	3.299205	0.387913	-1.941063
H	3.391341	0.688185	-1.201274	H	3.262268	1.864413	-0.976004
H	3.176121	0.880630	-2.962194	H	3.105313	1.959381	-2.754168
H	3.879086	3.058647	-1.267874	H	2.760224	4.093576	-0.662954
H	2.750830	4.429100	-1.297180	H	1.203860	4.919854	-0.884852
H	2.960688	3.507626	1.245628	H	1.179797	4.077128	1.507313
H	1.473530	4.373168	0.790772	H	-0.466570	4.013499	0.825574
H	-2.445429	2.405396	1.799872	H	-2.617633	0.340685	2.951615
H	-2.459155	2.362403	0.024061	H	-2.221327	1.575218	1.714660
H	-5.628865	1.248829	1.698111	H	-5.778850	1.199509	1.170313
H	-4.328770	1.089830	2.897092	H	-5.417887	0.165099	2.570863
H	-4.923590	-0.348505	2.051957	H	-5.736872	-0.577708	1.001877
H	-4.620134	-2.962035	-0.745988	H	-4.204746	-2.472500	-2.083040
H	-3.527481	-2.176989	-1.912302	H	-2.632159	-1.664814	-2.282593
H	-2.934299	-2.642142	-0.300425	H	-2.926104	-2.746140	-0.890142
H	-5.698917	0.485621	-0.500431	H	-5.017234	0.884455	-1.014102
H	-5.852527	-0.908731	-1.575390	H	-4.728986	-0.049742	-2.484632
H	-6.279642	-1.070219	0.142109	H	-5.940196	-0.615199	-1.313119
H	2.509465	3.070617	-2.407014	H	1.724968	3.715566	-2.069371
H	-3.867551	2.983291	0.907079	H	-3.663083	1.759352	2.708562
H	1.362232	2.796599	1.590841	H	0.204495	2.608404	1.679963
H	-0.937244	0.259588	1.801385				
3b (neutral form)							
C	-3.246494	2.257520	1.832140				
C	-3.636107	1.488519	0.702960				
C	-2.639566	0.839286	-0.084906				
C	-1.257139	0.981828	0.274965				
C	-0.934486	1.739053	1.379451				
C	-1.924039	2.377488	2.163034				
C	-3.069098	0.076455	-1.207327				
C	-4.399003	-0.029568	-1.527964				

C	-5.381639	0.617798	-0.744143	
C	-5.005105	1.356819	0.347003	
H	-2.327395	-0.451545	-1.796640	
P	0.091347	0.286233	-0.806594	
N	-0.246807	-1.376420	-0.755422	
C	0.229307	-2.383190	-0.096363	
N	0.809985	-2.376637	1.151010	
C	1.874738	-3.283924	1.530775	
N	1.459105	0.563704	0.171265	
C	2.469531	1.271610	-0.240969	
N	3.729330	0.961240	0.222316	
C	4.674817	1.993836	0.617789	
N	2.428430	2.334358	-1.120550	
C	1.288938	3.224681	-1.212037	
C	3.485386	2.594130	-2.080717	
N	0.171443	-3.642125	-0.683297	
C	-0.310414	-4.786143	0.077917	
C	-0.113080	-3.723191	-2.101546	
C	0.391992	-1.447899	2.179256	
C	3.923301	-0.318664	0.872451	
H	-4.701751	-0.618484	-2.388222	
H	-6.430552	0.525079	-1.007335	
H	-5.751482	1.856225	0.958898	
H	0.111449	1.830628	1.658094	
H	-1.625862	2.961857	3.028197	
H	-4.015121	2.746723	2.424130	
H	0.739658	3.092852	-2.151327	
H	0.605060	3.049552	-0.382306	
H	1.637283	4.263730	-1.158436	
H	3.054402	2.650362	-3.087297	
H	4.215256	1.785550	-2.061601	
H	4.001331	3.541639	-1.879153	
H	5.639825	1.865100	0.115725	
H	4.841234	1.950472	1.701234	
H	4.976517	-0.602371	0.788116	
H	3.654371	-0.283808	1.937574	
H	0.426115	-2.940648	-2.634394	
H	0.214752	-4.700962	-2.467661	
H	0.345885	-5.653118	-0.054237	
H	-1.319838	-5.064510	-0.253123	
H	-0.361125	-4.544143	1.138491	
H	0.214569	-2.001484	3.109785	
H	1.142422	-0.670071	2.346021	
H	-0.535239	-0.961224	1.880807	
H	2.250918	-3.806818	0.651579	
H	2.695547	-2.712570	1.979161	
H	1.543664	-4.027853	2.267802	
H	4.281891	2.980605	0.376256	
H	-1.184594	-3.611657	-2.319895	
H	3.299161	-1.070089	0.390816	
3c (protonated form)				3c (dication)

C	1.936200	-3.348207	0.708130	C	1.161917	3.028254	0.638921
N	2.149786	-2.169093	-0.008402	C	0.135608	2.982103	-0.339035
C	0.957533	-1.669190	-0.419294	C	-0.367994	4.209598	-0.857513
N	-0.002345	-2.526689	0.014536	C	0.195369	5.434597	-0.414211
C	0.596141	-3.570065	0.724857	C	1.205827	5.446029	0.510579
N	0.780268	-0.594288	-1.200519	C	1.685051	4.229625	1.045740
P	0.354330	0.876412	-0.703891	C	-1.432899	4.195480	-1.795091
N	-0.981520	1.064819	0.157120	C	-2.002889	3.021322	-2.217473
C	-2.282903	0.929383	-0.024796	C	-1.520403	1.797016	-1.721892
N	-3.024944	0.722710	-1.150450	C	-0.471602	1.775386	-0.818388
C	-4.386912	0.760907	-0.809977	P	0.042279	0.167420	-0.292264
C	-4.463185	0.943900	0.531530	N	1.542551	-0.061172	-0.270281
N	-3.155572	1.021492	1.014173	C	2.607913	-0.833436	-0.012464
C	-2.433520	0.653526	-2.497486	N	2.675435	-2.141177	0.307616
C	-3.081346	-0.396465	-3.398696	C	4.014133	-2.489708	0.434118
C	-5.502099	0.639142	-1.792920	C	4.752836	-1.362336	0.203444
C	-5.677175	1.064599	1.389625	N	3.861181	-0.341304	-0.079383
C	-2.675679	1.233746	2.389457	C	1.490417	-3.025465	0.406678
C	-2.653119	2.722897	2.724636	C	1.481300	-3.851788	1.689656
C	3.423804	-1.495596	-0.309245	C	4.500415	-3.854623	0.785715
C	4.053763	-0.875774	0.935771	C	6.230837	-1.187923	0.292597
C	-1.414087	-2.390256	-0.375602	C	4.144674	1.061753	-0.463331
C	-2.342668	-2.283053	0.829903	C	4.765771	1.134173	-1.855219
C	-0.160640	-4.652402	1.419514	N	-1.027703	-0.881406	0.104489
C	3.025686	-4.174663	1.305096	C	-2.379877	-0.828139	0.192683
C	1.638452	1.699021	0.282365	N	-3.134748	-0.068532	1.009426
C	2.916411	2.014909	-0.286944	C	-4.471165	-0.431428	0.827026
C	3.904428	2.604616	0.554294	C	-4.498422	-1.419696	-0.109692
C	3.603720	2.860582	1.917714	N	-3.181789	-1.655225	-0.496780
C	2.374563	2.552142	2.435295	C	-5.617662	0.176679	1.562371
C	1.388112	1.972889	1.608111	C	-2.576044	0.901452	1.979104
C	5.187358	2.904109	0.025471	C	-2.929038	0.522522	3.414572
C	5.491029	2.627759	-1.281740	C	-2.645761	-2.678793	-1.423963
C	4.514636	2.046461	-2.121459	C	-2.652777	-4.051218	-0.757264
C	3.262772	1.754146	-1.641971	C	-5.678501	-2.136042	-0.673448
H	2.543419	1.292595	-2.309269	C	1.333076	-3.853803	-0.865154
C	-3.418794	0.396289	3.427863	C	4.936533	1.796604	0.612822
C	-2.381004	2.039338	-3.134306	C	-2.933233	2.345006	1.629561
C	4.385084	-2.393901	-1.082954	C	-3.333601	-2.649035	-2.784868
C	-1.824719	-3.469193	-1.374987	H	1.536555	2.111222	1.078925
H	5.928285	3.350792	0.681931	H	-0.194712	6.362755	-0.819485
H	4.757353	1.828721	-3.156235	H	2.471478	4.244138	1.792563
H	6.476325	2.853238	-1.675465	H	1.632483	6.385536	0.843539
H	0.410767	1.744841	2.017014	H	-1.974347	0.875002	-2.070398
H	2.148829	2.751338	3.477170	H	-2.817223	3.024457	-2.931641
H	4.370719	3.304469	2.545590	H	-1.799338	5.144013	-2.175215
H	-1.645309	0.875025	2.353911	H	3.155931	1.516818	-0.519737
H	-4.386386	0.822876	3.697302	H	5.780047	0.730686	-1.882597
H	-3.569244	-0.628990	3.080250	H	4.152719	0.593851	-2.580147
H	-2.812038	0.360922	4.335962	H	4.816059	2.182159	-2.160035
H	-3.662370	3.145197	2.721903	H	5.984454	1.492184	0.640882

H	-2.043658	3.267474	1.998951	H	4.493942	1.639314	1.599580
H	-2.223995	2.871868	3.719139	H	4.906226	2.866166	0.391102
H	-5.832913	0.176507	2.007574	H	6.631591	-0.624595	-0.550648
H	-5.617625	1.933067	2.050341	H	6.511083	-0.672020	1.214822
H	-6.560389	1.190236	0.762793	H	6.717922	-2.162798	0.297849
H	-6.445261	0.880247	-1.301911	H	5.568732	-3.923969	0.581611
H	-5.384333	1.331580	-2.630418	H	4.347667	-4.075497	1.845006
H	4.842582	-3.158029	-0.450812	H	-3.977411	0.719813	3.644167
H	-5.589796	-0.372920	-2.196006	H	4.004538	-4.628246	0.197016
H	-1.855695	2.746519	-2.486463	H	1.746367	-3.238490	2.554033
H	-3.388101	2.424397	-3.317280	H	2.148830	-4.712997	1.643919
H	-1.854440	1.987600	-4.090694	H	0.467141	-4.229693	1.839199
H	5.189714	-1.773608	-1.486616	H	-2.322105	1.127902	4.091645
H	3.876885	-2.882294	-1.918033	H	-2.713000	-0.530895	3.605146
H	-4.015258	-0.052868	-3.844404	H	2.156823	-4.558839	-1.000584
H	-2.389026	-0.617458	-4.214348	H	0.405607	-4.428432	-0.800113
H	-3.268636	-1.324303	-2.853166	H	1.278338	-3.208173	-1.745310
H	3.323999	-0.277084	1.486235	H	-2.794598	2.546717	0.565994
H	-1.414092	0.299082	-2.338451	H	0.642885	-2.346021	0.468324
H	4.469316	-1.630561	1.607832	H	-3.962902	2.587222	1.899234
H	3.124415	-0.685905	-0.974280	H	-1.496440	0.784036	1.879565
H	4.869600	-0.216532	0.626850	H	-2.277354	3.012299	2.193698
H	3.731098	-3.572013	1.879891	H	-5.548894	1.264205	1.599634
H	3.587111	-4.716713	0.539228	H	-5.688549	-0.200855	2.585640
H	2.598777	-4.911428	1.985909	H	-6.548164	-0.070324	1.051291
H	-0.714144	-4.263692	2.278902	H	-5.893978	-1.813839	-1.695317
H	-0.870345	-5.156663	0.761262	H	-5.533098	-3.217966	-0.677803
H	0.533115	-5.409135	1.786097	H	-6.557078	-1.929036	-0.062749
H	-1.173453	-3.447504	-2.252087	H	-2.094752	-4.026601	0.182406
H	-2.851523	-3.283312	-1.701280	H	-2.177861	-4.774731	-1.424633
H	-1.795975	-4.471550	-0.943169	H	-3.667761	-4.399710	-0.551329
H	-1.438725	-1.438146	-0.901872	H	-1.607133	-2.379024	-1.569672
H	-1.930304	-1.587526	1.565235	H	-3.425459	-1.626052	-3.157885
H	-2.510718	-3.248250	1.312257	H	-4.322032	-3.110514	-2.763184
H	-3.313040	-1.900860	0.498893	H	-2.720767	-3.215774	-3.489424
H	0.328778	1.600358	-1.906529				
3c (neutral form)							
C	3.946239	-0.685268	0.150415				
N	2.921165	-0.673077	1.101440				
C	1.870444	-1.440765	0.661354				
N	2.247440	-1.915514	-0.569111				
C	3.531518	-1.462451	-0.881721				
N	0.777069	-1.746116	1.322490				
P	-0.511295	-0.690168	1.568304				
C	-3.441053	-2.021908	1.598735				
C	-2.924229	-1.716443	0.307099				
C	-3.743206	-2.009784	-0.825952				
C	-5.022417	-2.597519	-0.631046				
C	-5.485349	-2.876583	0.627947				
C	-4.683054	-2.581664	1.755637				
C	-3.274503	-1.691476	-2.126376				

C	-2.049618	-1.098658	-2.294806
C	-1.247852	-0.807410	-1.170740
C	-1.645791	-1.102791	0.113349
C	2.985272	-0.206363	2.491472
C	3.979204	-1.040504	3.301723
C	1.425644	-2.903096	-1.276173
C	1.960399	-4.316825	-1.049729
C	4.223322	-1.750596	-2.171626
C	5.198082	0.119727	0.259909
N	0.115289	0.790280	1.041300
C	-0.364500	1.770710	0.345175
N	0.425577	2.593177	-0.437235
C	-0.371439	3.560221	-1.062281
C	-1.647861	3.356985	-0.663827
N	-1.652819	2.246800	0.201067
C	1.821717	2.243777	-0.704886
C	2.017572	1.642933	-2.097695
C	0.172623	4.626241	-1.953825
C	-2.878802	4.096732	-1.069323
C	-2.742673	1.830803	1.086705
C	-2.959698	2.837094	2.217555
C	-4.026709	1.481661	0.334339
C	2.781474	3.396713	-0.418701
C	3.209214	1.296579	2.621885
C	1.226318	-2.579333	-2.755928
H	-5.632427	-2.816491	-1.503416
H	-5.056258	-2.801021	2.751207
H	-6.466083	-3.321207	0.764472
H	-0.283334	-0.329921	-1.319023
H	-1.691681	-0.849494	-3.289391
H	-3.904613	-1.917973	-2.982115
H	-2.387259	0.909197	1.548954
H	-3.798285	0.903268	-0.564277
H	-4.661097	0.866880	0.978926
H	-4.597087	2.369535	0.052554
H	-3.708659	2.451794	2.915327
H	-3.312724	3.802225	1.844019
H	-2.027910	2.998944	2.766236
H	-3.547306	3.470629	-1.668092
H	-3.449187	4.466312	-0.212697
H	-2.606728	4.962773	-1.674047
H	0.782367	5.344410	-1.396695
H	0.790908	4.220206	-2.758593
H	3.165565	1.568130	3.680624
H	-0.644816	5.178142	-2.419484
H	2.578726	3.835981	0.561662
H	2.722844	4.185154	-1.173003
H	3.809173	3.022069	-0.418329
H	2.418873	1.836873	2.098251
H	4.182317	1.614309	2.240308
H	1.329997	0.807625	-2.255154

H	1.861933	2.373561	-2.896280				
H	3.037796	1.256686	-2.184104				
H	3.893092	-0.782811	4.360982				
H	2.014841	1.448022	0.016308				
H	3.762764	-2.106184	3.188474				
H	1.986563	-0.423562	2.872537				
H	5.015214	-0.864455	3.000544				
H	5.888366	-0.155902	-0.538341				
H	5.716218	-0.035363	1.208869				
H	4.996830	1.191309	0.164306				
H	4.251916	-2.821022	-2.392231				
H	3.736372	-1.247669	-3.012945				
H	5.254802	-1.398648	-2.127568				
H	1.035294	-1.513873	-2.906343				
H	0.357317	-3.131560	-3.123413				
H	2.085494	-2.867322	-3.365786				
H	0.459316	-2.821348	-0.775326				
H	2.014223	-4.536019	0.019807				
H	2.957424	-4.446012	-1.481646				
H	1.292722	-5.045398	-1.518397				
H	-2.832155	-1.791564	2.466138				
3d (protonated form)				3d (dication)			
C	2.362708	1.861320	-1.132385	C	2.156275	2.107687	-0.678982
C	1.508437	2.123274	-0.026945	C	1.036857	2.494525	0.097980
C	1.872198	3.163963	0.875599	C	0.949911	3.847361	0.537378
C	3.060454	3.905347	0.644610	C	1.996194	4.752124	0.220021
C	3.860132	3.630531	-0.433802	C	3.078381	4.341080	-0.512514
C	3.504736	2.596165	-1.328593	C	3.150381	3.007379	-0.971000
C	1.044613	3.441098	1.996310	C	-0.182823	4.280340	1.273096
C	-0.098773	2.723819	2.223554	C	-1.214340	3.426960	1.571293
C	-0.472305	1.696464	1.329833	C	-1.147449	2.086347	1.157943
C	0.298325	1.397790	0.228367	C	-0.047856	1.622036	0.451529
P	-0.247010	0.056926	-0.867325	P	-0.076576	-0.107016	0.091869
N	-1.697249	-0.498117	-0.408036	N	-1.414018	-0.825925	-0.214195
C	-2.858342	0.121161	-0.577264	C	-2.625429	-0.358026	-0.628681
N	-3.983976	-0.583415	-0.193281	N	-3.722061	-0.957032	-0.078576
C	-5.231117	-0.059129	-0.318605	C	-4.969341	-0.594881	-0.458562
C	-5.445972	1.188085	-0.830704	C	-5.180486	0.376456	-1.405464
C	-4.330602	1.946003	-1.228714	C	-4.076285	0.998107	-1.989444
C	-3.069486	1.427908	-1.100010	C	-2.803818	0.628433	-1.603317
C	-3.759944	-1.937470	0.366112	C	-3.493337	-2.014347	0.948528
C	-5.016270	-2.686338	0.766775	C	-4.752324	-2.627803	1.526322
N	0.883463	-1.089607	-1.000261	N	1.285685	-0.821864	0.208620
C	1.322954	-1.830501	0.011261	C	1.649779	-2.130182	0.093904
C	0.737433	-1.961264	1.302450	C	0.783854	-3.225570	0.159048
C	1.297961	-2.766588	2.257058	C	1.281134	-4.511521	0.071063
C	2.467094	-3.492980	1.967783	C	2.652084	-4.709278	-0.083244
C	3.014340	-3.367740	0.723774	C	3.476232	-3.611053	-0.142670
N	2.470177	-2.563254	-0.227200	N	2.992151	-2.353065	-0.052815
C	3.089384	-2.413832	-1.565471	C	3.898405	-1.171502	-0.147235
C	4.344551	-3.234384	-1.792340	C	5.374956	-1.487602	-0.015157

H	3.324493	4.695473	1.341299	H	1.918125	5.778215	0.565025
H	4.143890	2.378692	-2.177952	H	3.999462	2.689462	-1.566491
H	4.766940	4.201394	-0.602857	H	3.874919	5.037021	-0.750918
H	-1.380785	1.134726	1.521485	H	-1.958499	1.419161	1.428770
H	-0.723731	2.938282	3.083182	H	-2.074905	3.769568	2.132627
H	1.338546	4.236083	2.675359	H	-0.223449	5.315299	1.598408
H	-0.180632	-1.421913	1.499491	H	-0.274818	-3.037222	0.276837
H	3.296010	-1.349085	-1.693487	H	3.580908	-0.483586	0.635668
H	2.321293	-2.674598	-2.295997	H	3.689784	-0.699411	-1.109760
H	4.685202	-3.031814	-2.809940	H	5.905169	-0.533156	-0.009301
H	4.160833	-4.309287	-1.715550	H	5.763024	-2.068600	-0.854685
H	5.154904	-2.956296	-1.113453	H	5.602296	-2.000270	0.922612
H	3.908311	-3.903183	0.442217	H	4.544160	-3.708277	-0.263438
H	2.933116	-4.143099	2.695433	H	3.082885	-5.698318	-0.157814
H	0.832879	-2.848467	3.233409	H	0.604993	-5.356770	0.120718
H	-4.464531	2.944231	-1.630686	H	-4.210609	1.764851	-2.743127
H	-6.455312	1.567048	-0.913081	H	-6.193527	0.635902	-1.680664
H	-2.205353	2.016715	-1.382970	H	-1.927894	1.081933	-2.048848
H	-6.047273	-0.684670	0.010071	H	-5.787655	-1.108362	0.022124
H	-3.199512	-2.495150	-0.386845	H	-2.879203	-2.776140	0.464972
H	-3.093548	-1.814632	1.222740	H	-2.894710	-1.555684	1.737059
H	-5.570032	-2.179627	1.561435	H	-5.368914	-1.895628	2.053055
H	-4.704970	-3.659112	1.153185	H	-4.435333	-3.375455	2.256017
H	-5.682817	-2.867304	-0.080474	H	-5.352547	-3.140494	0.771056
H	-0.299226	0.617148	-2.154462	H	2.226947	1.093976	-1.050194
H	2.124504	1.059086	-1.822167				
3d (neutral form)							
N	-0.172889	3.420355	0.299010				
C	-0.543934	2.179272	-0.243515				
C	-1.884539	2.138827	-0.787316				
C	-2.715224	3.215371	-0.739037				
C	-2.287435	4.433002	-0.147438				
C	-1.023044	4.483136	0.350934				
N	0.328911	1.222211	-0.189682				
P	0.107216	-0.303316	-0.933682				
N	1.454408	-1.168189	-0.366321				
C	2.675984	-0.835407	-0.656943				
C	3.142398	0.335891	-1.368808				
C	4.464783	0.566025	-1.591358				
C	5.447475	-0.345263	-1.122657				
C	5.016614	-1.449813	-0.457734				
N	3.695747	-1.704988	-0.238774				
C	3.325167	-2.903616	0.522787				
C	3.128441	-2.598494	2.002289				
C	1.165228	3.547448	0.888343				
C	1.210846	3.022959	2.317993				
C	-2.793920	-1.479865	-1.654484				
C	-2.429675	-1.510011	-0.277120				
C	-3.385198	-2.016611	0.655809				
C	-4.651732	-2.460806	0.187351				
C	-4.968697	-2.409047	-1.144366				

C	-4.025109	-1.912438	-2.074744				
C	-3.054753	-2.067103	2.033818				
C	-1.830745	-1.631517	2.472851				
C	-0.890472	-1.123382	1.551494				
C	-1.161232	-1.054404	0.202385				
H	2.393216	1.045379	-1.695508				
H	-3.788308	-2.456274	2.734548				
H	0.075055	-0.777411	1.908888				
H	-1.581348	-1.672346	3.528654				
H	-4.278801	-1.878351	-3.129589				
H	-5.939511	-2.749476	-1.489906				
H	-5.367733	-2.843315	0.909681				
H	4.770973	1.457834	-2.129577				
H	6.504851	-0.182011	-1.280727				
H	-3.715296	3.140740	-1.154841				
H	-2.930338	5.300788	-0.091087				
H	-2.217802	1.208580	-1.231737				
H	-0.618472	5.374700	0.815661				
H	1.852250	2.985427	0.254609				
H	1.440054	4.603745	0.850077				
H	0.935035	1.966626	2.337751				
H	0.524867	3.582842	2.960239				
H	2.222120	3.127557	2.719869				
H	5.700418	-2.193873	-0.066225				
H	4.117874	-3.640556	0.377942				
H	2.405410	-3.293581	0.087466				
H	2.847839	-3.510232	2.536140				
H	4.049296	-2.208382	2.445321				
H	2.332788	-1.861549	2.130137				
H	-2.073280	-1.107761	-2.375387				
3e (protonated form)				3e (dication)			
C	-2.741350	-1.384681	1.580674	C	-2.699601	-1.245703	1.373609
C	-2.317165	-1.951795	0.348068	C	-2.271277	-2.081572	0.314063
C	-3.228669	-2.788940	-0.357477	C	-3.175267	-3.054908	-0.195474
C	-4.519379	-3.028018	0.182924	C	-4.496567	-3.111417	0.317884
C	-4.899996	-2.458364	1.369735	C	-4.897733	-2.257656	1.312318
C	-3.997980	-1.628934	2.073810	C	-3.982277	-1.329235	1.855235
C	-1.031734	-1.704249	-0.234027	C	-0.958924	-2.036384	-0.259544
C	-0.697062	-2.269531	-1.443412	C	-0.550004	-2.966287	-1.202155
C	-1.606386	-3.099589	-2.136311	C	-1.449116	-3.943499	-1.665994
C	-2.841677	-3.352945	-1.602368	C	-2.735710	-3.966376	-1.191006
P	0.161981	-0.600074	0.566332	P	0.154051	-0.693261	0.013890
N	-0.432091	0.861645	0.832657	N	-0.349882	0.741724	0.139724
P	-1.330712	1.860929	-0.016458	P	-1.405005	1.938396	-0.181894
N	-0.411076	3.226378	-0.256626	N	-0.500688	3.305207	-0.194518
C	1.039966	3.190393	-0.368597	C	0.886333	3.358696	-0.643181
H	-2.075016	-0.733298	2.134107	H	-2.005861	-0.546087	1.822699
N	1.510131	-0.717616	-0.288302	N	1.624031	-1.140152	0.010520
P	3.021674	-0.493855	0.141370	P	3.113908	-0.482197	0.180269
N	3.805503	-1.957535	0.024877	N	4.125520	-1.712639	-0.193449
C	3.280959	-3.034247	-0.807226	C	3.837372	-3.113311	0.116012

N	3.634349	0.726019	-0.816975	N	3.296276	0.795831	-0.838621
C	5.029010	1.141472	-0.688395	C	4.201978	1.915530	-0.572948
N	3.385982	0.011647	1.681326	N	3.373427	0.097559	1.694941
C	3.339697	-0.924918	2.803607	C	4.069205	-0.701093	2.704339
C	3.096341	0.928445	-2.159382	C	2.958271	0.623728	-2.254117
N	-1.915056	1.402859	-1.505309	N	-2.208751	1.730551	-1.601383
C	-3.072332	0.529158	-1.683130	C	-3.037341	0.539435	-1.805678
N	-2.709076	2.193418	0.838286	N	-2.534613	2.009145	0.998524
C	-3.881602	2.858890	0.282816	C	-3.939439	2.355079	0.789892
C	-1.033425	1.433768	-2.666373	C	-1.664983	2.292671	-2.839571
C	-2.705415	2.144792	2.295261	C	-2.093079	2.052505	2.392582
C	-1.019106	4.432155	-0.802696	C	-1.157235	4.606714	-0.072588
C	3.171577	1.400107	2.086793	C	2.468458	1.108768	2.245548
C	5.242366	-2.048662	0.266838	C	5.512217	-1.439176	-0.568914
H	-5.203398	-3.667709	-0.366913	H	-5.180656	-3.851009	-0.085740
H	-3.549127	-3.986896	-2.128887	H	-3.440985	-4.701135	-1.566885
H	-4.302398	-1.181108	3.014207	H	-4.292548	-0.687272	2.673008
H	0.279438	-2.062017	-1.868601	H	0.454579	-2.926585	-1.608634
H	-0.237303	2.166599	-2.532015	H	-1.176021	3.246803	-2.647219
H	-1.813521	1.630933	2.651213	H	-1.068811	1.687396	2.487126
H	-0.579136	0.450095	-2.846863	H	-0.949970	1.609203	-3.312145
H	-2.730388	3.155141	2.721327	H	-2.138400	3.075472	2.780932
H	-3.588377	1.596904	2.642497	H	-2.743896	1.417148	3.000015
H	-3.583859	0.367923	-0.734640	H	-3.429313	0.173623	-0.855822
H	-3.772866	0.987362	-2.390199	H	-3.882855	0.803286	-2.445569
H	-2.763794	-0.444139	-2.078909	H	-2.466040	-0.263265	-2.287284
H	-4.781430	2.283159	0.527389	H	-4.577604	1.545805	1.159319
H	-3.993461	3.866109	0.703006	H	-4.179830	3.274124	1.334146
H	-3.808101	2.938882	-0.801371	H	-4.142121	2.515285	-0.267857
H	-2.066644	4.508023	-0.512832	H	-2.151755	4.495803	0.360648
H	-0.954470	4.465735	-1.898782	H	-1.250128	5.100294	-1.046369
H	-0.499641	5.306440	-0.399645	H	-0.563082	5.241363	0.590077
H	1.486294	3.944343	0.289372	H	1.466354	3.961572	0.062137
H	1.361238	3.401127	-1.397528	H	0.965884	3.811280	-1.638354
H	3.686971	-2.996517	-1.826561	H	4.099885	-3.726310	-0.750531
H	2.195167	-2.974506	-0.853157	H	2.776995	-3.241833	0.327865
H	3.560893	-3.993310	-0.360168	H	4.422110	-3.451624	0.978483
H	5.818319	-1.963378	-0.663239	H	5.779787	-2.069098	-1.421163
H	5.466684	-3.016977	0.725070	H	6.198401	-1.652497	0.257982
H	5.565380	-1.267803	0.956302	H	5.635202	-0.396575	-0.862358
H	5.378177	1.005156	0.335682	H	4.491969	1.930200	0.476347
H	5.686164	0.580573	-1.365016	H	5.103405	1.840312	-1.191190
H	5.105928	2.204898	-0.935046	H	3.695246	2.853961	-0.815356
H	3.619789	0.314453	-2.904205	H	3.854622	0.408180	-2.845629
H	4.169954	-0.713997	3.484901	H	4.607901	-0.023868	3.371389
H	3.218748	1.980979	-2.432929	H	2.500648	1.543393	-2.628430
H	2.400357	-0.825821	3.362183	H	3.366091	-1.298088	3.295561
H	2.035543	0.682083	-2.175176	H	2.247665	-0.192720	-2.388137
H	3.887738	1.651133	2.874574	H	3.042064	1.807036	2.860035
H	2.155714	1.554136	2.472743	H	1.692521	0.643731	2.864974
H	3.332394	2.073019	1.246009	H	1.986133	1.672408	1.445866

H	3.430498	-1.950110	2.446887	H	4.795504	-1.364464	2.236458
H	-5.890602	-2.641278	1.772191	H	-5.908784	-2.305954	1.700643
H	-1.318934	-3.529738	-3.089372	H	-1.121784	-4.656212	-2.413188
H	1.414643	2.209128	-0.084413	H	1.307253	2.353929	-0.674280
H	-1.609854	1.716728	-3.552438	H	-2.493021	2.469303	-3.529597
H	0.351659	-1.131002	1.854268				
3e (neutral form)							
C	-4.078555	-3.746311	0.033897				
C	-2.844426	-3.213375	0.493142				
C	-2.159300	-2.245359	-0.298840				
C	-2.758853	-1.842944	-1.525706				
C	-3.954320	-2.372729	-1.942290				
C	-4.623911	-3.338215	-1.155949				
C	-2.285169	-3.622117	1.733888				
C	-1.098556	-3.091225	2.163240				
C	-0.419455	-2.131072	1.375730				
C	-0.919996	-1.694635	0.171331				
P	0.048518	-0.497669	-0.889897				
N	-0.955708	0.847136	-0.952065				
P	-1.328866	2.066531	-0.049373				
N	-0.195267	3.249508	0.312779				
C	0.179853	4.248519	-0.677853				
H	-2.266527	-1.085128	-2.125023				
N	1.310504	-0.127102	0.176080				
P	2.813715	-0.463151	-0.126523				
N	3.657319	-0.271989	1.309441				
C	5.107809	-0.381549	1.328984				
N	3.434165	0.444206	-1.399393				
C	4.801456	0.302480	-1.880664				
N	3.289400	-2.014323	-0.585038				
C	3.143586	-3.079478	0.403101				
C	2.842163	1.733822	-1.720647				
N	-2.489803	2.943756	-0.903741				
C	-3.325893	2.263196	-1.882338				
N	-1.891909	1.671652	1.494362				
C	-2.891143	0.612237	1.571332				
C	-3.190288	4.004401	-0.192408				
C	-2.025062	2.628024	2.586103				
C	0.866804	2.973866	1.271441				
C	2.991532	-2.482484	-1.935907				
C	3.107125	0.495622	2.413913				
H	-2.814246	-4.360214	2.330636				
H	-4.587113	-4.484635	0.648303				
H	0.518651	-1.709200	1.724830				
H	-4.392117	-2.047622	-2.881068				
H	2.020348	0.456080	2.372018				
H	3.416839	-2.713279	1.392726				
H	3.448206	0.058950	3.359693				
H	2.113411	-3.462512	0.441611				
H	3.809831	-3.906748	0.137924				

H	5.445352	-1.090839	0.572079				
H	5.602215	0.585017	1.156869				
H	5.427189	-0.757175	2.307172				
H	3.719964	-3.250228	-2.218443				
H	1.984838	-2.918580	-2.001942				
H	3.055102	-1.659859	-2.647483				
H	5.176000	-0.700597	-1.676224				
H	5.477420	1.033978	-1.416773				
H	4.822736	0.459487	-2.965218				
H	2.883331	1.893378	-2.804152				
H	3.376552	2.563886	-1.234805				
H	1.794689	2.679659	0.767965				
H	0.580569	2.156916	1.931561				
H	1.059485	3.869904	1.874206				
H	1.074124	3.950914	-1.241804				
H	0.400691	5.194650	-0.170394				
H	-0.638783	4.409634	-1.378419				
H	-2.505246	4.534797	0.471694				
H	-3.586078	4.724777	-0.915722				
H	-4.032193	3.621934	0.404301				
H	-3.692607	2.994314	-2.611331				
H	-3.055659	3.001185	2.669019				
H	-4.198424	1.778256	-1.418091				
H	-1.764765	2.141908	3.533889				
H	-2.737648	1.504379	-2.395685				
H	-3.901581	1.032761	1.680816				
H	-2.693203	-0.039408	2.430213				
H	-2.865223	-0.000536	0.672480				
H	-1.364736	3.481436	2.441362				
H	-0.672732	-3.402610	3.112744				
H	-5.568910	-3.750666	-1.495227				
H	1.798543	1.754590	-1.406669				
H	3.427873	1.547413	2.389263				
3f (protonated form)				3f (dication)			
C	3.022635	-2.641337	-1.398212	C	2.375731	1.554490	-2.081226
N	3.073887	-1.166086	-1.501563	N	2.767406	1.248321	-0.684490
C	4.086609	-0.744437	-2.489942	C	3.591094	2.341216	-0.106707
C	4.948431	-1.990471	-2.680879	C	3.947867	3.199735	-1.318615
C	3.931749	-3.124686	-2.532408	C	2.731487	3.034082	-2.231719
P	2.600697	-0.265057	-0.197155	P	2.874062	-0.306129	-0.180886
N	1.138704	-0.673462	0.285881	N	1.587840	-1.190823	-0.684541
P	-0.163809	-0.957649	-0.606470	P	0.062365	-0.995166	-0.615068
N	-1.193460	0.233168	-0.900356	N	-0.662551	0.352001	-0.611973
P	-1.797695	1.412261	-0.020048	P	-1.806372	1.242558	0.134394
N	-1.263945	1.635024	1.531460	N	-2.871649	0.405804	1.038491
C	-1.708411	0.689217	2.581158	C	-4.321999	0.301544	0.759917
C	-0.493506	0.562691	3.502737	C	-4.727500	-0.953087	1.529420
C	0.202823	1.914841	3.347465	C	-3.791928	-0.939623	2.740044
C	0.064437	2.189308	1.851890	C	-2.459600	-0.484378	2.144293
N	3.601019	-0.521367	1.081224	N	4.146246	-1.131774	-0.772432
C	5.061924	-0.604466	0.927009	C	5.514481	-0.578245	-0.695297

C	5.579560	-0.307886	2.335349	C	6.401963	-1.803177	-0.927322
C	4.474543	-0.871086	3.233392	C	5.542983	-2.694174	-1.827694
C	3.191892	-0.487751	2.492699	C	4.138932	-2.532072	-1.246790
N	2.823551	1.298205	-0.686079	N	2.987798	-0.209687	1.450021
C	2.047416	1.874339	-1.797939	C	2.016529	0.568627	2.253976
C	1.924069	3.350921	-1.423112	C	1.669906	-0.369269	3.407684
C	3.217350	3.620424	-0.651222	C	2.986199	-1.114819	3.637838
C	3.411052	2.344320	0.171442	C	3.497097	-1.373295	2.218587
C	-0.999929	-2.373616	0.162051	C	-0.822306	-2.514107	-0.486592
C	-2.085167	-3.045239	-0.490237	C	-2.193670	-2.670821	-0.886883
C	-2.721411	-4.122879	0.190961	C	-2.852455	-3.872903	-0.499501
C	-2.271970	-4.495828	1.485916	C	-2.143152	-4.861687	0.230199
C	-1.227863	-3.842398	2.083213	C	-0.819444	-4.703690	0.553963
C	-0.584366	-2.780901	1.409251	C	-0.152075	-3.521477	0.194370
C	-3.799713	-4.804341	-0.432633	C	-4.206150	-4.079099	-0.871309
C	-4.232946	-4.439252	-1.680272	C	-4.877420	-3.145475	-1.617543
C	-3.604852	-3.370394	-2.359071	C	-4.213024	-1.971627	-2.033536
C	-2.562009	-2.691346	-1.782249	C	-2.907590	-1.739364	-1.678441
H	-2.118983	-1.855406	-2.311712	H	-2.417787	-0.838975	-2.023452
N	-1.459835	2.856673	-0.753088	N	-0.999161	2.248358	1.146365
C	-1.607239	2.947871	-2.222357	C	0.018483	3.157858	0.576088
C	-1.667113	4.452513	-2.492014	C	0.399788	4.047567	1.758095
C	-2.331325	5.007285	-1.230635	C	-0.901878	4.131267	2.559907
C	-1.678870	4.177441	-0.127396	C	-1.443541	2.704279	2.480764
N	-3.429340	1.163055	0.077464	N	-2.588127	2.017766	-1.072802
C	-4.329122	2.180756	0.644900	C	-3.430120	3.195425	-0.768102
C	-5.693228	1.487917	0.656394	C	-3.195170	4.115893	-1.964084
C	-5.329001	0.019159	0.880531	C	-3.002615	3.127340	-3.115324
C	-4.075607	-0.161245	0.024811	C	-2.166946	2.005867	-2.493872
H	-3.955267	-3.081178	-3.344428	H	-4.736196	-1.244405	-2.645238
H	0.256591	-2.275224	1.872237	H	0.887514	-3.387908	0.471718
H	-5.058012	-4.964973	-2.149124	H	-5.910899	-3.309765	-1.900641
H	-0.885375	-4.135870	3.069521	H	-0.285911	-5.473644	1.097730
H	-4.275988	-5.622273	0.100041	H	-4.696300	-4.996252	-0.560983
H	-2.771797	-5.315380	1.994117	H	-2.669637	-5.765487	0.520854
H	0.843724	1.665015	1.289490	H	-1.899488	-1.342982	1.754160
H	0.112100	3.254342	1.615220	H	-1.828366	0.037407	2.867298
H	1.246267	1.905815	3.670129	H	-3.704129	-1.910865	3.229364
H	-0.323993	2.684248	3.921328	H	-4.137122	-0.209825	3.478788
H	-0.777114	0.331192	4.531008	H	-5.783839	-0.937586	1.802538
H	0.162923	-0.231486	3.133632	H	-4.542082	-1.840641	0.916667
H	-1.997038	-0.281663	2.164754	H	-4.510266	0.224847	-0.311903
H	-2.576396	1.100485	3.109278	H	-4.838211	1.186772	1.147493
H	-0.713333	4.619211	0.150662	H	-0.988069	2.077271	3.256225
H	-2.171295	6.078129	-1.090622	H	-0.753418	4.454534	3.591442
H	-2.281423	4.100290	0.779635	H	-2.529110	2.643751	2.581108
H	-3.421651	-0.945373	0.410051	H	-2.367431	1.039115	-2.960111
H	-4.327961	-0.421365	-1.009397	H	-1.095204	2.214155	-2.577875
H	-3.410790	4.822166	-1.259088	H	-1.598023	4.825412	2.077550
H	-6.124535	-0.672936	0.597315	H	-2.503967	3.564922	-3.981539
H	-5.085796	-0.149856	1.935097	H	-3.971544	2.735304	-3.438986

H	-6.353480	1.895191	1.424348	H	-4.026931	4.804289	-2.121630
H	-6.181523	1.610655	-0.315690	H	-2.284569	4.704048	-1.810736
H	-4.331749	3.085949	0.030508	H	-3.134861	3.650603	0.182369
H	-4.019354	2.458091	1.661984	H	-4.481142	2.896378	-0.694968
H	-2.533952	2.458322	-2.548101	H	-0.417426	3.754401	-0.236073
H	-2.213676	4.680900	-3.408779	H	0.773497	5.019319	1.432075
H	-0.653949	4.856615	-2.588661	H	1.178573	3.564538	2.357806
H	-0.770092	2.460137	-2.726521	H	0.853489	2.583347	0.168412
H	5.462310	-1.995934	-3.644164	H	4.139227	4.237189	-1.039632
H	5.702081	-2.049082	-1.888212	H	4.843721	2.803098	-1.807047
H	4.646725	0.122751	-2.135029	H	4.465907	1.952304	0.416959
H	3.592552	-0.466003	-3.428624	H	2.993285	2.907728	0.615983
H	5.353892	-1.610476	0.599023	H	5.657049	0.176432	-1.477047
H	6.557995	-0.755467	2.518631	H	7.360660	-1.533027	-1.372653
H	5.663803	0.774619	2.478336	H	6.594503	-2.306219	0.025439
H	4.558298	-1.960944	3.293348	H	5.564636	-2.324338	-2.857531
H	4.497316	-0.469644	4.248126	H	5.863226	-3.737382	-1.829677
H	2.369759	-1.183002	2.674309	H	3.348393	-2.684208	-1.982061
H	2.859818	0.518007	2.781640	H	3.975964	-3.221872	-0.410259
H	3.401705	-2.967701	-0.421198	H	2.946609	0.938591	-2.786118
H	4.387266	-4.090176	-2.305003	H	2.932983	3.296723	-3.271267
H	2.888401	2.419932	1.132981	H	3.084231	-2.310516	1.827232
H	1.066681	1.395243	-1.885337	H	1.140097	0.854634	1.665174
H	3.165565	4.508132	-0.018027	H	2.866470	-2.043133	4.198349
H	1.054176	3.484075	-0.773211	H	0.886379	-1.069067	3.096671
H	1.801080	3.991993	-2.298707	H	1.318156	0.173157	4.286992
H	4.052796	3.744441	-1.347683	H	3.690225	-0.475335	4.178860
H	2.582641	1.743127	-2.746235	H	2.496383	1.484536	2.616003
H	4.465240	2.141635	0.377735	H	4.586596	-1.424467	2.159275
H	5.435340	0.111324	0.187228	H	5.701295	-0.111449	0.276983
H	1.998697	-3.012276	-1.501508	H	1.309995	1.361826	-2.226544
H	0.208792	-1.414376	-1.884197	H	1.903664	3.657197	-1.878116
H	3.352977	-3.230449	-3.455503				
3f (neutral form)							
C	3.531949	-0.396154	-1.806061				
N	2.953414	-1.541381	-1.074102				
C	3.835361	-2.714973	-1.103179				
C	4.792539	-2.393878	-2.251710				
C	4.944116	-0.873919	-2.151203				
P	1.681832	-1.391968	-0.036083				
N	0.910172	-2.830363	0.177737				
C	-0.073771	-3.303317	-0.814929				
C	-0.466417	-4.680738	-0.289469				
C	0.842765	-5.187872	0.320656				
C	1.395879	-3.943363	1.017067				
N	0.657057	-0.379863	-0.685741				
P	0.030559	1.071766	-0.625174				
C	1.024497	2.259787	0.310783				
C	1.862960	3.098624	-0.476291				
C	2.769327	3.981518	0.164292				
C	2.782127	4.028374	1.583108				

C	1.915809	3.259266	2.319661
C	1.027694	2.365073	1.678700
C	3.597176	4.805434	-0.641883
C	3.508652	4.762015	-2.010980
C	2.572128	3.913269	-2.644217
C	1.753861	3.102112	-1.896995
N	-1.478713	1.235724	-0.150775
P	-2.785231	0.333475	-0.178535
N	-2.754700	-0.804330	-1.377731
C	-2.160940	-0.472814	-2.692125
C	-2.896086	-1.380709	-3.679731
C	-3.341657	-2.562053	-2.816342
C	-3.746721	-1.888127	-1.507976
N	2.306569	-1.043105	1.455266
C	3.557330	-0.288457	1.635405
C	3.769827	-0.357275	3.144919
C	2.345637	-0.249767	3.699304
C	1.486418	-1.013003	2.679976
N	-4.038471	1.397358	-0.300906
C	-5.448245	0.976747	-0.269551
C	-6.163164	2.188267	0.327457
C	-5.341751	3.360792	-0.214669
C	-3.898061	2.855877	-0.133085
N	-3.079552	-0.577893	1.179516
C	-2.149526	-1.683159	1.505457
C	-2.190302	-1.784241	3.031766
C	-2.489308	-0.350236	3.469283
C	-3.500236	0.111110	2.421063
H	0.979987	-3.857929	2.027724
H	0.346199	1.763962	2.272897
H	2.500505	3.916101	-3.726557
H	1.913039	3.329098	3.402120
H	4.149404	5.393191	-2.617298
H	3.474091	4.701923	2.079130
H	4.298641	5.478403	-0.158508
H	4.427107	0.436446	3.505039
H	4.212938	-1.321951	3.410833
H	4.369653	-0.748447	1.068157
H	3.451490	0.755471	1.308034
H	2.244960	-0.664575	4.703699
H	2.042976	0.799508	3.738986
H	0.521478	-0.521427	2.509494
H	1.282413	-2.033084	3.018837
H	4.387070	-2.833112	-0.158974
H	5.637070	-0.621768	-1.341398
H	5.318103	-0.415623	-3.068853
H	3.256912	-3.627205	-1.277988
H	4.331233	-2.666741	-3.206705
H	5.738933	-2.930351	-2.162937
H	2.936443	-0.180809	-2.697637
H	2.485047	-3.948909	1.100278

H	3.547700	0.512416	-1.194073
H	0.708606	-6.020187	1.014071
H	1.524886	-5.509492	-0.474088
H	-0.856182	-5.324261	-1.080684
H	0.392156	-3.400043	-1.801463
H	-1.233055	-4.587638	0.487462
H	-0.906642	-2.600104	-0.894368
H	-2.284630	0.587676	-2.933829
H	-3.770095	-0.865261	-4.090945
H	-2.250021	-1.673028	-4.508701
H	-4.160205	-3.135283	-3.255345
H	-2.502511	-3.244075	-2.638960
H	-4.768185	-1.493974	-1.582119
H	-3.703801	-2.562910	-0.651220
H	-3.249419	3.278871	-0.903449
H	-2.464055	-2.613236	1.024417
H	-1.136004	-1.456059	1.156040
H	-1.255860	-2.179035	3.436632
H	-3.001790	-2.448339	3.345587
H	-3.509594	1.196011	2.294941
H	-4.515838	-0.203980	2.688221
H	-2.879420	-0.278762	4.486413
H	-1.583807	0.264187	3.405253
H	-5.576439	0.069956	0.328976
H	-5.485722	4.283652	0.351101
H	-5.809466	0.771224	-1.285315
H	-5.618802	3.557547	-1.256275
H	-7.216915	2.230674	0.045702
H	-6.098674	2.155472	1.420202
H	-3.454801	3.097792	0.841473
H	0.988829	2.417104	-2.197646
H	-1.112951	-0.686452	-2.723372
TS2(2a)			
C	0.602109	4.696222	1.354116
C	0.425461	3.511103	2.114216
C	0.256144	2.274421	1.435370
C	0.279520	2.245557	0.002729
C	0.436124	3.424449	-0.691643
C	0.601800	4.653531	-0.015122
C	0.054831	1.093727	2.203871
C	0.038255	1.139310	3.577720
C	0.216932	2.367793	4.248533
C	0.405205	3.523842	3.532456
P	-0.124050	-0.394079	1.210746
N	1.002413	-1.535295	1.549631
C	2.308467	-1.442981	1.524402
C	3.091808	-0.153461	1.462946
P	0.041648	0.626554	-0.868888
N	-1.409591	0.111148	-1.446733
C	-2.637705	0.401896	-1.129559
C	-3.050463	1.485666	-0.164730

N	1.235340	-0.424297	-1.294509
C	2.436038	-0.210653	-1.761386
C	3.066706	1.146304	-1.945587
N	3.190910	-1.280407	-2.070619
C	4.520420	-1.168405	-2.658740
C	2.697669	-2.632059	-1.846816
N	-1.615828	-0.974779	1.572590
C	-2.177888	-1.992669	0.961536
C	-1.493528	-2.868926	-0.060406
N	-3.446967	-2.306407	1.271545
C	-4.160844	-3.414312	0.649520
C	-4.227270	-1.501332	2.200620
N	3.024301	-2.577548	1.593822
C	2.363718	-3.874956	1.567963
C	4.478676	-2.600293	1.693648
N	-3.634443	-0.318278	-1.692978
C	-3.362541	-1.271216	-2.758960
C	-5.042530	-0.021498	-1.470183
C	0.042693	1.642047	-3.655149
O	-0.760312	2.531708	-3.738519
O	0.749849	0.857062	-4.224496
H	0.420356	3.423360	-1.775417
H	0.726866	5.562824	-0.592182
H	0.731061	5.639361	1.876242
H	-0.114707	0.230043	4.150601
H	0.202296	2.393703	5.332458
H	0.539498	4.470955	4.046115
H	-5.230635	0.270520	-0.437960
H	-5.619450	-0.925967	-1.669871
H	-2.291880	-1.447416	-2.824140
H	-3.878299	-2.213616	-2.553393
H	4.578245	-0.336332	-3.359711
H	5.291143	-1.046713	-1.889908
H	2.311000	-3.064647	-2.775263
H	3.519052	-3.253629	-1.482211
H	1.899893	-2.608986	-1.107119
H	-5.400468	0.770530	-2.137829
H	-3.723890	-0.880199	-3.716235
H	4.852658	-1.765845	2.285129
H	2.981451	-4.573344	0.999722
H	2.227425	-4.263381	2.582418
H	-4.999122	-3.685095	1.291507
H	-4.557206	-3.132980	-0.332541
H	-3.524511	-4.292310	0.542060
H	-3.630058	-0.659344	2.540330
H	-5.131917	-1.138918	1.702627
H	-4.522802	-2.106927	3.062329
H	4.774477	-3.521267	2.196706
H	1.389304	-3.778256	1.093521
H	4.100260	1.159335	-1.595291
H	3.053643	1.411695	-3.006298

H	2.512031	1.906275	-1.399963				
H	-3.450216	1.040120	0.749971				
H	-2.198695	2.104820	0.104935				
H	-3.815244	2.130701	-0.601897				
H	3.469668	0.101203	2.457864				
H	3.944110	-0.235183	0.786066				
H	2.465785	0.670294	1.128477				
H	4.946179	-2.578717	0.702926				
H	-0.593852	-2.390222	-0.443709				
H	-1.206364	-3.818174	0.402526				
H	-2.150008	-3.086081	-0.903582				
H	4.727035	-2.083422	-3.214454				
H	0.253825	1.426342	-2.246737				
	TS1(2b)				TS2(2b)		
C	-1.688584	-0.997842	4.579628	C	0.124800	-0.646100	5.054300
C	-0.391736	-0.968213	4.004185	C	-0.898500	-0.312500	4.131500
C	-0.246543	-0.563206	2.645673	C	-0.565200	-0.204000	2.752900
C	-1.415234	-0.157555	1.936386	C	0.762600	-0.449700	2.300300
C	-2.655342	-0.181357	2.526260	C	1.723800	-0.750000	3.238500
C	-2.796097	-0.619919	3.861030	C	1.407500	-0.852500	4.613300
C	1.042323	-0.547729	2.026557	C	-1.587900	0.156800	1.828500
C	2.136351	-0.865341	2.803275	C	-2.878700	0.374300	2.244800
C	2.001005	-1.257568	4.155640	C	-3.209600	0.242200	3.612400
C	0.765148	-1.322631	4.743174	C	-2.242700	-0.088100	4.529900
P	1.246536	-0.155914	0.163507	P	-1.020600	0.260000	0.120800
N	2.855367	0.362302	0.325672	N	-1.098300	1.802000	-0.330200
C	3.242982	1.554828	-0.022650	C	-1.788300	2.540500	-1.171100
N	2.517282	2.697661	0.221165	N	-2.293900	3.726100	-0.733800
C	2.462120	3.814318	-0.703221	C	-2.456300	3.961200	0.690900
P	-1.058242	0.320992	0.242576	P	1.151400	-0.316200	0.447500
N	-1.997404	-0.430355	-0.864802	N	1.208800	-1.944500	0.181200
C	-2.887296	-1.387754	-0.779790	C	1.994800	-2.639300	-0.604900
N	-3.907176	-1.388896	-1.687925	N	3.355200	-2.474800	-0.649800
C	-4.180937	-0.187495	-2.453263	C	4.132300	-2.666900	-1.861400
N	-1.260280	1.941732	0.202596	N	2.524100	0.602300	0.628200
C	-1.757919	2.813087	-0.632223	C	2.751800	1.862600	0.388700
N	-1.854718	2.679229	-1.988344	N	3.968700	2.255200	-0.083300
C	-2.936142	3.278222	-2.755187	C	4.560600	3.538400	0.258100
N	-2.219726	3.996462	-0.115925	N	1.846400	2.870800	0.628500
C	-1.952683	5.270066	-0.772369	C	1.056500	2.889900	1.845000
C	-2.460334	4.086470	1.313086	C	1.636200	3.965100	-0.296600
N	1.066611	-1.662616	-0.484657	N	-1.770300	-0.780600	-0.877700
C	1.787355	-2.379750	-1.300587	C	-2.721800	-1.671800	-0.662400
N	1.167805	-3.024637	-2.337987	N	-2.894400	-2.414400	0.468400
C	-0.143236	-2.581623	-2.776772	C	-4.218200	-2.735200	0.978500
N	3.131529	-2.608130	-1.172455	N	-3.621500	-1.887000	-1.656800
C	3.764764	-2.629372	0.132914	C	-4.176300	-3.204100	-1.937100
C	4.008497	-2.860453	-2.302107	C	-3.796000	-0.898000	-2.703100
N	4.428726	1.734728	-0.684638	N	-1.975700	2.232500	-2.481300
C	5.059118	0.596511	-1.321118	C	-1.009200	1.400200	-3.179100
C	5.308163	2.859526	-0.409304	C	-3.137000	2.667500	-3.244400

C	1.735268	2.846511	1.437039	C	-2.290300	4.928200	-1.559300
N	-2.908246	-2.404642	0.135740	N	1.476100	-3.629900	-1.376400
C	-1.705259	-3.013343	0.670707	C	2.173900	-4.880600	-1.625500
C	-4.150285	-2.905671	0.699470	C	0.075500	-3.608100	-1.752000
C	-4.447417	-2.619481	-2.247728	C	4.108800	-2.173300	0.554900
C	-0.949308	1.840877	-2.750282	C	4.877800	1.291200	-0.668300
C	1.513195	-4.385989	-2.722376	C	-1.797500	-2.918200	1.274400
H	-3.532855	0.128950	1.964959	O	2.436800	1.058000	-2.657700
H	-3.779463	-0.646886	4.317424	C	1.860400	0.020200	-2.656100
H	-1.791868	-1.322739	5.611272	O	1.458800	-0.989600	-3.132200
H	3.124750	-0.810733	2.363831	H	-3.652300	0.637900	1.528700
H	2.889837	-1.512483	4.724719	H	-4.232400	0.407900	3.933400
H	0.655807	-1.632235	5.778815	H	-2.497600	-0.182300	5.581700
H	-3.900817	-3.480172	-1.863854	H	2.752400	-0.897300	2.925300
H	-5.510095	-2.737502	-2.013152	H	2.192000	-1.098200	5.322200
H	-4.332124	-2.599236	-3.336368	H	-0.120800	-0.729500	6.108900
H	-3.927915	0.689446	-1.858884	H	-3.681400	-3.958100	-1.326000
H	-5.243550	-0.164843	-2.707321	H	-5.254300	-3.240000	-1.750400
H	-3.597802	-0.159586	-3.383026	H	-3.996900	-3.443900	-2.989500
H	-4.987567	-2.286961	0.379399	H	-3.577400	0.090300	-2.302600
H	-4.080685	-2.856579	1.792336	H	-4.832300	-0.930100	-3.049300
H	-0.814959	-2.581681	0.209100	H	-3.133700	-1.090200	-3.555700
H	-1.649695	-2.878898	1.756719	H	-4.979200	-2.177100	0.434600
H	-3.704536	3.659634	-2.083769	H	-4.259000	-2.438800	2.032400
H	-2.583096	4.094822	-3.396162	H	-0.833900	-2.625900	0.854000
H	-1.385232	0.860953	-2.963194	H	-1.872200	-2.546400	2.301300
H	-0.021480	1.693978	-2.193723	H	-3.919400	3.012200	-2.568600
H	-0.709794	2.350841	-3.688365	H	-2.893900	3.466700	-3.952300
H	-2.878429	5.808399	-0.997849	H	-1.227500	0.334900	-3.073700
H	-1.338327	5.894386	-0.114073	H	-0.017700	1.603600	-2.775100
H	-1.399835	5.111541	-1.697344	H	-1.015000	1.676900	-4.235500
H	-2.863377	3.144400	1.682156	H	-3.303800	5.257000	-1.808800
H	-1.539752	4.311514	1.867473	H	-1.791200	5.729700	-1.006400
H	-3.183531	4.885903	1.493805	H	-1.731900	4.754500	-2.478400
H	-4.342761	-3.945706	0.411631	H	-2.600400	3.016500	1.212300
H	-3.382294	2.511659	-3.396800	H	-1.579300	4.466000	1.113600
H	-1.725595	-4.089991	0.458253	H	-3.333200	4.595600	0.844500
H	0.658239	2.810404	1.237341	H	-4.438600	-3.806300	0.909700
H	1.993564	2.052520	2.138023	H	-3.522500	1.816600	-3.812700
H	1.976923	3.810898	1.900500	H	-1.850400	-4.013500	1.299800
H	1.412208	4.060602	-0.901425	H	-0.003300	2.716800	1.639800
H	2.936159	3.541186	-1.645287	H	1.419300	2.124100	2.530400
H	2.953149	4.710767	-0.303244	H	1.168100	3.868300	2.328800
H	5.497179	3.451396	-1.311615	H	0.565200	4.040000	-0.517300
H	6.268370	2.491473	-0.029682	H	2.165100	3.766200	-1.229100
H	5.627282	0.941160	-2.189732	H	1.975300	4.927700	0.108300
H	5.746225	0.075103	-0.641192	H	4.648600	4.188500	-0.619300
H	-0.285039	-1.530117	-2.534344	H	5.562500	3.375200	0.668400
H	-0.225203	-2.731641	-3.857287	H	5.433800	1.768900	-1.480200
H	1.900298	-4.436461	-3.745739	H	5.596400	0.918200	0.072900
H	0.616617	-5.012127	-2.661099	H	-0.293200	-2.584200	-1.729700

N	0.510834	1.236190	-0.602957	N	2.190411	1.308672	0.853804
C	1.486242	1.798228	-1.307414	C	3.489696	1.247136	0.585335
N	1.904063	1.526770	-2.579623	N	4.453944	0.467602	1.162560
C	2.927740	2.408789	-2.937478	C	5.698060	0.776097	0.599758
C	3.128178	3.241648	-1.884351	C	5.496257	1.759674	-0.310045
N	2.241262	2.853403	-0.880318	N	4.127118	2.044127	-0.318172
C	1.214521	0.558502	-3.443639	C	6.952732	0.025705	0.897648
C	0.442224	1.257011	-4.563284	C	4.228573	-0.233169	2.434643
C	3.678969	2.350288	-4.225627	C	4.890283	0.504575	3.599217
C	4.122509	4.344174	-1.736440	C	3.449461	3.183274	-0.952029
C	1.997688	3.483256	0.420953	C	3.778777	4.460363	-0.177358
C	1.174358	4.758875	0.260228	C	6.485412	2.392306	-1.230110
C	2.133290	-0.547226	-3.949891	N	1.870596	-1.327991	0.376169
C	3.270622	3.699689	1.237851	C	1.782530	-2.325940	-0.474777
C	5.565128	-0.556009	-2.275831	N	1.100279	-3.490366	-0.295883
C	1.295333	-4.020772	2.108854	C	1.463041	-4.393010	-1.301041
N	-2.506279	0.491211	1.194671	C	2.339159	-3.755034	-2.118992
C	-2.448391	1.770252	0.874376	N	2.521701	-2.467062	-1.610061
N	-2.093331	2.788000	1.706030	C	0.268105	-3.704571	0.901158
C	-2.266194	4.005487	1.044805	C	1.106385	-4.317103	2.019989
C	-2.739392	3.724769	-0.198127	C	0.923978	-5.778185	-1.420236
N	-2.874778	2.338357	-0.286536	C	2.986554	-4.254862	-3.366200
C	-1.688504	2.532375	3.096531	C	3.486100	-1.439787	-2.034623
C	-0.196501	2.763097	3.318398	C	3.429758	-1.145853	-3.532908
C	-2.017882	5.340292	1.663526	C	-1.008430	-4.496018	0.624738
C	-3.088446	4.672883	-1.295657	C	4.894140	-1.792349	-1.562411
C	-3.383835	1.519629	-1.395797	C	4.568855	-1.717325	2.376305
C	-4.757492	1.972094	-1.883867	C	3.729016	3.298978	-2.448060
C	-2.567169	3.283299	4.095311	C	-1.378394	-2.895787	-2.794098
C	-2.362795	1.391197	-2.519436	C	-2.678460	-2.507583	3.228577
C	-5.698180	-2.759272	1.539537	C	-4.925888	0.909823	-0.444959
C	-1.869564	-4.562402	-2.480029	C	0.282260	4.942367	-1.686437
H	0.756073	-1.267589	6.183389	H	-0.996344	0.081095	6.097345
H	-2.491098	-2.089905	3.493712	H	1.850107	-1.602070	3.362639
H	-1.470425	-2.233672	5.760843	H	0.869466	-1.469466	5.638836
H	3.132866	0.742316	1.146641	H	-2.955740	2.527768	1.101268
H	4.028672	0.910348	3.443247	H	-3.724422	2.894327	3.359073
H	2.780810	-0.065687	5.344109	H	-2.698583	1.703557	5.269947
H	0.835727	-2.680029	0.549892	H	0.204901	3.192673	-0.466491
H	1.634248	-3.304713	2.861810	H	-0.481327	4.316331	1.667719
H	0.218389	-4.158544	2.236114	H	1.108351	4.789411	1.047989
H	1.779317	-4.982841	2.286934	H	-0.253911	5.897293	0.879841
H	0.266238	-4.895488	-0.307353	H	1.352488	5.117678	-1.562371
H	1.975467	-5.363113	-0.332248	H	-0.198649	5.916202	-1.807587
H	1.399056	-4.051922	-1.382538	H	0.132102	4.362957	-2.601028
H	4.048457	-4.612943	2.591406	H	-2.499578	6.300187	0.811663
H	3.745756	-5.529426	1.110260	H	-1.914179	6.726389	-0.800868
H	5.378203	-4.997064	1.499346	H	-3.641512	6.691014	-0.476904
H	7.007712	-2.529476	-0.643914	H	-5.618722	4.569155	-2.166243
H	6.991790	-2.006518	1.044017	H	-5.974432	3.801913	-0.611518
H	1.533858	-1.282596	-4.493831	H	-2.745826	-0.965158	-4.421474

H	6.837568	-3.715920	0.644786	H	-5.406066	5.465709	-0.661063
H	4.877191	-1.090169	-2.934932	H	-4.653089	2.339132	-3.620364
H	6.487891	-1.136630	-2.192753	H	-6.049794	2.371598	-2.520338
H	5.817739	0.400683	-2.742915	H	-5.515953	0.847803	-3.212202
H	2.606556	-1.038703	-3.098223	H	-4.165694	-0.890506	-3.367138
H	2.895357	-0.174477	-4.637799	H	-3.700296	-2.420475	-4.129736
H	5.423419	0.544737	1.030093	H	-4.211016	0.706447	0.355672
H	6.839289	0.023899	0.098652	H	-5.713716	1.558273	-0.049911
H	5.978672	1.494181	-0.361456	H	-5.379731	-0.040714	-0.742800
H	-0.258653	0.546645	-5.011651	H	-0.852368	-2.660546	-3.721997
H	4.023798	0.303487	-1.082450	H	-3.450826	0.843664	-1.983414
H	-0.128959	2.101890	-4.172549	H	-0.639033	-2.957519	-1.994422
H	0.487217	0.093910	-2.777437	H	-1.832262	-0.882931	-2.288852
H	1.097658	1.618517	-5.359305	H	-1.864849	-3.870459	-2.906265
H	4.331376	3.220107	-4.310519	H	-5.602442	-4.377670	-1.629792
H	3.020235	2.349878	-5.096272	H	-4.216979	-4.224223	-2.707836
H	4.311171	1.459471	-4.283198	H	-5.497821	-3.004526	-2.728676
H	3.658977	5.267087	-1.378933	H	-5.079050	-4.088028	2.003445
H	4.923325	4.079684	-1.039875	H	-6.336938	-3.012088	1.381041
H	4.581298	4.562003	-2.701494	H	-5.889179	-4.463435	0.485044
H	3.952933	2.850497	1.148090	H	-5.370704	-0.585232	2.121419
H	2.996857	3.802965	2.291469	H	-4.621070	-0.488475	3.721082
H	3.805234	4.605628	0.943490	H	-5.385448	-1.994072	3.204744
H	1.380841	2.744301	0.932799	H	-2.830461	-0.655674	2.205930
H	0.212029	4.537217	-0.209471	H	-1.644832	-2.622599	2.892890
H	1.697440	5.506179	-0.343313	H	-3.154399	-3.492084	3.280040
H	0.984995	5.199005	1.243165	H	-2.652184	-2.085678	4.237027
H	-3.506906	0.536477	-0.938685	H	3.159229	-0.542966	-1.506330
H	-2.231513	2.335467	-3.056248	H	3.987937	-1.878741	-4.119053
H	-1.396143	1.089113	-2.107653	H	2.401184	-1.118611	-3.899083
H	-2.706567	0.642800	-3.240159	H	3.881357	-0.166687	-3.710769
H	-5.443665	2.132852	-1.047932	H	4.906259	-1.945637	-0.481456
H	-5.171474	1.185639	-2.521440	H	5.574367	-0.969332	-1.799150
H	-4.709624	2.886501	-2.479178	H	5.268066	-2.697580	-2.049416
H	-2.711307	4.331483	-2.262244	H	2.586352	-3.760441	-4.255693
H	-4.169272	4.816899	-1.385556	H	4.068925	-4.104575	-3.354055
H	-2.641582	5.648057	-1.095468	H	2.806264	-5.324832	-3.472936
H	-2.860978	5.661555	2.282788	H	1.042432	-6.341166	-0.490714
H	-1.123450	5.342808	2.288308	H	-0.135862	-5.782726	-1.689359
H	-6.600513	-2.951652	0.953010	H	5.979727	0.429588	3.583721
H	-1.873382	6.090484	0.884197	H	1.465482	-6.315726	-2.199107
H	-2.339898	4.351044	4.130436	H	1.425391	-5.332847	1.765817
H	-2.392035	2.875570	5.094277	H	0.518070	-4.362985	2.941039
H	-3.625718	3.156657	3.854007	H	1.995547	-3.709658	2.208518
H	-5.998861	-2.624997	2.582167	H	4.539923	0.069120	4.538957
H	-5.051217	-3.638391	1.478108	H	4.613287	1.561811	3.586941
H	0.391427	2.146842	2.636190	H	-1.523635	-4.133589	-0.267129
H	0.085249	3.811380	3.183478	H	-0.825294	-5.566181	0.518446
H	0.065757	2.472318	4.339304	H	-1.683794	-4.364442	1.471818
H	-6.735468	-0.293826	0.686509	H	5.638057	-1.896986	2.245692
H	-1.881718	1.463655	3.218401	H	-0.035324	-2.696077	1.190754

H	-5.954291	-0.041214	2.246866	H	4.270714	-2.187000	3.318619
H	-4.067863	-1.387961	1.684372	H	3.157927	-0.144992	2.593453
H	-5.205536	0.614826	0.787365	H	4.016333	-2.194964	1.564465
H	-6.895949	-1.873667	-2.634501	H	7.797215	0.506209	0.402914
H	-6.713637	-0.473694	-1.578443	H	6.896482	-1.002963	0.528260
H	-7.191465	-2.037295	-0.907260	H	7.179702	-0.013719	1.964739
H	-4.011764	-1.863033	-4.484840	H	6.309281	2.104889	-2.270522
H	-4.062418	-3.601216	-4.166799	H	6.463401	3.483281	-1.172958
H	-5.536384	-2.646077	-4.068399	H	7.492973	2.073090	-0.962526
H	-0.892049	-4.975699	-2.743737	H	3.240714	5.314843	-0.596196
H	-2.573140	-4.838589	-3.269738	H	4.846942	4.690769	-0.222792
H	-2.197702	-5.025725	-1.545768	H	3.496114	4.354538	0.873626
H	-1.030169	-2.860159	-1.510508	H	2.392368	2.946120	-0.825806
H	-0.212941	-2.647932	-3.747368	H	2.971057	3.947274	-2.895438
H	-1.251570	-1.252597	-3.411674	H	3.658319	2.322536	-2.930288
H	-1.830462	-2.574086	-4.450140	H	4.704903	3.739553	-2.659875
H	-0.021728	-1.131987	-1.074313	H	-0.038787	-0.127293	-1.358080
				C	0.619251	0.465109	-2.771498
				O	1.486758	1.168975	-2.368669
				O	-0.012200	-0.066766	-3.625160
TS2(2d)							
C	-3.599573	1.060172	-0.955421				
C	-2.649884	0.053989	-1.314769				
N	-3.159223	-1.050316	-1.978642				
C	-4.485145	-1.185777	-2.254013				
C	-5.396631	-0.235041	-1.907361				
C	-4.927107	0.919872	-1.244080				
N	-1.368064	0.025564	-1.033567				
P	-0.405424	1.217949	-0.436891				
P	0.376233	-0.256922	1.219807				
N	-0.347640	-1.730186	1.226579				
C	-1.641555	-1.979121	1.229120				
N	-2.036411	-3.243123	0.816650				
C	-3.345946	-3.619998	0.764797				
C	-4.356953	-2.775473	1.106771				
C	-4.011945	-1.479109	1.547975				
C	-2.702410	-1.100726	1.617517				
C	-1.007437	-4.212628	0.406562				
C	-0.359604	-4.899813	1.600428				
C	-2.223579	-2.091909	-2.431805				
C	-1.556684	-1.709831	-3.745797				
N	1.068307	1.574840	-1.079131				
C	1.884857	0.726410	-1.659263				
C	1.624720	-0.639943	-2.009874				
C	2.582860	-1.421477	-2.586030				
C	3.861197	-0.892764	-2.877567				
C	4.093056	0.412656	-2.571252				
N	3.149380	1.200210	-1.981303				
C	3.469465	2.611721	-1.712529				
C	2.934155	3.534310	-2.799177				
C	-0.869128	2.391964	0.910921				

C	-0.670570	2.016422	2.277979
C	-1.061065	2.907921	3.314556
C	-1.618000	4.166218	2.968068
C	-1.779078	4.518281	1.654197
C	-1.406099	3.626254	0.622827
C	-0.878994	2.512227	4.664641
C	-0.330364	1.293215	4.977327
C	0.069953	0.411841	3.950205
C	-0.093287	0.765875	2.632286
N	1.995121	-0.351062	1.318025
C	2.850763	-1.266047	0.922838
N	4.169780	-0.860699	0.784304
C	5.159207	-1.717462	0.404534
C	4.915536	-3.027151	0.126290
C	3.587461	-3.493210	0.254539
C	2.590702	-2.644346	0.639418
C	4.520691	0.534300	1.094175
C	4.745777	0.742568	2.585069
H	0.638362	-1.028716	-1.789280
H	-1.912063	4.846043	3.762051
H	-1.543469	3.930916	-0.409025
H	-2.198338	5.483813	1.393354
H	0.511238	-0.547221	4.204719
H	-0.198490	1.004143	6.014287
H	-1.182954	3.194993	5.452477
H	2.358930	-2.457003	-2.819332
H	4.639493	-1.489891	-3.332133
H	-5.624874	1.697541	-0.952098
H	-6.443378	-0.378394	-2.137544
H	-3.237613	1.928468	-0.420909
H	-4.761114	-2.098253	-2.767496
H	-1.479936	-2.217164	-1.645388
H	-2.789666	-3.020601	-2.523978
H	-1.040734	-0.752359	-3.644773
H	-2.296268	-1.627947	-4.546913
H	-0.827813	-2.475562	-4.023503
H	1.567702	-2.971899	0.755137
H	3.698225	1.155733	0.742355
H	5.416364	0.777415	0.519482
H	5.558532	0.108716	2.950130
H	3.834846	0.509921	3.141057
H	5.010196	1.786061	2.772896
H	6.147984	-1.281333	0.337363
H	5.725339	-3.676012	-0.178177
H	3.356405	-4.533551	0.049862
H	-4.788503	-0.776809	1.830770
H	-5.384675	-3.104782	1.040703
H	-2.439883	-0.107477	1.957084
H	-3.523147	-4.632932	0.426223
H	-1.492623	-4.938735	-0.247313
H	-0.267663	-3.668632	-0.182583

H	0.110944	-4.166121	2.258439				
H	0.407160	-5.595106	1.249627				
H	-1.101786	-5.463204	2.171915				
H	-1.061846	2.241706	-1.461687				
H	5.039667	0.898507	-2.772768				
H	4.555587	2.684278	-1.635697				
H	3.037701	2.867092	-0.744628				
H	3.229708	4.563198	-2.578995				
H	3.341588	3.260654	-3.776284				
H	1.843944	3.489847	-2.838925				
C	-1.160648	2.832613	-2.839936				
O	-1.438570	1.918730	-3.557821				
O	-0.917211	3.997102	-2.697132				
TS1(2e)				TS2(2e)			
C	-1.184713	-0.387331	1.882746	C	1.381575	0.136801	1.934669
C	-0.036984	-0.009359	2.650494	C	0.240032	-0.178023	2.721756
C	-0.096560	0.022114	4.073645	C	0.323088	-0.276955	4.139619
C	-1.286937	-0.383231	4.724944	C	1.564603	-0.007684	4.765780
C	-2.367826	-0.781918	3.984031	C	2.653413	0.340768	4.004603
C	-2.315849	-0.774391	2.572173	C	2.558078	0.411148	2.596192
C	1.180588	0.374460	2.020260	C	-1.011982	-0.414192	2.084927
C	2.227857	0.880727	2.747026	C	-2.102595	-0.818116	2.812990
C	2.148900	0.950801	4.155987	C	-2.007578	-0.959242	4.216600
C	1.025211	0.500315	4.801951	C	-0.831804	-0.672162	4.864628
P	1.101690	0.136389	0.240595	P	-0.985872	-0.066997	0.312004
N	1.483528	-1.427113	-0.117968	N	-1.620381	1.369898	-0.034600
P	2.509244	-2.445812	0.512268	P	-2.642772	2.375988	0.615205
N	3.282092	-3.238162	-0.748499	N	-1.823617	3.530935	1.494996
C	2.495943	-3.647532	-1.903544	C	-2.495921	4.782669	1.824257
P	-1.293100	-0.169259	-0.022970	P	1.227960	0.125264	0.018251
N	-2.572791	-1.249251	-0.119177	N	1.969168	-1.289733	-0.323751
P	-3.324643	-1.976974	-1.274554	P	2.338385	-2.656626	0.343012
N	-4.617539	-1.179316	-1.993169	N	1.330567	-3.402137	1.435425
C	-5.897210	-1.125311	-1.293272	C	0.067649	-3.979301	0.996013
N	-1.811176	1.346954	-0.338580	N	2.013047	1.553352	-0.072417
P	-2.109753	2.667122	0.446553	P	2.735367	2.536011	-1.048579
N	-3.472190	2.510447	1.410021	N	2.955316	3.948923	-0.190249
C	-4.476755	1.506351	1.089577	C	3.465026	5.138804	-0.850692
N	2.136764	1.228192	-0.374908	N	4.245529	2.061286	-1.617176
P	2.889903	1.770530	-1.629019	C	5.365262	2.177073	-0.687928
N	3.826844	3.107917	-1.231681	N	1.902866	2.903636	-2.447644
C	3.181489	4.416098	-1.228646	C	2.510637	3.323595	-3.703376
N	4.013556	0.724607	-2.284401	C	4.300170	0.830430	-2.406183
C	5.300702	1.105370	-2.847215	N	-1.555718	-1.310524	-0.490644
N	1.853610	2.199104	-2.860348	P	-2.608946	-2.101024	-1.332285
C	2.371329	2.584513	-4.164774	N	-1.859808	-2.684556	-2.692218
C	3.513247	-0.552857	-2.773930	C	-2.631250	-3.224918	-3.800714
N	3.762498	-1.878027	1.439381	N	-3.298915	-3.391366	-0.533078
C	3.896057	-2.044612	2.876818	C	-2.848064	-4.763742	-0.702080
N	1.700007	-3.516103	1.520077	N	-3.930969	-1.190707	-1.772387
C	2.373839	-4.759802	1.880716	C	-5.275334	-1.714622	-1.972181

C	4.783760	-1.043408	0.820334	C	-3.986930	-3.151501	0.727291
C	0.252409	-3.666882	1.430847	N	-3.547284	3.020100	-0.634968
C	4.481934	-4.038599	-0.554797	C	-2.900005	3.320989	-1.905441
N	-2.239042	3.856962	-0.732032	N	-3.789232	1.773283	1.652109
C	-2.738527	3.518569	-2.056772	C	-3.886437	2.072821	3.071572
N	-1.003911	3.333683	1.495283	C	-4.743247	3.815404	-0.392110
C	0.228560	3.924123	0.987547	C	-4.811531	0.875608	1.127600
C	-2.491975	5.242706	-0.362691	C	-0.370191	3.635728	1.487689
N	-2.359311	-2.340654	-2.610557	N	3.783715	-2.540360	1.188256
C	-2.904139	-2.653773	-3.927243	C	4.745130	-1.510608	0.825766
N	-4.022942	-3.364942	-0.640357	N	2.392024	-3.773048	-0.910432
C	-4.635301	-4.308433	-1.567778	C	2.825130	-3.339991	-2.232810
C	-1.133027	-3.083502	-2.335632	C	4.411622	-3.723716	1.762237
C	-0.988607	3.096977	2.932443	C	2.667545	-5.178972	-0.650421
C	-4.025427	3.654107	2.124559	C	1.426173	-3.239111	2.879294
C	-3.436271	-3.998930	0.532639	C	0.543217	3.396873	-2.255389
C	-4.287006	0.092633	-2.636761	C	3.032932	3.981017	1.261322
C	0.472037	2.586526	-2.624904	C	-3.694308	0.081695	-2.444434
C	4.731039	2.932565	-0.096951	C	-0.440762	-3.007186	-2.714092
H	-1.330509	-0.361797	5.810176	O	-0.587101	0.685969	-3.227664
H	0.968002	0.524285	5.886528	C	0.478263	0.173879	-3.151838
H	-3.192234	-1.063282	2.007981	O	1.446259	-0.362334	-3.577775
H	3.123411	1.210897	2.228788	H	1.640830	-0.081532	5.846851
H	-4.021006	0.664676	0.568189	H	-0.767819	-0.756536	5.945928
H	4.534103	-0.829123	-0.220104	H	3.436540	0.692338	2.024506
H	-1.773001	2.396061	3.217331	H	-3.047832	-1.011584	2.319088
H	-0.215125	-2.720586	1.169980	H	4.225113	-0.657358	0.393200
H	-4.927195	1.136702	2.017831	H	-4.482821	0.419987	0.190211
H	4.852018	-0.086534	1.350679	H	2.220880	-2.540163	3.138991
H	-0.024243	2.674316	3.229791	H	0.092267	2.692515	1.205360
H	-0.033850	-4.419520	0.681378	H	5.281666	-1.178125	1.721769
H	-1.134923	4.039127	3.476593	H	-4.988995	0.071264	1.849697
H	-0.134776	-3.988153	2.403621	H	0.483082	-2.846806	3.272477
H	-3.253780	4.394341	2.336125	H	-0.024932	4.401078	0.778675
H	2.990131	-2.484065	3.292169	H	1.624748	-4.205542	3.360439
H	-4.825638	4.140433	1.550088	H	-0.022885	3.911890	2.489425
H	4.753234	-2.686677	3.118602	H	3.664482	-4.475708	2.016943
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H	4.048032	-1.069142	3.350310	H	5.138685	-4.174153	1.072507
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H	1.982115	-5.118386	2.837501	H	4.938302	-3.445678	2.681626
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H	2.216839	-5.543029	1.125926	H	-0.075608	-4.957853	1.470487
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H	3.447468	-4.603948	1.999453	H	-0.774081	-3.326297	1.258998
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H	5.152765	-3.897630	-1.410074	H	2.301224	-5.467197	0.335633
H	-2.027031	5.901949	-1.103791	H	-5.173592	3.579998	0.582154
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C	4.535182	-4.276510	0.400436	C	3.441303	0.108763	-4.375767
C	5.454405	-3.254596	-0.268205	C	4.731245	-0.726731	-4.223164
C	4.499843	-2.441598	-1.151830	C	4.261738	-2.016984	-3.549172
N	1.334860	-2.138113	-0.110589	N	1.393675	-1.604898	-0.709401
P	1.032104	-0.686289	0.549946	P	1.000316	-0.447675	0.304143
N	2.103874	0.459441	0.137081	C	0.845499	-1.078333	1.988779
P	3.345023	1.280855	0.617629	C	-0.192011	-0.420268	2.701944
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C	1.771258	4.634315	1.977094	C	1.437463	-2.303791	3.975554
C	2.732773	5.179031	0.917921	C	1.623121	-2.026222	2.600526
C	3.715913	4.022040	0.736936	C	-1.214128	0.211983	4.817558
P	-0.997248	0.470854	0.272310	C	-1.974675	1.132297	4.137980
C	-0.802607	0.759428	2.166696	C	-1.937474	1.211510	2.723898
C	0.087582	-0.045403	2.950075	C	-1.092030	0.417033	1.986142
C	0.056174	0.010956	4.373048	P	-1.126254	0.233525	0.069975
C	-0.776823	0.968966	5.004504	N	-1.543356	1.796635	-0.139435
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C	1.672200	-1.803163	4.482041	C	-5.179825	0.766787	-2.522277
C	1.766513	-1.805587	3.072353	C	-5.813755	2.116854	-2.177840
C	1.023243	-0.923816	2.331118	C	-4.732070	2.788917	-1.339669
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C	-5.706874	0.721290	2.718135	C	6.236501	2.933544	-0.635544
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C	-6.045874	-3.333871	-1.247200	C	4.175598	0.005519	4.369728
C	-5.714884	-2.252476	-0.216169	C	4.288432	0.196379	2.847948
N	-1.858955	1.915631	0.105724	N	1.928709	-3.850823	-1.805362
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C	-1.025520	3.037471	-3.735655	C	-4.078470	-2.612961	-1.930335
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C	0.868747	-0.659253	-2.964877	C	-1.476798	-3.429728	1.707642
C	0.857701	-0.481794	-4.482149	C	-1.375317	-4.939771	1.966457
C	2.329502	-0.664716	-4.852005	C	-2.446408	-5.544340	1.055368
C	2.769489	-1.813671	-3.944317	C	-3.567660	-4.508759	1.134083
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C	6.333386	2.042365	-1.816675	C	-3.051767	6.444057	-0.488586
C	5.906941	1.665321	-0.395430	C	-2.432969	5.427689	-1.455138
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C	3.839093	1.302312	3.326860	C	-1.336452	3.247588	-3.954547
C	4.936799	0.679079	4.184250	C	-0.034011	3.840242	-4.494827
C	5.113321	-0.709900	3.559429	C	1.035422	3.012125	-3.777468
C	4.843019	-0.494899	2.060013	C	0.464870	2.853659	-2.367682
H	6.514604	0.832530	-0.019957	O	-0.628788	0.187820	-3.748693
H	2.434353	-2.500690	2.571030	C	-0.830230	-0.729572	-3.019590
H	-2.234838	2.315067	2.252677	O	-1.044692	-1.875680	-2.802952
H	2.264241	-2.503105	5.063346	H	6.291797	1.447749	0.937147
H	-2.170672	2.557835	4.720376	H	2.386966	-2.552005	2.038102
H	0.823868	-0.854548	6.200069	H	-2.595730	1.903104	2.208576
H	-0.786946	1.030118	6.089007	H	2.049560	-3.062098	4.453273
H	4.663508	0.637146	5.240814	H	-2.646471	1.785512	4.687546
H	5.856566	1.264608	4.087403	H	0.443339	-1.752896	5.786855
H	3.844837	2.394935	3.349595	H	-1.292459	0.111453	5.896172
H	2.850495	0.951091	3.656859	H	3.070556	1.225432	5.829682
H	6.103232	-1.134417	3.737882	H	4.395644	2.072556	5.008434
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H	4.503131	4.060677	1.505589	H	3.477303	-0.805924	4.588474
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H	0.817059	5.164648	2.012234	H	5.317857	0.403223	2.540839
H	4.197802	4.026700	-0.245457	H	3.763817	4.249512	2.382886
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H	0.745352	3.014457	0.917621	H	3.890912	4.660240	0.660109

H	6.010270	2.494916	0.308381	H	1.925799	6.046836	0.740917
H	1.440748	2.526689	2.460412	H	2.588671	6.353179	2.356079
H	7.407990	1.924305	-1.970155	H	0.343459	3.740566	0.508021
H	6.071245	3.086423	-2.021150	H	5.541849	2.963931	1.456707
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H	3.544161	2.001815	-2.293334	H	7.325243	3.005982	-0.595796
H	5.900717	0.100775	-2.677117	H	5.827214	3.942303	-0.759676
H	3.532374	0.233590	-2.139744	H	5.767585	2.465342	-2.742773
H	1.070946	0.287889	-2.452297	H	3.592696	2.453666	-1.709137
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H	0.453655	0.487785	-4.782396	H	1.901307	0.129748	-2.780389
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H	3.840399	-1.781298	-3.733377	H	5.229078	-0.917628	-5.176030
H	-0.941716	-3.482711	-0.796771	H	5.442547	-0.214964	-3.568571
H	4.993789	-2.094360	-2.063990	H	3.881681	-2.727460	-4.297832
H	4.127140	-1.556708	-0.621148	H	5.036539	-2.518953	-2.966522
H	5.993624	-2.622194	0.440144	H	-0.146131	-3.754517	-1.364078
H	6.195228	-3.770258	-0.887871	H	5.462484	-1.340863	-1.174262
H	2.625626	-5.038583	-0.387802	H	4.505135	-0.805564	0.205100
H	4.033126	-5.379313	-1.401979	H	6.432058	-1.675893	1.362583
H	5.066768	-5.143999	0.797611	H	6.712883	-2.902315	0.118066
H	3.976321	-3.807792	1.218468	H	3.124088	-4.185559	0.750329
H	2.027413	-5.072286	-3.230464	H	4.508497	-4.735933	-0.198417
H	-1.677700	-6.043850	-1.457487	H	5.628403	-4.222723	1.861438
H	0.661735	-4.215542	-3.974027	H	4.514069	-2.906145	2.238342
H	-1.741358	-4.762880	-2.678441	H	3.738048	-4.818269	-2.375102
H	-0.283903	-6.433025	-3.741609	H	0.074943	-6.485211	-1.113691
H	0.574983	-6.708121	-2.214551	H	2.492866	-4.762749	-3.634344
H	-0.029679	-4.853711	-0.154234	H	0.036878	-5.741602	-2.721109
H	-4.107429	1.366701	1.372776	H	2.151265	-7.002119	-2.770110
H	-5.379151	0.431761	0.565924	H	2.536065	-6.487734	-1.116737
H	-6.044155	1.753472	2.836873	H	0.847375	-4.461332	-0.078728
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H	-5.372530	-0.079820	4.742823	H	-5.610997	0.091784	0.617004
H	-4.152338	1.066966	4.180890	H	-6.449379	1.050105	3.012623
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H	-6.342370	-1.364897	-0.377665	H	-4.547255	0.304058	4.323344
H	-7.105218	-3.340520	-1.512461	H	-3.205139	-1.444327	3.564386
H	-5.873462	-2.582129	0.813561	H	-4.579439	-2.536726	3.306202
H	-1.312437	-2.355234	2.926430	H	-6.550110	-1.611294	-0.367842
H	-0.620780	-2.992306	1.430210	H	-7.331050	-3.461405	-1.676966
H	-5.790902	-4.324365	-0.854298	H	-6.010818	-2.937232	0.666405
H	-0.538602	-5.015618	2.711417	H	-1.314015	-2.858275	2.627103
H	-1.839256	-4.472752	3.778050	H	-0.744534	-3.087319	0.971061
H	-3.020489	-6.090376	2.397739	H	-5.987305	-4.494272	-1.172206
H	-2.140320	-5.577515	0.946140	H	-0.371438	-5.322287	1.765956
H	-4.167311	-4.310105	0.708566	H	-1.612368	-5.158361	3.012713

C	1.595063	-2.794272	-1.195924	C	-3.203305	1.849768	-1.225779
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C	3.602242	-2.892171	-2.655284	C	-4.939151	-1.498670	0.910280
N	2.656816	0.178856	0.466020	C	-5.675797	-0.191533	1.178141
C	3.049728	1.400425	0.263178	C	-1.676918	-2.626231	-2.578460
N	4.180704	1.655832	-0.465587	C	-1.179913	-1.815436	-3.770754
C	5.111881	2.719480	-0.128343	C	-4.343605	-1.917074	-4.110834
N	2.420448	2.507938	0.778643	C	-6.469583	-1.125844	-1.822177
C	1.687244	2.433808	2.027500	C	-0.606758	-1.365410	2.455007
C	2.295494	3.754517	0.048041	C	0.739922	-0.916746	2.588028
N	-1.866721	-0.367811	-0.908412	C	1.404898	-1.096406	3.833203
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C	-4.537701	-2.053851	0.894880	C	-1.245543	-2.008937	3.486144
N	-3.939859	-0.977625	-1.670392	C	2.717073	-0.579954	3.981851
C	-4.761893	-2.113609	-2.063697	C	3.310142	0.090181	2.940433
C	-3.937869	0.141213	-2.594345	C	2.639635	0.238446	1.704569
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N	0.878760	-3.530504	-2.093170	N	2.169995	1.763591	-2.325494
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C	-0.536738	-3.268942	-2.276723	C	3.352302	3.469706	-1.510239
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H	-3.753380	0.652588	4.216280	C	1.320449	4.931022	0.610711
H	-2.069337	-0.468731	5.622350	C	4.359920	4.540842	-1.259210
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H	-4.414505	-3.018797	-1.566991	N	3.790838	-1.846908	-0.480661
H	-5.817388	-1.953770	-1.821720	C	4.507645	-2.849700	0.176211
H	-4.670942	-2.259114	-3.144611	C	3.602071	-3.707220	0.710159
H	-3.500160	1.013078	-2.110599	N	2.331913	-3.222799	0.386036
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H	-2.113480	-2.447290	2.027830	C	0.867070	-4.966012	-0.537584
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H	-2.341941	5.253333	0.790668	H	-1.072130	-2.741190	5.516580
H	-4.959217	-3.052942	0.736861	H	3.138407	0.769044	0.899510
H	-2.644949	2.469066	-3.869210	H	4.307801	0.503941	3.059309
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H	2.831604	4.576596	0.538038	H	1.594902	-5.775108	-0.422872
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H	1.511887	-4.795037	-3.675591	H	1.299048	-0.347839	-4.888020
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C	-4.445926	-0.217872	3.047904	P	3.462204	0.812748	0.875038
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C	2.404338	-2.820893	2.686386	C	1.095176	-2.180900	4.421991
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C	-4.214348	-2.488636	-3.062141	P	-3.577386	-1.062670	0.685693
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C	3.768819	2.054086	-2.317976	N	-1.151457	4.591828	-0.787199
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H	-0.239266	-1.454319	5.838600	C	1.229808	3.679420	-4.224049
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H	2.883177	-1.930416	3.093340	C	-4.413333	1.435281	-2.693517
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H	2.879985	-3.711669	3.116702	C	2.792721	-0.924762	-4.760818
H	-1.695126	1.907289	3.660310	C	2.890116	-2.113876	-3.806709
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H	5.058131	4.149714	-1.325056	H	2.578121	4.299513	3.177888
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H	4.084045	1.321972	-1.563330	H	4.783393	3.420098	0.175561
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H	1.194312	2.639803	-4.762392	H	5.901308	0.628151	-3.266727
H	-5.166008	-2.273395	-2.562552	H	4.046422	1.505711	-1.991591
H	0.658461	4.264092	-4.279641	H	6.080053	-0.762277	-2.180828
H	-4.320992	-2.230435	-4.124450	H	3.715180	-0.232348	-1.867385
H	-0.722969	1.659816	-3.431572	H	1.192027	0.210152	-2.618486
H	-4.238928	0.077254	-2.412043	H	-0.038439	-0.987637	-3.009309
H	0.411928	5.904697	-2.255670	H	0.712275	-1.230570	-5.265690
H	-0.538554	-1.545247	-5.212596	H	1.113772	0.476357	-5.024848
H	-1.204755	3.310841	-2.972123	H	3.116979	-1.181322	-5.771249
H	-3.097033	-0.059823	-3.775303	H	3.423121	-0.104367	-4.398654

H	1.512988	6.758725	-1.151450	H	2.615933	-3.044700	-4.317738
H	-0.666988	-3.294666	-4.929953	H	3.898749	-2.234812	-3.407501
H	-0.849552	2.089599	-1.721678	H	-1.436050	-3.136450	-1.071217
H	-2.518774	0.274929	-2.114720	H	4.669112	-2.675666	-1.622856
H	-0.755931	4.972761	-0.085691	H	3.745737	-2.103201	-0.231945
H	1.274177	-1.240601	-3.589561	H	5.321891	-3.530983	0.890656
H	0.456763	5.883541	0.841699	H	5.438312	-4.620867	-0.496202
H	1.312051	-2.988234	-3.262835	H	1.661243	-5.225483	-0.346422
H	0.312064	4.120644	1.055095	H	3.050735	-5.814559	-1.266571
H	1.073126	-1.820823	-1.936635	H	3.941014	-5.861338	0.995391
H	2.171619	5.649978	-2.361403	H	3.072904	-4.378037	1.427851
H	-2.076461	-2.243588	-4.684844	H	1.377311	-5.131675	-3.384580
H	2.993199	1.846725	4.552734	H	-2.625158	-5.388827	-2.092977
H	-1.899829	-2.795498	4.606645	H	0.342110	-3.933744	-4.188181
H	3.432135	-0.906383	-2.315601	H	-2.280270	-4.016022	-3.159036
H	-2.868220	2.756035	-1.178292	H	-1.102784	-5.868628	-4.276200
H	5.853437	0.270444	0.530880	H	-0.503910	-6.470389	-2.720335
H	-5.665512	-1.297551	0.769390	H	-0.892725	-4.733597	-0.536959
H	0.765157	0.441934	-1.436484	H	-4.072918	1.898873	1.347344
				H	-5.441265	1.225335	0.442069
				H	-5.983175	2.626651	2.695114
				H	-6.813181	1.081043	2.433311
				H	-5.769691	0.684821	4.603953
				H	-4.333788	1.599793	4.136210
				H	-3.410537	-0.449784	3.563557
				H	-4.986099	-1.258003	3.465425
				H	-6.537414	-0.341278	-0.698287
				H	-7.548627	-2.166228	-1.891258
				H	-6.432449	-1.594735	0.543366
				H	-1.793440	-2.395862	2.881026
				H	-1.273951	-2.812463	1.243288
				H	-6.507106	-3.362205	-1.106444
				H	-1.379379	-5.043185	2.094732
				H	-2.507793	-4.577642	3.371836
				H	-4.002464	-5.739587	1.848283
				H	-3.174154	-5.066201	0.430841
				H	-5.028916	-3.542008	0.638028
				H	-4.945069	-3.553951	2.409298
				H	-3.737580	-2.957644	-1.518353
				H	-5.386614	-3.054799	-3.268715
				H	-5.664172	-1.306701	-3.207820
				H	-3.425812	-1.403809	-2.311121
				H	1.478081	3.527656	-5.276944
				H	2.404151	1.956753	-3.641061
				H	1.236886	4.756406	-4.024292
				H	-0.960621	3.773919	-4.049322
				H	-0.324101	2.169771	-4.427783
				H	-0.006877	5.711368	-2.172630
				H	-0.705148	7.818225	-1.234850
				H	-2.317401	7.192998	-0.854658
				H	0.286010	6.498750	0.594214

N	2.535797	3.500409	0.340305	C	6.593340	-1.013583	-1.024839
C	2.984873	3.269678	1.704371	C	6.425493	-2.349238	-0.815725
C	2.621004	4.848555	-0.200607	C	5.131349	-2.814055	-0.483124
H	2.773807	-0.419393	1.931320	C	4.094223	-1.936838	-0.376251
H	2.603435	-2.032646	3.818142	C	5.760873	1.318649	-1.163676
H	0.818706	-3.753958	3.780480	C	7.179003	1.737471	-1.505510
H	-3.117226	-2.769941	-0.440512	N	0.954993	1.489188	-0.874000
H	-2.909955	-4.719805	1.073931	C	1.088376	2.661588	-0.312932
H	-1.102705	-4.741496	2.768000	N	0.327470	3.700321	-0.866509
H	2.844969	4.832971	-1.267461	C	0.310302	4.950296	-0.325960
H	3.436369	5.376586	0.295086	C	1.051663	5.281484	0.767082
H	3.870231	2.626630	1.728096	C	1.892033	4.289920	1.325608
H	3.222917	4.228117	2.165753	C	1.919730	3.033005	0.799571
H	6.269262	-1.139948	-2.808461	C	-0.433027	3.376549	-2.090210
H	6.553510	-2.135160	-1.364202	C	-1.313156	4.490933	-2.623889
H	4.462373	-4.114616	-2.412767	H	1.322920	-0.721752	5.290708
H	4.023875	-3.667782	-0.744986	H	3.508808	0.090878	1.719663
H	2.889283	-3.358698	-2.065312	H	3.485993	-0.294733	4.145215
H	1.697078	5.420059	-0.044704	H	-3.240341	-0.830558	1.675468
H	2.200901	2.776207	2.285803	H	-3.160450	-1.092339	4.116578
H	-6.078353	1.617605	-2.834755	H	-0.967923	-0.983169	5.275058
H	-5.426404	-2.183565	-1.823413	H	2.575241	2.273678	1.199352
H	-5.539851	-1.500919	-0.192171	H	-1.036902	2.496660	-1.866871
H	-0.609636	3.746282	3.346572	H	0.295286	3.061907	-2.842569
H	-2.285046	3.187995	3.514629	H	-1.825742	4.108721	-3.509460
H	-0.921650	2.086575	3.846072	H	-0.743340	5.372585	-2.929042
H	-1.027488	3.242458	-0.144623	H	-2.080806	4.790914	-1.904507
H	-1.563622	4.440911	1.063225	H	-0.326374	5.672779	-0.815410
H	0.134343	3.907511	1.028332	H	1.003432	6.285315	1.166744
H	-6.916711	0.111049	-3.217647	H	2.525479	4.532690	2.172865
H	-6.951347	-1.442944	-1.278748	H	4.965250	-3.871073	-0.300964
H	5.538007	0.358718	-1.183248	H	7.271915	-3.017533	-0.896846
H	4.799044	0.557153	-2.776484	H	3.104575	-2.279131	-0.097813
H	3.978255	1.165297	-1.323088	H	7.559901	-0.599903	-1.272867
H	0.866734	3.677131	-1.716432	H	5.071146	1.609951	-1.959680
H	2.258281	2.872007	-2.453548	H	5.414239	1.830817	-0.262310
H	0.813756	1.933412	-2.039811	H	7.886296	1.510971	-0.702960
H	-3.859494	1.689633	-3.207475	H	7.178366	2.820580	-1.646648
H	-4.399191	2.444898	-1.698942	H	7.535724	1.285011	-2.434866
H	-2.737706	1.882221	-1.847480	H	-3.887872	-2.336562	-0.029648
H	-7.274223	0.967172	-1.701305	H	0.527546	-3.760520	-0.758196
H	-1.206103	-0.116935	2.955066	H	-0.053213	-3.746793	-2.408017
H	-2.713807	0.801994	3.115924	H	1.652597	-5.479424	-2.077895
H	-2.594710	-0.504442	1.935210	H	0.137391	-6.263487	-2.517775
H	6.225127	-2.892763	-2.934079	H	0.705563	-6.284217	-0.827746
H	-1.086072	-0.230738	-1.924079	H	-1.503226	-6.485756	-1.080668
				H	-3.809443	-6.641985	-0.217545
				H	-5.027955	-4.500127	0.334359
				H	-2.364006	4.218476	0.939351
				H	-4.734562	4.819312	0.291119
				H	-1.552622	1.942205	0.554099

		H	-6.150057	3.062988	-0.708108		
		H	-5.040565	0.191330	-2.125945		
		H	-5.579040	-0.274833	-0.526622		
		H	-7.522262	1.331947	-0.692469		
		H	-7.486885	0.150410	-1.999287		
		H	-6.976494	1.805312	-2.322964		
		H	-0.662628	0.189931	-1.074177		
2a(dication)-HCOO⁻ complex			2b (dication)-HCOO⁻ complex				
C	0.845611	4.890788	0.285527	C	1.145874	2.715856	3.087344
C	0.529482	3.887830	1.236190	C	-0.122074	2.504432	2.492537
C	0.314802	2.550819	0.797786	C	-0.292853	1.546904	1.438829
C	0.396356	2.235097	-0.604469	C	0.893904	0.926520	0.919624
C	0.704690	3.254880	-1.484065	C	2.102800	1.156982	1.555016
C	0.938808	4.575641	-1.041991	C	2.240098	2.022598	2.652733
C	0.018716	1.566622	1.783475	C	-1.646689	1.289237	1.020504
C	-0.076450	1.891723	3.116058	C	-2.680919	2.055858	1.510494
C	0.121575	3.221585	3.539333	C	-2.475437	3.084505	2.451172
C	0.423904	4.192023	2.617619	C	-1.224045	3.269962	2.961979
P	-0.128268	-0.089284	1.111648	P	-2.112748	-0.159424	0.027228
N	1.008585	-1.109506	1.733168	O	-1.477962	0.084230	-1.402714
C	2.308992	-0.998891	1.738990	C	-0.153078	-0.537605	-1.927148
C	3.097300	0.209163	1.294113	O	-0.183976	-1.773439	-2.167283
P	0.013325	0.490409	-1.157836	P	1.223988	0.040026	-0.684196
N	-1.512408	-0.051270	-1.409185	N	2.164418	1.054883	-1.557531
C	-2.683751	0.450930	-1.167864	C	2.407379	2.334870	-1.385172
C	-2.918346	1.816655	-0.571646	N	3.686417	2.778074	-1.484970
N	1.142611	-0.696683	-1.316238	C	4.784301	1.828654	-1.432905
C	2.367883	-0.679182	-1.751915	N	2.017884	-1.276893	-0.170574
C	3.097208	0.538787	-2.264990	C	3.130188	-1.872168	-0.513540
N	3.062380	-1.836381	-1.722425	N	3.738938	-1.821729	-1.733507
C	4.407714	-1.974596	-2.264254	C	5.185939	-1.823895	-1.875936
C	2.466779	-3.033710	-1.148243	N	3.765528	-2.631596	0.431898
N	-1.610745	-0.618817	1.604020	C	4.400083	-3.900077	0.099113
C	-2.112039	-1.775510	1.240278	C	3.411608	-2.474450	1.829112
C	-1.347392	-2.833337	0.481296	N	-3.721390	-0.099906	-0.109240
N	-3.385385	-2.045262	1.580091	C	-4.461984	-0.358297	-1.172431
C	-4.000017	-3.359281	1.434948	N	-4.202146	-1.314126	-2.103193
C	-4.198956	-1.029240	2.230644	C	-3.410031	-2.498557	-1.801273
N	3.016855	-2.043378	2.213453	N	-1.595924	-1.533157	0.672649
C	2.295640	-3.244959	2.612527	C	-0.960964	-1.903685	1.761492
C	4.474228	-2.064826	2.223751	N	-0.988422	-1.228971	2.953907
N	-3.768114	-0.300775	-1.460434	C	0.189830	-1.096738	3.792282
C	-3.611416	-1.567450	-2.155322	N	-5.602168	0.361254	-1.352213
C	-5.126541	0.046358	-1.070742	C	-5.774829	1.622724	-0.654079
H	0.759691	3.045510	-2.542096	C	-6.819332	-0.228581	-1.894434
H	1.182408	5.338938	-1.772781	N	-0.257052	-3.059030	1.734334
H	1.011352	5.907509	0.628757	C	0.052649	-3.704971	0.467798
H	-0.303736	1.120291	3.845265	C	-0.111003	-3.898392	2.915158
H	0.042020	3.470793	4.591711	C	-2.193186	-0.607892	3.470318
H	0.588569	5.217310	2.935169	N	1.447765	3.275289	-1.136989

H	-5.140441	0.666469	-0.175857	C	0.093199	3.122927	-1.635730
H	-5.663603	-0.875507	-0.836543	C	1.657673	4.388989	-0.225619
H	-2.678824	-1.561399	-2.717815	C	4.028452	4.096745	-1.999949
H	-3.594638	-2.404852	-1.448738	C	2.998661	-1.609448	-2.964556
H	4.556621	-1.337449	-3.135088	C	-4.491720	-1.115423	-3.515376
H	5.171692	-1.740211	-1.514017	H	3.000160	0.682671	1.171093
H	1.972590	-3.638185	-1.916352	H	3.212486	2.162300	3.111245
H	3.252875	-3.629415	-0.678781	H	1.227317	3.438681	3.893161
H	1.729062	-2.746784	-0.399873	H	-3.688925	1.813950	1.199784
H	-5.659881	0.563536	-1.876014	H	-3.315224	3.675536	2.798814
H	-4.454477	-1.703840	-2.836691	H	-1.044005	4.005744	3.739864
H	4.881792	-1.107144	2.548042	H	3.141443	4.584872	-2.401541
H	3.004836	-3.967418	3.013445	H	4.469679	4.732133	-1.225679
H	1.549763	-3.005223	3.373520	H	4.754212	3.982109	-2.810528
H	-4.721570	-3.493112	2.242275	H	4.486276	0.947670	-0.867153
H	-4.529463	-3.453458	0.480296	H	5.641891	2.304181	-0.950151
H	-3.262980	-4.156332	1.519087	H	5.078750	1.510196	-2.440273
H	-3.872625	-0.040615	1.913590	H	2.598106	4.261675	0.309932
H	-5.242279	-1.180270	1.947649	H	0.846524	4.393035	0.510269
H	-4.112288	-1.091597	3.320798	H	0.063919	2.352846	-2.405442
H	4.809451	-2.821401	2.931954	H	-0.611724	2.857868	-0.841805
H	1.774873	-3.690094	1.759315	H	5.661990	-1.715579	-0.901692
H	4.118475	0.585066	-1.882692	H	5.551391	-2.740616	-2.352556
H	3.144133	0.511023	-3.357974	H	3.099463	-0.576920	-3.313222
H	2.577272	1.447935	-1.975396	H	1.941914	-1.834160	-2.807887
H	-2.911047	1.740362	0.520952	H	3.394085	-2.290392	-3.725611
H	-2.113376	2.488364	-0.866259	H	5.470576	-3.889657	0.328561
H	-3.861963	2.258118	-0.889529	H	3.928563	-4.700655	0.679328
H	3.523788	0.721102	2.161927	H	4.265017	-4.124172	-0.958186
H	3.919693	-0.077485	0.635339	H	3.170351	-1.434158	2.040371
H	2.465936	0.918912	0.765391	H	2.545908	-3.091617	2.098178
H	4.883663	-2.309375	1.237022	H	4.263604	-2.777363	2.442872
H	-0.630536	-2.356423	-0.188522	H	1.662997	5.353961	-0.744293
H	-0.789425	-3.456760	1.185954	H	5.477776	-0.973894	-2.501731
H	-1.994850	-3.471524	-0.118561	H	-0.227661	4.070622	-2.080028
H	4.545447	-3.007521	-2.586175	H	-2.039593	0.460893	3.648699
O	0.149575	1.061619	-2.890196	H	-3.016676	-0.734672	2.767821
C	0.003129	0.334469	-3.975939	H	-2.468102	-1.082325	4.420037
O	-0.200604	-0.857821	-4.062633	H	0.339285	-0.034696	4.018085
H	0.100480	0.975075	-4.869962	H	1.067658	-1.454361	3.255964
				H	0.094047	-1.644800	4.736957
				H	0.915330	-3.901818	3.297181
				H	-0.379371	-4.923868	2.646818
				H	1.057564	-4.134288	0.528988
				H	-0.662889	-4.514758	0.275384
				H	-2.370082	-2.383382	-2.125177
				H	-3.417888	-2.684680	-0.728531
				H	-5.253114	-1.814206	-3.878554
				H	-3.571352	-1.278987	-4.085241
				H	-4.829500	-0.095073	-3.692683
				H	-6.521571	2.213478	-1.189027

		H	-6.113894	1.476571	0.378477		
		H	-4.835789	2.175190	-0.644549		
		H	-6.683858	-1.299224	-2.041670		
		H	-7.634751	-0.081170	-1.179574		
		H	-7.103428	0.231094	-2.846331		
		H	-0.780965	-3.563887	3.706548		
		H	-3.868275	-3.350834	-2.313082		
		H	0.018279	-2.981911	-0.348127		
		H	0.015085	0.171346	-2.765721		
2c (dication)-HCOO⁻ complex			2d (dication)-HCOO⁻ complex				
C	5.630527	2.786053	-1.398897	C	-3.115289	0.178100	1.275670
N	4.346895	2.818279	-0.840353	C	-2.409870	-1.060992	1.396141
C	4.123063	1.655267	-0.164150	N	-3.206418	-2.197132	1.452706
N	5.248738	0.897519	-0.297872	C	-4.565403	-2.141533	1.374492
C	6.194240	1.603088	-1.049812	C	-5.235802	-0.965496	1.230216
N	3.090863	1.346059	0.603194	C	-4.476612	0.223984	1.184856
P	1.552788	0.956545	0.280834	N	-1.110959	-1.253095	1.461935
N	1.249485	-0.587685	0.028442	P	0.092073	-0.188648	1.112826
C	2.050476	-1.631584	0.071354	N	1.531807	-0.923324	1.400750
N	2.582555	-2.269575	-1.004424	C	1.953294	-1.949152	0.689429
C	3.347993	-3.350260	-0.563039	C	1.211310	-2.718866	-0.266533
C	3.270861	-3.373450	0.794449	C	1.763593	-3.792933	-0.902065
N	2.440114	-2.317784	1.179111	C	3.102674	-4.164371	-0.644512
C	2.349203	-1.768546	-2.370471	C	3.814209	-3.409038	0.236978
C	3.582266	-1.074124	-2.941264	N	3.271595	-2.332692	0.872596
C	4.085558	-4.273984	-1.471283	C	4.108961	-1.565030	1.809302
C	3.954450	-4.285545	1.756273	C	3.929766	-2.035391	3.245501
C	1.957361	-1.928857	2.516948	C	-2.562558	-3.510089	1.628893
C	1.563961	-3.121465	3.384992	C	-2.250116	-3.792488	3.091572
C	3.483334	3.998090	-0.675110	C	0.053311	1.238837	2.198925
C	4.120066	5.010931	0.276175	C	-0.263385	2.448498	1.516553
C	5.433773	-0.332305	0.492753	C	-0.446309	3.625984	2.294895
C	6.107146	0.001240	1.821955	C	-0.262100	3.563949	3.700269
C	7.543271	1.075420	-1.404484	C	0.074841	2.388308	4.322562
C	6.172866	3.851340	-2.291676	C	0.220136	1.209257	3.562885
C	0.660355	1.483157	1.784466	C	-0.817731	4.833658	1.652154
C	-0.457821	0.748900	2.336766	C	-0.998787	4.864089	0.296646
C	-0.598865	0.788497	3.761472	C	-0.778732	3.706257	-0.480917
C	0.137219	1.729768	4.532815	C	-0.402711	2.505991	0.084428
C	1.037352	2.567805	3.941563	P	-0.035208	0.974553	-0.919811
C	1.342167	2.381395	2.576113	O	-0.233936	1.895109	-2.533402
C	-1.472658	-0.110584	4.423114	C	0.670579	2.667709	-3.081453
C	-2.240071	-0.988260	3.706412	O	1.653708	3.150725	-2.552781
C	-2.239372	-0.896501	2.303178	N	1.461739	0.473751	-1.365583
C	-1.407266	-0.042493	1.606046	C	2.642021	0.809311	-0.919876
P	-1.833745	0.151632	-0.180645	C	2.973248	1.840900	0.022512
N	-1.659092	-1.274330	-0.917523	C	4.259703	2.078397	0.402364
C	-2.482337	-2.295714	-1.022156	C	5.320922	1.305784	-0.129033
N	-2.322349	-3.498213	-0.393444	C	5.007568	0.337960	-1.030836
C	-3.280195	-4.403103	-0.856688	N	3.722312	0.086169	-1.412156
C	-4.047981	-3.745222	-1.761867	C	3.485231	-0.924848	-2.453532

N	-3.555399	-2.438761	-1.853994	C	3.447407	-0.296087	-3.839490
C	-1.246959	-3.719230	0.582019	N	-1.192786	-0.085724	-1.404013
C	-1.776287	-4.302788	1.893100	C	-2.432339	0.106037	-1.777171
C	-3.972528	-1.372920	-2.774912	N	-3.176805	-1.041091	-2.030037
C	-5.440445	-1.002642	-2.592075	C	-4.490428	-0.995740	-2.391106
C	-5.247208	-4.250140	-2.493730	C	-5.164916	0.177467	-2.526652
C	-3.413792	-5.806202	-0.366279	C	-4.456291	1.376129	-2.280955
N	-3.426225	0.523184	-0.165104	C	-3.141743	1.343387	-1.920214
C	-3.973599	1.721054	-0.095871	C	-2.523758	-2.351912	-1.894787
N	-3.904133	2.758673	-0.986129	C	-1.666475	-2.706344	-3.101083
C	-4.719856	3.807323	-0.543537	H	-0.961878	5.726839	2.252466
C	-5.299615	3.408756	0.616066	H	-0.912454	3.782680	-1.549922
N	-4.839879	2.116899	0.883605	H	-1.296136	5.781813	-0.198514
C	-3.203831	2.651935	-2.274058	H	0.459872	0.272608	4.056935
C	-4.176535	2.603811	-3.451426	H	0.214252	2.358222	5.397608
C	-4.833483	5.125864	-1.233494	H	-0.397295	4.472093	4.280052
C	-6.273740	4.142014	1.476585	H	2.165214	2.446410	0.407479
C	-5.043658	1.299820	2.085317	H	2.539722	-1.411968	-2.223035
C	-4.259682	1.861285	3.269315	H	4.281716	-1.666985	-2.372521
C	-6.518953	1.058513	2.395777	H	2.658281	0.457429	-3.890624
C	-2.116210	3.710403	-2.433830	H	3.244017	-1.065280	-4.588620
C	-0.107393	-4.535228	-0.023891	H	4.403036	0.177733	-4.080939
C	-3.587631	-1.695270	-4.217471	H	5.756513	-0.291359	-1.495738
C	2.941143	-1.003515	3.227474	H	6.350532	1.469580	0.157922
C	1.784360	-2.838547	-3.299510	H	4.470348	2.868942	1.114948
C	3.031986	4.602147	-2.001705	H	-4.960489	2.331913	-2.378258
C	6.149494	-1.453450	-0.255238	H	-6.208365	0.174631	-2.810202
H	-0.032996	1.764302	5.605037	H	-2.599544	2.256706	-1.727746
H	2.204369	2.893775	2.164846	H	-4.956718	-1.958481	-2.559002
H	1.585146	3.301585	4.522328	H	-1.914549	-2.310238	-0.991922
H	-2.963803	-1.485889	1.747270	H	-3.313400	-3.089844	-1.743011
H	-2.896847	-1.692941	4.205314	H	-0.856844	-1.983459	-3.219717
H	-1.524387	-0.081210	5.507453	H	-2.266927	-2.725594	-4.014472
H	-4.595056	0.343701	1.808661	H	-1.229706	-3.698032	-2.955810
H	-7.006020	1.936510	2.825641	H	0.193463	-2.411896	-0.469085
H	-7.062639	0.760570	1.495367	H	3.825401	-0.518154	1.704013
H	-6.597308	0.248866	3.126335	H	5.143441	-1.677029	1.480145
H	-4.641334	2.835122	3.588661	H	4.206024	-3.088266	3.350079
H	-3.202798	1.965567	3.009037	H	2.891713	-1.906858	3.559241
H	-4.331387	1.174209	4.116203	H	4.568635	-1.444202	3.906170
H	-7.274007	3.702843	1.418529	H	4.849466	-3.615216	0.478465
H	-5.972631	4.151469	2.526862	H	3.567643	-5.009813	-1.132683
H	-6.348770	5.180042	1.151063	H	1.172931	-4.356055	-1.616969
H	-5.599964	5.731065	-0.748353	H	-4.973343	1.181581	1.072866
H	-3.894052	5.684336	-1.189342	H	-6.314541	-0.960864	1.157675
H	-0.427239	-5.539859	-0.312874	H	-2.535884	1.091363	1.239559
H	-5.115728	5.027378	-2.283782	H	-5.071960	-3.096913	1.429763
H	-1.513364	3.761622	-1.525558	H	-3.241708	-4.258315	1.217171
H	-2.525030	4.699122	-2.656622	H	-1.648501	-3.508282	1.035305
H	-1.460077	3.425191	-3.260891	H	-1.564171	-3.039535	3.485146
H	0.705475	-4.638281	0.700168	H	-1.777752	-4.773702	3.181397

H	0.293587	-4.029214	-0.904627	H	-3.163440	-3.792295	3.692624
H	-4.625847	3.575927	-3.668329	H	0.424320	2.866716	-4.139557
H	-3.638011	2.281876	-4.347184				
H	-4.979396	1.888995	-3.258209				
H	-2.731997	-3.849099	2.167133				
H	-2.696730	1.691940	-2.212006				
H	-1.908700	-5.385740	1.840383				
H	-0.867705	-2.712647	0.773877				
H	-1.068284	-4.093860	2.697494				
H	-3.834340	-5.847637	0.642684				
H	-2.454503	-6.328682	-0.351523				
H	-4.079823	-6.366093	-1.024052				
H	-6.176976	-3.869429	-2.060167				
H	-5.234878	-3.979546	-3.551206				
H	-5.281381	-5.338997	-2.437081				
H	-2.523644	-1.938157	-4.281112				
H	-3.777797	-0.819523	-4.844418				
H	-4.159477	-2.530743	-4.629413				
H	-3.384837	-0.513896	-2.453253				
H	-5.629512	-0.742016	-1.548058				
H	-6.119263	-1.801742	-2.895882				
H	-5.668195	-0.131973	-3.211961				
H	1.048374	-1.364311	2.297562				
H	3.160008	-0.123018	2.618991				
H	2.501222	-0.668691	4.171463				
H	3.878474	-1.523032	3.451330				
H	1.047794	-3.889176	2.805123				
H	0.882088	-2.767922	4.162782				
H	2.423179	-3.579091	3.879529				
H	4.732021	-4.849761	1.239615				
H	4.435968	-3.723002	2.560978				
H	3.268309	-5.006189	2.209178				
H	3.409039	-4.969931	-1.975731				
H	4.647150	-3.733169	-2.236169				
H	3.832646	5.151940	-2.499782				
H	4.800022	-4.866109	-0.897804				
H	1.466105	-2.358655	-4.228637				
H	0.911357	-3.324672	-2.857638				
H	2.521036	-3.602443	-3.557658				
H	2.219290	5.307175	-1.807244				
H	2.661042	3.824444	-2.673079				
H	3.943060	-0.302426	-2.257100				
H	4.396232	-1.775339	-3.147381				
H	3.313669	-0.588852	-3.882798				
H	4.391183	4.530600	1.220068				
H	1.587391	-1.000521	-2.226141				
H	5.015338	5.471086	-0.148304				
H	2.600976	3.609230	-0.167098				
H	3.401622	5.807127	0.487363				
H	5.623321	3.895017	-3.236398				
H	7.216499	3.640781	-2.526264				

H	6.135241	4.842176	-1.833680				
H	8.116357	1.849007	-1.915891				
H	8.110173	0.783129	-0.516572				
H	7.482439	0.210476	-2.070100				
H	7.227777	-1.297910	-0.311748				
H	5.755971	-1.576541	-1.265793				
H	5.978107	-2.385444	0.288093				
H	4.415737	-0.663039	0.700157				
H	5.527083	0.748274	2.369646				
H	7.118809	0.387729	1.665175				
H	6.177670	-0.900774	2.436142				
O	-0.958291	1.257730	-0.741750				
C	1.094654	1.917433	-1.239118				
O	1.484721	1.553080	-2.330217				
H	0.633239	2.907714	-1.077028				
2e (dication)-HCOO⁻ complex				2f (dication)-HCOO⁻ complex			
C	0.948847	0.300064	4.440752	C	5.332058	-3.164730	0.590693
C	0.056940	-0.410479	3.593257	N	5.138098	-2.235893	-0.540695
C	0.105639	-0.234854	2.174086	C	6.021054	-1.058090	-0.378113
C	1.266717	0.437517	1.652601	C	6.849244	-1.353851	0.881245
C	2.114619	1.099758	2.515594	C	5.966211	-2.310006	1.685623
C	1.922709	1.099994	3.913017	P	3.596153	-1.961443	-1.121521
C	-0.861037	-1.321546	4.180097	N	2.809930	-3.408356	-1.053481
C	-1.744231	-2.011149	3.401253	C	3.235594	-4.570779	-1.842926
C	-1.843058	-1.684865	2.033200	C	2.424917	-5.721057	-1.241440
C	-0.991263	-0.794151	1.410612	C	1.133112	-5.028736	-0.800061
P	-1.692336	-0.113726	-0.162320	C	1.621444	-3.694897	-0.234883
C	-0.809366	-0.478717	-1.755189	N	2.843416	-0.872954	-0.284430
O	-0.543904	-1.604898	-2.127233	P	1.573468	0.068119	-0.046521
P	1.867268	0.141569	-0.053608	N	1.877692	1.655690	-0.092701
O	0.864746	0.690683	-1.060288	P	3.131197	2.497898	0.378725
N	1.999965	-1.460447	-0.185331	N	4.434061	2.258063	-0.611918
P	2.704770	-2.705095	0.442548	C	4.210192	1.972536	-2.044549
N	1.578212	-3.869142	0.817404	C	5.593688	2.151370	-2.672996
C	0.324753	-3.949427	0.082953	C	6.254712	3.202062	-1.777432
N	3.307041	0.892938	-0.128130	C	5.796070	2.771028	-0.386248
P	3.966860	1.711749	-1.304007	C	1.027789	-0.283342	1.684685
N	3.203735	1.827266	-2.789104	C	-0.006579	0.443356	2.371880
C	2.923889	0.594543	-3.525696	C	0.074373	0.525370	3.793394
N	3.798213	-3.288549	-0.681493	C	0.999370	-0.286929	4.501822
C	4.444895	-4.577231	-0.496647	C	1.842187	-1.125153	3.826806
N	3.554653	-2.590270	1.881364	C	1.890230	-1.068212	2.417441
C	4.874748	-1.975953	1.875472	C	-0.790337	1.400017	4.507256
C	4.491722	-2.404932	-1.605519	C	-1.742753	2.128749	3.851799
N	-1.769186	1.474336	-0.087417	C	-1.953557	1.901283	2.473646
P	-2.416573	2.630528	0.755657	C	-1.146605	1.054816	1.746235
N	-2.387710	2.555343	2.417168	P	-1.857392	0.361281	0.214034
C	-3.128004	1.510389	3.116858	N	-1.916691	-1.193637	0.531844
N	-3.100642	-0.859820	-0.321067	P	-2.897871	-2.367081	0.867975
P	-4.212290	-1.396692	-1.286149	N	-4.281545	-2.020560	1.725931
N	-5.600316	-1.498179	-0.376611	C	-4.059104	-1.551807	3.117194

C	-5.950519	-0.458159	0.581090	C	-5.117978	-0.466439	3.329803
N	-4.044031	2.769814	0.439599	C	-6.225596	-0.857143	2.351066
C	-4.992419	3.475264	1.292685	C	-5.436179	-1.321680	1.129669
N	-1.596418	4.000083	0.296623	N	-3.259274	1.108694	-0.016027
C	-2.103400	5.323522	0.621962	P	-3.874016	1.882430	-1.255194
C	-4.519174	2.578962	-0.924121	N	-2.851460	2.979511	-1.932632
N	-4.563805	-0.499780	-2.642369	C	-2.903729	3.471352	-3.317816
C	-3.571636	-0.338890	-3.696190	C	-2.379673	4.901959	-3.201465
N	-3.810987	-2.885097	-1.896805	C	-1.347818	4.790504	-2.076881
C	-2.973096	-3.814631	-1.155798	C	-2.011119	3.834552	-1.080559
C	-5.841568	0.133079	-2.920009	N	-5.217554	2.652433	-0.684277
C	-4.392178	-3.444980	-3.108532	C	-5.869017	3.718340	-1.459400
C	-6.680422	-2.412117	-0.712135	C	-7.169216	3.986120	-0.689432
N	4.234904	3.268093	-0.760976	C	-6.842170	3.538734	0.738827
C	5.114317	4.169758	-1.488873	C	-5.987324	2.294832	0.508149
N	5.429826	1.027978	-1.716420	N	-4.381553	0.991977	-2.562915
C	6.290595	0.534364	-0.651952	C	-3.410490	0.178762	-3.327738
C	3.309037	3.938861	0.137586	C	-4.082760	-1.188827	-3.424102
C	6.119632	1.234206	-2.981642	C	-5.565322	-0.825215	-3.512376
C	2.160467	2.833839	-2.970998	C	-5.690214	0.307045	-2.491429
C	2.853145	-2.405562	3.147483	N	3.895705	-1.532682	-2.697702
C	1.833100	-5.027265	1.660845	C	2.763743	-1.196655	-3.586637
C	-0.183341	3.952510	-0.058437	C	3.163515	-1.800987	-4.930976
C	-1.266177	3.090607	3.178215	C	4.685304	-1.653200	-4.920255
H	-0.835766	-1.462985	5.256548	C	5.056590	-2.004732	-3.478346
H	0.844037	0.182498	5.515078	N	-3.429093	-3.148444	-0.494693
H	-2.676389	-2.083362	1.468336	C	-2.360050	-3.638852	-1.398610
H	2.997910	1.572424	2.100665	C	-3.089942	-4.609754	-2.321951
H	-3.862991	1.892369	-1.459372	C	-4.150034	-5.221812	-1.402928
H	5.399643	-2.193972	0.944510	C	-4.615742	-4.023904	-0.572297
H	-3.857870	1.047319	2.451155	N	-2.043270	-3.427543	1.806196
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H	-5.521479	2.140565	-0.892288	C	-1.546869	-5.309696	3.132022
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H	-2.455243	0.730533	3.487922	C	-0.876382	-3.070691	2.626142
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				H	0.708482	0.495179	-2.221179

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