Electronic Supplementary Information

Deciphering the Active Species and Reaction Mechanism in Water Oxidation Catalyzed by the Copper Complex with Redox-Active Ligand

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1. The overall potential energy surface of the water oxidation reaction.

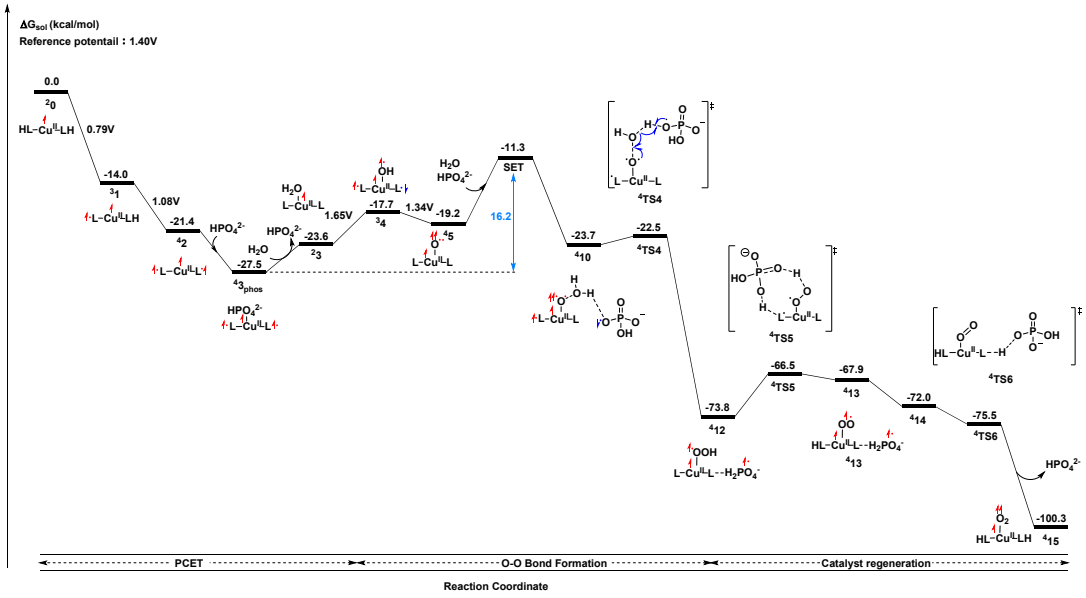


Fig. S1 The overall potential energy surface of the water oxidation reaction.

The Gibbs free energy diagram for the entire process is depicted along with the intermediate in the catalytic cycle. From the diagrams, it can be observed that the rate-determining step occurs at the SET, with an free energy barrier of 16.2 kcal/mol ($^4\mathbf{3}_{\mathbf{phos}}$→**SET**).

2. Estimation of activation barriers for single electron transfer by Marcus-Hush theory.

The Marcus theory of electron transfer was proposed by Rudolph A. Marcus, building upon the foundation of the Libby electron transfer theory.

(I) Internal reorganization energy (λ_i)

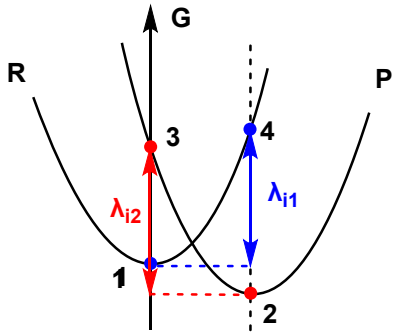


Fig. S2 Marcus model for single electron transfer reaction: R → P

The reaction : $A + B = C + D \Leftrightarrow A + B = A^+ + B^-$

$\lambda_{i1} = [E^+(A^+) + E^-(B^-)] - [E(A) + E(B)] = E_4 - E_1$

$\lambda_{i2} = [E^+(A) + E^-(B)] - [E(A^+) + E(B^-)] = E_3 - E_2$

$$\lambda_i = \frac{|\lambda_{i1} - \lambda_{i2}|}{2} \qquad \text{(eq.1)}$$

(II) External reorganization energy (λ_o)

$$\lambda_o = (332\text{kcal/mol})\left(\frac{1}{2a_1} - \frac{1}{2a_2} - \frac{1}{R}\right)\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon}\right) \qquad \text{(eq.2)}$$

Where a_1 and a_2 are the radii of reactant A and B , respectively, $R = a_1 + a_2$, ε_{op} and ε are the optical dielectric constant (1.78) and the static dielectric constant(78.36) of water solvent , respectively.

(III) Activation energy barrier for single-electron transfer ($\Delta G^{o\ddagger}$)

The total reorganization energy $\lambda = \lambda_i + \lambda_o$,

$$\Delta G^{o\neq} = (\Delta G_r + \lambda)^2 / 4\lambda \qquad \text{(eq. 3)}$$

Where ΔG_r is the Gibbs free energy change during electron gain or loss reactions.

3. The coordination of HPO_4^{2-} and water for some intermediates.

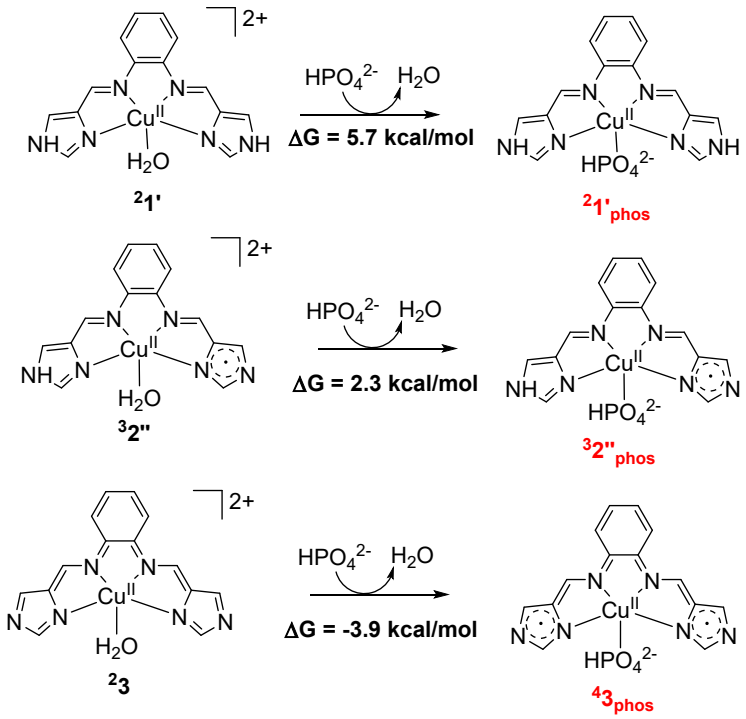


Fig. S3 The reaction free energy of the ligand exchange reaction

For intermediates **^{2}1'** and **^{3}2''**, the coordination of HPO_4^{2-} with Cu results in a higher reaction free energy compared to water coordination, as depicted in the Fig. 3. However, for intermediate 3, the coordination with HPO_4^{2-} is more stable than with water. Starting from **^{4}3$_{phos}$**, an extra water cannot further coordinate as the Cu center, suggesting the **^{4}3$_{phos}$** is saturated coordination complex. Consequently, HPO_4^{2-} dissociates to create a vacancy for water to occupy, thereby facilitating the reaction, leading to the formation of **^{2}3** coordination.

4. The DFT calculated free energy diagram of H-atom abstraction from water.

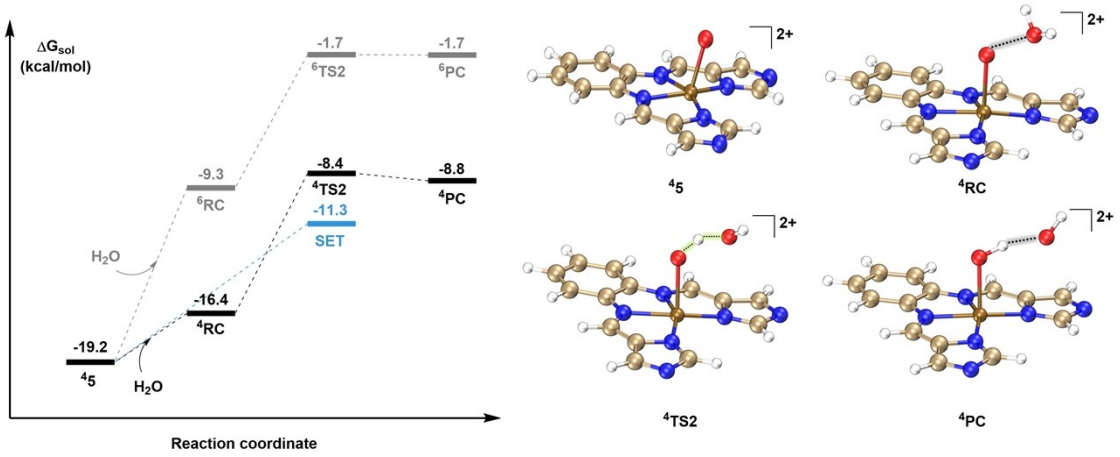


Fig. S4 The free energy diagram of H-atom abstraction from water.

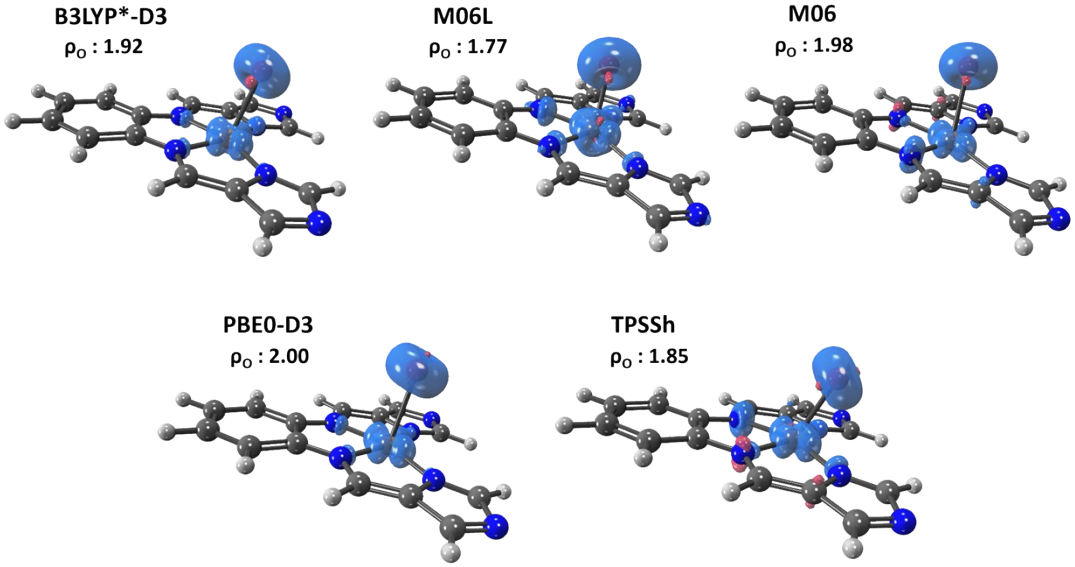
We have computed the process involving the formation of Cu-OH* and OH* from Cu(II)-O** and H_2O, considering both quartet and sextet spin states. The calculations indicate that the reaction pathway for the quadruplet state is lower than that for the sextet state in free energy, ranging from ^{4}5 to ^{4}TS2, with an activation energy of 10.8 kcal/mol higher than the SET energy by 2.9 kcal/mol. Therefore, this pathway does not hold an advantage.

5. Gibbs free energy of Cu^{II}-O•• at different functionals.

Table S1 Gibbs free energy of Cu^{II}-O•• at different functionals (kcal/mol)

	B3LYP*-D3	M06L	M06	PBE0-D3	TPSSh
Doublet	1.1	3.7	2.7	3.2	2.4
Quartet	0	0	0	0	0
Sextet	6.8	6.3	1.7	5.5	6.3

For the Cu^{II}-O•• intermediate ^{4}5 , we considered the doublet state, quartet and sextet states, and performed calculations using five different functionals: B3LYP*-D3, M06L, M06, PBE0-D3, and TPSSh. The results indicate that the quartet state is the most stable, and spin density analysis also suggests that the oxygen atom of Cu^{II}-oxyl complex is in a biradical state (Cu^{II}-O••).



6. The DFT calculated energies of all optimized structures

Table S2. The DFT calculated energies of all optimized structures

Species	Gc hartree	G(gas) hartree	Esp + G_{SOL} hartree	G hartree	Final G（1.9） hartree
H_2O	0.003564	-76.354759	-76.03024812	-76.0266841	-76.0198316 **(4.3)**
O_2	-0.016089	-150.220889	-149.575865	-149.591954	-149.5889261
HPO_4^{2-}	-0.002999	-642.487273	-640.636351	-640.63935	-640.6363224
$H_2PO_4^-$	0.008233	-643.258643	-641.105459	-641.097226	-641.0941983
Cu					
^{2}0	0.208346	-2508.305846	-2500.878357	-2500.67001	-2500.66698
^{3}1	0.193525	-2507.634628	-2500.231102	-2500.03758	-2500.03455
^{4}2	0.177812	-2506.950802	-2499.5724	-2499.39459	-2499.39156
^{4}3$_{phos}$	0.197031	-3150.124071	-3140.237776	-3140.040745	-3140.037717
^{2}3	0.200318	-2583.336556	-2575.618311	-2575.41799	-2575.41497
^{3}4	0.185989	-2582.647884	-2574.939912	-2574.75392	-2574.75089
^{2}1’	0.226723	-2584.682214	-2586.422701	-2586.19598	-2586.19295
^{3}2’	0.215371	-2583.99202	-2585.726435	-2585.51106	-2585.50804
^{4}3’	0.200504	-2583.321677	-2585.056006	-2584.85550	-2584.85247
^{3}2’’	0.212621	-2584.012019	-2585.754651	-2585.54203	-2585.53900
^{3}6	0.23075	-3302.176604	-3291.646522	-3291.41577	-3291.41274
^{3}TS1	0.229897	-3302.162711	-3291.615907	-3291.38601	-3291.38298
^{3}7	0.202157	-2658.788528	-2650.56347	-2650.36131	-2650.35828
^{4}5	0.176605	-2581.975607	-2574.27811	-2574.1015	-2574.09848
^{4}8	0.196231	-2658.349889	-2650.313115	-2650.116884	-2650.113856
^{4}TS2	0.191303	-2658.328521	-2650.295476	-2650.104173	-2650.101145
^{4}9	0.218886	-3301.50391	-3290.98365	-3290.76476	-3290.76173
^{4}TS3	0.216838	-3301.48907	-3290.97981	-3290.76297	-3290.75995
^{4}10	0.18913	-2658.15983	-2649.93657	-2649.74744	-2649.74441
^{4}11	0.222474	-3301.58898	-3291.06706	-3290.84459	-3290.84156
^{4}TS4	0.218887	-3301.58656	-3291.05193	-3290.83304	-3290.83001
^{4}12	0.223503	-3301.58983	-3291.05881	-3290.83530	-3290.83228
^{4}13	0.2185	-3301.58407	-3291.06021	-3290.84171	-3290.83868
^{4}TS5	0.213828	-3301.58699	-3291.06115	-3290.84732	-3290.84429
^{4}14	0.203936	-2658.52437	-2650.45452	-2650.25059	-2650.24756

- The $\mathbf{G_C}$ designate the thermal correction of Enthalpy and Gibbs Free Energy at B3LYP-D3/def2-SVP level.
- The **G(gas)** designate Enthalpy and Gibbs Free Energy in the gas phase at the B3LYP-D3/def2-SVP level.
- The $\mathbf{E_{SP} + G_{SOL}}$ designates the sum of single point energy at B3LYP-D3/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.

7. The cartesian coordinates for all structures

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	8	O	0.00000000	0.00000000	0.12022500
2	1	H	0.00000000	-0.75711800	-0.48089800
3	1	H	0.00000000	0.75711800	-0.48089800

O_2

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	8	O	0.00000000	0.00000000	0.59997900
2	8	O	0.00000000	0.00000000	-0.59997900

HPO_4^{2-}

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	15	P	-0.16277300	0.00039400	-0.07219300
2	8	O	-0.90876200	1.30005000	0.29495600
3	8	O	1.28983200	-0.00976800	0.98879300
4	1	H	1.89774300	0.00046400	0.23513500
5	8	O	-0.90166700	-1.31115800	0.26299600
6	8	O	0.58857900	0.02007900	-1.44077500

$H_2PO_4^-$

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	15	P	0.00000000	0.11865700	0.13551100
2	8	O	-0.00038600	1.61173500	0.23925800
3	8	O	-1.29908100	-0.33864400	-0.83656000
4	1	H	-1.57328000	-1.18170900	-0.45182000
5	8	O	1.29871600	-0.33789500	-0.83727900
6	8	O	0.00069800	-0.86237100	1.29355400
7	1	H	1.57370600	-1.18074200	-0.45263000

^{2}0

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.60639800	-0.00000600	-0.00008200
2	7	N	0.92943700	1.30034200	-0.00025400
3	7	N	0.92930100	-1.30046300	-0.00019300
4	6	C	4.61732900	-0.70249400	0.00027800
5	6	C	3.41744600	-1.41237400	0.00013200
6	6	C	2.20324700	-0.71188900	-0.00012300
7	6	C	2.20326400	0.71170500	-0.00019100
8	6	C	3.41751800	1.41213300	-0.00007800
9	6	C	4.61736300	0.70220600	0.00017400
10	1	H	5.56489400	-1.24539500	0.00042400
11	1	H	3.43464300	-2.50355500	0.00011600
12	1	H	3.43474200	2.50331500	-0.00022700
13	1	H	5.56495900	1.24505300	0.00024700
14	6	C	-2.92261800	-2.19312800	0.00021300
15	6	C	-0.83217400	-2.80836400	-0.00001200
16	6	C	-1.58574700	-3.96563600	-0.00007200
17	7	N	-2.89026400	-3.54899800	0.00006900
18	1	H	-3.70698000	-4.15839400	0.00011000
19	1	H	-3.84639000	-1.61683500	0.00053500
20	1	H	-1.30079900	-5.01593200	-0.00020500
21	6	C	-1.58539200	3.96578300	0.00021100
22	6	C	-0.83193600	2.80844600	0.00005200
23	6	C	-2.92243400	2.19339700	-0.00006600
24	7	N	-2.88995100	3.54926100	0.00015300
25	1	H	-3.70660800	4.15873400	0.00024300
26	1	H	-1.30033800	5.01605100	0.00039400
27	1	H	-3.84624900	1.61718700	-0.00015700
28	6	C	0.58879300	-2.54784700	0.00000200
29	6	C	0.58903200	2.54774900	-0.00005400
30	1	H	1.31113100	3.37349500	-0.00005800
31	1	H	1.31073500	-3.37372800	0.00000200
32	7	N	-1.69435600	-1.71157700	0.00012500

33	7	N	-1.69421500	1.71172700	-0.00016400

^{3}1

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.62329900	0.12348100	-0.00000200
2	7	N	1.12473200	1.14053300	0.00000300
3	7	N	0.68485400	-1.41350500	0.00000100
4	6	C	4.41898500	-1.39898500	0.00001100
5	6	C	3.12056500	-1.92027800	0.00000700
6	6	C	2.03196300	-1.04700000	0.00000500
7	6	C	2.25921500	0.38296500	0.00000600
8	6	C	3.58673000	0.88431400	0.00000900
9	6	C	4.64881700	-0.00299400	0.00001200
10	1	H	5.27071200	-2.08358700	0.00001300
11	1	H	2.97577000	-3.00191600	0.00000600
12	1	H	3.77236800	1.95950000	0.00001000
13	1	H	5.67377900	0.37434900	0.00001400
14	6	C	-3.25814200	-1.67034100	-0.00000900
15	6	C	-1.29565700	-2.61647100	-0.00000400
16	6	C	-2.22987000	-3.63896500	-0.00000700
17	7	N	-3.44525900	-3.01743500	-0.00001000
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22	6	C	-0.35134100	2.90725400	0.00000000
23	6	C	-2.49516300	2.68917500	-0.00000600
24	7	N	-2.29265800	4.05124700	-0.00000500
25	1	H	-0.50852800	5.19278200	0.00000000
26	1	H	-3.49776500	2.25654000	-0.00000800
27	6	C	0.14307300	-2.59342000	0.00000000
28	6	C	0.97487500	2.46540500	0.00000300
29	1	H	1.81808300	3.16481200	0.00000600
30	1	H	0.71899700	-3.52743400	0.00000100
31	7	N	-1.97045000	-1.39404800	-0.00000500
32	7	N	-1.38264700	1.96507600	-0.00000300

^{4}2

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.65938900	0.00002100	-0.00029200
2	7	N	-0.89833100	1.29852600	0.00040900
3	7	N	-0.89826600	-1.29857300	-0.00028800
4	6	C	-4.57865100	-0.70234800	0.00013700
5	6	C	-3.37400300	-1.41786000	-0.00016000
6	6	C	-2.15275200	-0.72290400	-0.00002700
7	6	C	-2.15278800	0.72279700	0.00037200
8	6	C	-3.37407200	1.41769100	0.00067100
9	6	C	-4.57868700	0.70211700	0.00055900
10	1	H	-5.52686300	-1.24532100	0.00004300
11	1	H	-3.39662600	-2.50921900	-0.00049800
12	1	H	-3.39675300	2.50904800	0.00098600
13	1	H	-5.52692400	1.24504500	0.00078900
14	6	C	2.93309900	-2.23954900	-0.00011600
15	6	C	0.85361600	-2.79294200	-0.00061400
16	6	C	1.70095900	-3.98782400	0.00009600
17	7	N	2.95427300	-3.61713400	0.00030800
18	1	H	3.85007100	-1.64563800	-0.00006300
19	1	H	1.37961900	-5.03294800	0.00029700
20	6	C	1.70069400	3.98791900	0.00020500
21	6	C	0.85346900	2.79298400	0.00007600
22	6	C	2.93298300	2.23968400	-0.00005300
23	7	N	2.95408700	3.61727200	0.00027700
24	1	H	1.37929500	5.03302500	0.00055600
25	1	H	3.84999300	1.64582400	-0.00071300
26	6	C	-0.54267300	-2.57012800	-0.00045100
27	6	C	-0.54280300	2.57009800	0.00047500
28	1	H	-1.25721900	3.40151700	0.00065900
29	1	H	-1.25704600	-3.40158000	-0.00034800
30	7	N	1.70915000	-1.70520900	-0.00086300
31	7	N	1.70906200	1.70529500	0.00012100

$^{4}3_{phos}$

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.00193400	0.21636200	-0.49735200
2	7	N	1.21846200	-1.40928200	-0.40404100
3	7	N	1.81879700	1.09625500	-0.24986900
4	6	C	5.07446800	-0.34984600	0.78017500
5	6	C	4.14189100	0.62380400	0.47174700
6	6	C	2.83514800	0.25071700	0.07391200
7	6	C	2.49386600	-1.15809200	-0.00190300
8	6	C	3.47467100	-2.12709100	0.32361400
9	6	C	4.74100900	-1.72618800	0.70665400
10	1	H	6.08037900	-0.05727500	1.08983200
11	1	H	4.40790600	1.67987500	0.54085000
12	1	H	3.22638400	-3.18854000	0.27406600
13	1	H	5.49402600	-2.47571900	0.96016000
14	6	C	-1.60781200	2.91888400	-0.86529700
15	6	C	0.52717500	2.98060000	-0.57864200
16	6	C	-0.00680200	4.31404900	-0.59551500
17	7	N	-1.31427600	4.26342200	-0.77306200
18	1	H	-2.62267300	2.52810100	-0.94232300
19	1	H	0.53964400	5.25144900	-0.47157500
20	6	C	-1.79526100	-3.40551400	-1.26872000
21	6	C	-0.73682200	-2.45609400	-1.03919900
22	6	C	-2.53837700	-1.43084100	-1.59626100
23	7	N	-2.89340100	-2.76428200	-1.61380600
24	1	H	-1.74431300	-4.49226800	-1.17466400
25	1	H	-3.25250000	-0.62994900	-1.78493300
26	6	C	1.77698200	2.42084300	-0.29193100
27	6	C	0.58415900	-2.55726200	-0.58984400
28	1	H	1.04704400	-3.53370200	-0.40057100
29	1	H	2.65209700	3.05235000	-0.09279200
30	7	N	-0.55355500	2.12845900	-0.78601000
31	7	N	-1.27466500	-1.20120100	-1.28461800
32	15	P	-2.19453000	-0.10826100	1.64226600
33	8	O	-2.80494300	0.47808600	2.94442300
34	8	O	-2.44226600	-1.73550400	1.61089400
35	1	H	-3.38908300	-1.92274200	1.68652500
36	8	O	-3.11385400	0.54271000	0.57861200
37	8	O	-0.68548300	0.03426200	1.45503800

[2]3

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.64216100	0.00000000	0.09785900
2	7	N	0.93767100	-1.28987800	-0.10310100
3	7	N	0.93767100	1.28987800	-0.10310100
4	6	C	4.56104200	0.72458400	-0.13950600
5	6	C	3.39856900	1.44570600	-0.11982700
6	6	C	2.14725900	0.75101400	-0.09634200
7	6	C	2.14725900	-0.75101400	-0.09634200
8	6	C	3.39856900	-1.44570600	-0.11982700
9	6	C	4.56104200	-0.72458400	-0.13950600
10	1	H	5.52258300	1.24445600	-0.15312400
11	1	H	3.42386700	2.53620200	-0.11555900
12	1	H	3.42386700	-2.53620200	-0.11555900
13	1	H	5.52258300	-1.24445600	-0.15312400
14	6	C	-2.87423000	2.26498100	-0.21683500
15	6	C	-0.78939100	2.80995900	-0.22520100
16	6	C	-1.62547900	4.00254100	-0.35739600
17	7	N	-2.87986100	3.64781500	-0.35142500
18	1	H	-3.80396300	1.69225400	-0.18228200
19	1	H	-1.29231600	5.03933200	-0.45387700
20	6	C	-1.62547900	-4.00254200	-0.35739600
21	6	C	-0.78939100	-2.80995900	-0.22520100
22	6	C	-2.87423000	-2.26498100	-0.21683500
23	7	N	-2.87986000	-3.64781500	-0.35142500
24	1	H	-1.29231600	-5.03933200	-0.45387700
25	1	H	-3.80396300	-1.69225400	-0.18228200
26	6	C	0.56921200	2.59390200	-0.20257200
27	6	C	0.56921200	-2.59390200	-0.20257200
28	1	H	1.29129700	-3.41328200	-0.28264900
29	1	H	1.29129700	3.41328200	-0.28264900
30	7	N	-1.67851400	1.72117800	-0.13611500
31	7	N	-1.67851400	-1.72117800	-0.13611500
32	8	O	-0.51420200	0.00000000	2.30157400
33	1	H	-0.75029100	-0.76852800	2.84280100
34	1	H	-0.75029100	0.76852800	2.84280100

^{3}4

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.62217400	0.07565600	0.04713000
2	7	N	-1.03734200	1.25740000	-0.06105400
3	7	N	-0.86641200	-1.31694000	-0.10932800
4	6	C	-4.52658000	-0.98997800	-0.08101000
5	6	C	-3.31320600	-1.63195100	-0.09207400
6	6	C	-2.11587800	-0.85605300	-0.08264500
7	6	C	-2.21477500	0.63493200	-0.05945000
8	6	C	-3.50435100	1.24656600	-0.05249400
9	6	C	-4.62216300	0.45035400	-0.06185500
10	1	H	-5.44985300	-1.57522600	-0.08566100
11	1	H	-3.26624600	-2.72168500	-0.10529900
12	1	H	-3.60117100	2.33294900	-0.03386400
13	1	H	-5.61464500	0.90843700	-0.05260100
14	6	C	3.00784700	-2.05108600	-0.25772800
15	6	C	0.95686000	-2.72264300	-0.21347400
16	6	C	1.86170700	-3.86215400	-0.32397500
17	7	N	3.09409100	-3.42930400	-0.35342800
18	1	H	3.89997300	-1.42024600	-0.25343900
19	1	H	1.59426300	-4.92054600	-0.38321200
20	6	C	1.34453200	4.13674000	-0.21661400
21	6	C	0.58802400	2.88808400	-0.13498000
22	6	C	2.70410800	2.47969400	-0.17330400
23	7	N	2.61939400	3.86256600	-0.23986800
24	1	H	0.94525900	5.15369000	-0.25766400
25	1	H	3.66843600	1.96611400	-0.17727300
26	6	C	-0.41622300	-2.59080600	-0.17411600
27	6	C	-0.75751600	2.58117200	-0.10844700
28	1	H	-1.53213000	3.35457600	-0.14069300
29	1	H	-1.08315100	-3.45885100	-0.20636500
30	7	N	1.77708600	-1.57983200	-0.17805700
31	7	N	1.54350000	1.85704100	-0.10805200
32	8	O	0.86006800	-0.53825600	2.14659800
33	1	H	1.64914300	-0.34093800	2.69802600

^{2}1’

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.57536900	0.00003500	0.14544500
2	7	N	0.96279100	1.29904500	-0.11992300
3	7	N	0.96274000	-1.29906000	-0.11989000
4	6	C	4.65155200	-0.70222800	-0.09151300
5	6	C	3.45094500	-1.41138800	-0.09708100
6	6	C	2.23605200	-0.71187100	-0.10560400
7	6	C	2.23607800	0.71180900	-0.10562000
8	6	C	3.45099700	1.41128200	-0.09711000
9	6	C	4.65157700	0.70207800	-0.09152700
10	1	H	5.59895000	-1.24526700	-0.08024800
11	1	H	3.46633200	-2.50271800	-0.08470300
12	1	H	3.46642000	2.50261200	-0.08475400
13	1	H	5.59899600	1.24508300	-0.08027200
14	6	C	-2.88490000	-2.22345900	-0.13329900
15	6	C	-0.79421400	-2.80408500	-0.29065600
16	6	C	-1.53693800	-3.95982000	-0.44102400
17	7	N	-2.84380600	-3.56605800	-0.33708000
18	1	H	-3.65483000	-4.17827900	-0.40558900
19	1	H	-3.81248100	-1.66539300	-0.01672400
20	1	H	-1.24303400	-4.99387000	-0.60912600
21	6	C	-1.53680100	3.95989700	-0.44096200
22	6	C	-0.79411200	2.80413300	-0.29066100
23	6	C	-2.88481500	2.22357700	-0.13322800
24	7	N	-2.84367900	3.56618000	-0.33697300
25	1	H	-3.65468300	4.17843300	-0.40542300
26	1	H	-1.24286600	4.99394300	-0.60904000
27	1	H	-3.81241000	1.66554200	-0.01661900
28	6	C	0.62540000	-2.53157100	-0.30744000
29	6	C	0.62549300	2.53156800	-0.30746600
30	1	H	1.34718200	3.33816200	-0.48926600
31	1	H	1.34706000	-3.33818900	-0.48924600
32	7	N	-1.66351000	-1.73102300	-0.10101200
33	7	N	-1.66344100	1.73109600	-0.10101400
34	8	O	-0.64022600	-0.00014100	2.34395300

35	1	H	-0.47578100	0.77040500	2.90610200
36	1	H	-0.47688700	-0.77115500	2.90578200

^{3}2’

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.60603100	0.03415700	0.10581700
2	7	N	0.94978100	1.31510600	-0.09511000
3	7	N	0.93288900	-1.28458700	-0.12974800
4	6	C	4.62403300	-0.71719100	-0.12620700
5	6	C	3.41820700	-1.41748700	-0.12847100
6	6	C	2.20926400	-0.70716700	-0.12096200
7	6	C	2.21921200	0.71686400	-0.10408300
8	6	C	3.43991300	1.40628900	-0.09569600
9	6	C	4.63468000	0.68698100	-0.10966700
10	1	H	5.56722000	-1.26766800	-0.13134500
11	1	H	3.42463900	-2.50892000	-0.13212700
12	1	H	3.46546500	2.49717100	-0.07146900
13	1	H	5.58633300	1.22265300	-0.10186800
14	6	C	-2.93652100	-2.15629100	-0.15751400
15	6	C	-0.85105500	-2.76635800	-0.24878100
16	6	C	-1.60522000	-3.92318200	-0.33012700
17	7	N	-2.90696600	-3.51100400	-0.26921900
18	1	H	-3.72401600	-4.11855800	-0.30340800
19	1	H	-3.86010300	-1.58373600	-0.08935100
20	1	H	-1.31956700	-4.96915300	-0.42307600
21	6	C	-1.52618900	4.01369000	-0.25441200
22	6	C	-0.79319400	2.84416700	-0.18191900
23	6	C	-2.88958000	2.27424500	-0.04679900
24	7	N	-2.83542400	3.62607700	-0.16626700
25	1	H	-3.64110800	4.24925800	-0.18776000
26	1	H	-1.22325500	5.05383700	-0.35694900
27	1	H	-3.82203400	1.71906900	0.04159100
28	6	C	0.56829600	-2.51916500	-0.26388200
29	6	C	0.62167600	2.55997000	-0.21597300
30	1	H	1.35161200	3.36802000	-0.35145400
31	1	H	1.27802900	-3.34368300	-0.40944300
32	7	N	-1.71139700	-1.67510900	-0.14502400
33	7	N	-1.67238000	1.76967600	-0.05429200
34	8	O	-0.26862400	-0.56004600	2.14431100
35	1	H	0.54402500	-0.28177500	2.61805600

^{4}3’

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.59379200	0.04802900	0.06915300
2	7	N	-1.10387300	1.15026200	-0.14565100
3	7	N	-0.79850200	-1.41910000	-0.05258100
4	6	C	-4.52506300	-1.21014100	-0.00860300
5	6	C	-3.25575300	-1.79746500	0.00672300
6	6	C	-2.12336900	-0.98291000	-0.04760100
7	6	C	-2.27576100	0.45521800	-0.10857700
8	6	C	-3.57605900	1.02396000	-0.12656200
9	6	C	-4.68233200	0.19444200	-0.07652200
10	1	H	-5.41108800	-1.84820800	0.03476900
11	1	H	-3.16560400	-2.88334600	0.06661500
12	1	H	-3.70627400	2.10624100	-0.17202900
13	1	H	-5.68634800	0.62424700	-0.08478200
14	6	C	3.12535800	-1.91306000	-0.13697900
15	6	C	1.10933300	-2.73193500	-0.15219800
16	6	C	1.97565800	-3.80928600	-0.24374000
17	7	N	3.22780300	-3.26716500	-0.23098900
18	1	H	4.10147100	-3.78978200	-0.28807300
19	1	H	3.98901100	-1.24947700	-0.11351600
20	1	H	1.79451700	-4.88037500	-0.31559600
21	6	C	1.13090800	4.12599900	-0.36274900
22	6	C	0.44939400	2.84976600	-0.24916200
23	6	C	2.58724300	2.56731600	-0.20134300
24	7	N	2.42873500	3.92487400	-0.33440700
25	1	H	0.68034200	5.11651100	-0.46335900
26	1	H	3.57435400	2.10343300	-0.14511400
27	6	C	-0.32531800	-2.62384300	-0.14014700
28	6	C	-0.89351000	2.46030000	-0.23933000
29	1	H	-1.70339400	3.19463800	-0.31305500
30	1	H	-0.95417000	-3.51970400	-0.22119800
31	7	N	1.85935300	-1.55682200	-0.08677500

32	7	N	1.44928900	1.87964200	-0.15472000
33	8	O	0.73999600	0.76583600	2.11965700
34	1	H	1.58323900	0.87429300	2.60926300

^{3}2’’

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.59891300	0.10533700	0.13126200
2	7	N	-1.13780000	1.14109300	-0.14973700
3	7	N	-0.73530300	-1.41583100	-0.08045100
4	6	C	-4.46833600	-1.35132500	-0.08177700
5	6	C	-3.17724300	-1.88805300	-0.05349300
6	6	C	-2.07606200	-1.02967900	-0.08297300
7	6	C	-2.28323200	0.40098400	-0.13104800
8	6	C	-3.60377100	0.91786400	-0.16341400
9	6	C	-4.67871000	0.04560400	-0.13820400
10	1	H	-5.32913000	-2.02389600	-0.05758900
11	1	H	-3.04414500	-2.97010900	-0.00243800
12	1	H	-3.77487500	1.99496800	-0.19816300
13	1	H	-5.69817400	0.43690900	-0.15682200
14	6	C	3.20546100	-1.76129200	-0.16289100
15	6	C	1.22186500	-2.64775100	-0.25225200
16	6	C	2.12658300	-3.68670800	-0.40215000
17	7	N	3.35844400	-3.10312900	-0.34049600
18	1	H	4.25061800	-3.58959500	-0.42099800
19	1	H	4.04390800	-1.07001200	-0.08650500
20	1	H	1.98458700	-4.75654200	-0.54450200
21	6	C	1.00464900	4.18324900	-0.42044800
22	6	C	0.35937400	2.88619800	-0.27594300
23	6	C	2.49673800	2.67223400	-0.16960900
24	7	N	2.30298700	4.02541400	-0.35256500
25	1	H	0.52376400	5.15362100	-0.56691600
26	1	H	3.49631300	2.24227800	-0.07741600
27	6	C	-0.21680800	-2.59188200	-0.25258600
28	6	C	-0.97195400	2.45268000	-0.28843200
29	1	H	-1.80315100	3.15426600	-0.42255200
30	1	H	-0.81065800	-3.50024400	-0.41818800
31	7	N	1.92803100	-1.45380200	-0.10537800
32	7	N	1.38295600	1.95326200	-0.11575300
33	8	O	0.52761800	0.22102600	2.32537400
34	1	H	0.90877200	0.94570500	2.84222000
35	1	H	0.33622600	-0.48211300	2.96225800

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.74008600	0.67732700	0.40988100
2	7	N	-0.52634400	-1.26063400	1.04031300
3	7	N	-2.54082200	-0.10605100	-0.08421800
4	6	C	-3.60704800	-3.64291100	-0.43217000
5	6	C	-3.67526900	-2.26310500	-0.53422600
6	6	C	-2.61818100	-1.46905600	-0.03711800
7	6	C	-1.48439900	-2.11628600	0.58587700
8	6	C	-1.44052000	-3.52805100	0.66313400
9	6	C	-2.48905000	-4.27719900	0.16379300
10	1	H	-4.42222200	-4.25371700	-0.82723500
11	1	H	-4.53463400	-1.79013000	-1.01221600
12	1	H	-0.57375200	-4.02090200	1.10564300
13	1	H	-2.45385000	-5.36733900	0.21810100
14	6	C	-1.68309900	3.74369700	0.12608200
15	6	C	-3.02298400	2.13550600	-0.36983400
16	6	C	-3.63042100	3.38964500	-0.67188500
17	7	N	-2.79502000	4.37410400	-0.36009800
18	1	H	-0.80104200	4.28927900	0.46525800
19	1	H	-4.62175900	3.56708900	-1.09347800
20	6	C	2.84403500	-0.23863000	2.17781200
21	6	C	1.45521300	-0.38702000	1.81624000
22	6	C	2.08126000	1.64141300	1.50132300
23	7	N	3.21315200	1.01255300	1.97650400
24	1	H	3.53036700	-1.02003000	2.50423700
25	1	H	2.07442300	2.69131400	1.21255400
26	6	C	-3.41918200	0.79321200	-0.48255800
27	6	C	0.63174500	-1.51000100	1.61346300
28	1	H	0.98274800	-2.51786000	1.86177000
29	1	H	-4.41168200	0.52642700	-0.86838600
30	7	N	-1.76209700	2.42115100	0.15072700

31	7	N	1.01156200	0.86168200	1.42637900
32	8	O	0.07544600	0.65009100	-1.54606700
33	1	H	1.07295700	0.82465600	-1.45012700
34	15	P	3.54086400	-0.11275200	-1.09920700
35	8	O	3.90379400	-0.71807700	-2.48689800
36	8	O	4.92155500	0.28505100	-0.35134100
37	1	H	4.71947600	0.83397500	0.42821200
38	8	O	2.62365000	1.11057000	-1.12317400
39	8	O	2.91812400	-1.36367000	-0.40287100
40	8	O	0.53088700	-1.64295900	-1.59475500
41	1	H	1.42448400	-1.63131100	-1.15788000
42	1	H	0.72074300	-1.39760100	-2.51089700

^{3}TS1

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.66654200	0.59039600	-0.51121300
2	7	N	0.99651700	-1.37137300	-0.90640500
3	7	N	2.59949700	0.39907200	0.06010200
4	6	C	4.54231100	-2.65871400	0.88418800
5	6	C	4.23814400	-1.30814300	0.80436200
6	6	C	3.03545800	-0.89348100	0.19314200
7	6	C	2.13197800	-1.88529100	-0.33976400
8	6	C	2.46437500	-3.25271800	-0.23316100
9	6	C	3.65519000	-3.63017700	0.36768500
10	1	H	5.47338900	-2.97680600	1.35876500
11	1	H	4.92167100	-0.56624900	1.22099500
12	1	H	1.78115900	-4.01020600	-0.62004000
13	1	H	3.90875800	-4.68949500	0.44955800
14	6	C	0.63245300	3.79423100	-0.36763600
15	6	C	2.40048500	2.69714400	0.17797100
16	6	C	2.60059800	4.09366400	0.39823600
17	7	N	1.50370400	4.75921000	0.05534200
18	1	H	-0.37953100	4.02219000	-0.70593500
19	1	H	3.49456800	4.58704900	0.78489000
20	6	C	-2.48971400	-1.41754800	-2.12222200
21	6	C	-1.14107400	-1.16457200	-1.74773500
22	6	C	-2.23165100	0.69000600	-1.82259000
23	7	N	-3.15686600	-0.26387800	-2.16029000
24	1	H	-2.96658500	-2.38096000	-2.30311800
25	1	H	-2.48570500	1.74523900	-1.72757100
26	6	C	3.17335300	1.54026500	0.38288100
27	6	C	-0.05963100	-1.98925100	-1.38584600
28	1	H	-0.13493600	-3.08082700	-1.45992100
29	1	H	4.19182500	1.60315800	0.78805000
30	7	N	1.11267100	2.55752900	-0.32463900
31	7	N	-1.02348500	0.20865700	-1.57434300
32	8	O	-0.08699200	0.20488600	1.40008100
33	1	H	-1.01784500	0.54246600	1.40732100
34	15	P	-3.70831300	-0.18507200	1.12040400
35	8	O	-4.32979200	-0.05943800	2.53776000
36	8	O	-4.87560700	-0.04822900	0.03916600
37	1	H	-4.53410300	-0.16934800	-0.88073000
38	8	O	-2.71234900	0.99242600	1.10246700
39	8	O	-3.01730100	-1.56343000	0.82911100
40	8	O	-0.65209500	-1.70275900	1.46000400
41	1	H	-1.97124900	-1.63120600	1.15295500
42	1	H	-0.53124400	-1.64506900	2.41974100

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.61366100	0.10108800	-0.15974700
2	7	N	0.90333500	-1.23238800	-0.32851400
3	7	N	0.99057400	1.34107600	-0.17475000
4	6	C	4.62731000	0.63048400	-0.14115900
5	6	C	3.46832400	1.38344100	-0.12546300
6	6	C	2.21151700	0.73499000	-0.18247300
7	6	C	2.16060900	-0.71715400	-0.26104600
8	6	C	3.36985000	-1.45522300	-0.27264100
9	6	C	4.57806900	-0.78874500	-0.21373600
10	1	H	5.59768000	1.12969600	-0.09569400
11	1	H	3.52231800	2.47155500	-0.06622600
12	1	H	3.34620600	-2.54446300	-0.32841100
13	1	H	5.51121700	-1.35609700	-0.22248300
14	6	C	-2.80048200	2.42177200	-0.20062900

15	6	C	-0.70170400	2.91030800	-0.18389200
16	6	C	-1.48911900	4.10931000	-0.18666800
17	7	N	-2.77191300	3.79212800	-0.19560300
18	1	H	-3.73488100	1.85797000	-0.21065500
19	1	H	-1.13306100	5.14149000	-0.18263300
20	6	C	-1.75484600	-3.81777300	-0.55718400
21	6	C	-0.89044200	-2.67497500	-0.46413400
22	6	C	-2.95126100	-2.04900900	-0.46650000
23	7	N	-3.01324500	-3.41729400	-0.55558000
24	1	H	-1.46621500	-4.86884800	-0.62191600
25	1	H	-3.84671100	-1.42539500	-0.44532200
26	6	C	0.66810700	2.62997100	-0.17862500
27	6	C	0.49450200	-2.49150600	-0.42014900
28	1	H	1.18479700	-3.34207800	-0.46163600
29	1	H	1.41564000	3.43226000	-0.18689300
30	7	N	-1.60808700	1.84491000	-0.19353300
31	7	N	-1.72427500	-1.55514800	-0.40966200
32	8	O	-0.70585400	-0.14886800	2.16137300
33	8	O	-0.14986900	-1.40950600	2.56802300
34	1	H	-0.90954200	-1.81137000	3.02585100
35	1	H	-0.22281300	0.48239200	2.72280300

[4]5

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.60926500	0.07427900	0.01394000
2	7	N	-1.05751600	1.24333200	-0.04679900
3	7	N	-0.86487600	-1.33051100	-0.07951500
4	6	C	-4.52086600	-1.03293100	-0.04248500
5	6	C	-3.30802100	-1.66753800	-0.05802000
6	6	C	-2.11311100	-0.88241800	-0.05380600
7	6	C	-2.22467400	0.61644500	-0.03426000
8	6	C	-3.52306800	1.21827200	-0.01999500
9	6	C	-4.62893400	0.41285800	-0.02339800
10	1	H	-5.44148800	-1.62270300	-0.04276000
11	1	H	-3.25409300	-2.75690600	-0.06988300
12	1	H	-3.62833200	2.30383800	-0.00299200
13	1	H	-5.62668700	0.85952000	-0.00995300
14	6	C	3.01389300	-2.03506500	-0.20892400
15	6	C	0.96654400	-2.72808000	-0.19281800
16	6	C	1.88612400	-3.85880400	-0.27615900
17	7	N	3.11399500	-3.41295200	-0.28714900
18	1	H	3.89952300	-1.39556000	-0.18951900
19	1	H	1.63131500	-4.92089300	-0.32617000
20	6	C	1.30926200	4.13907900	-0.18539200
21	6	C	0.55512500	2.88694800	-0.12320200
22	6	C	2.67451300	2.48346600	-0.17865200
23	7	N	2.58377500	3.86832900	-0.21929200
24	1	H	0.90751900	5.15579000	-0.20444400
25	1	H	3.64094100	1.97392400	-0.19283100
26	6	C	-0.40300900	-2.60766000	-0.14969300
27	6	C	-0.78367400	2.57572800	-0.08297500
28	1	H	-1.56415800	3.34343400	-0.09066300
29	1	H	-1.06619500	-3.47840000	-0.17874300
30	7	N	1.77717300	-1.57515000	-0.16253300
31	7	N	1.51738200	1.85747400	-0.12279200
32	8	O	1.24285100	-0.41144700	2.13861700

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.49919300	0.32160000	-0.09489400
2	7	N	0.49270700	-1.45424500	-0.28080000
3	7	N	1.45571500	0.93322000	-0.09289300
4	6	C	4.60910700	-0.95749900	-0.04194300
5	6	C	3.79345800	0.14692400	-0.01020000
6	6	C	2.37968900	-0.02835500	-0.08801700
7	6	C	1.82376800	-1.40729100	-0.19862000
8	6	C	2.71905000	-2.51709300	-0.22961400
9	6	C	4.07175500	-2.29026000	-0.15269200
10	1	H	5.69335300	-0.83294900	0.01810700
11	1	H	4.22215300	1.14635700	0.07561100
12	1	H	2.33507400	-3.53471400	-0.31345900
13	1	H	4.76539600	-3.13470600	-0.17473000
14	6	C	-1.70834500	3.27466300	-0.26596400
15	6	C	0.42282400	2.99191700	-0.13315600

16	6	C	0.10135700	4.41841300	-0.16532000
17	7	N	-1.19197600	4.56278600	-0.24699700
18	1	H	-2.78329800	3.09146400	-0.33091000
19	1	H	0.80129800	5.25750700	-0.13192400
20	6	C	-2.88668700	-2.99009400	-0.71911000
21	6	C	-1.66847600	-2.19878100	-0.55292200
22	6	C	-3.38767000	-0.90745300	-0.64824000
23	7	N	-3.91275900	-2.18797600	-0.77164700
24	1	H	-2.96715800	-4.07791800	-0.79048800
25	1	H	-4.02945900	-0.02344200	-0.66573400
26	6	C	1.60367600	2.27652200	-0.07529000
27	6	C	-0.32957500	-2.51501600	-0.44228200
28	1	H	0.03066400	-3.54782500	-0.49421600
29	1	H	2.58041700	2.77033800	-0.03516300
30	7	N	-0.80608000	2.31564500	-0.20071400
31	7	N	-2.07930700	-0.85733700	-0.51392500
32	8	O	-0.51874200	0.21034000	2.15327300
33	8	O	-1.86799700	-1.52456500	2.43038400
34	1	H	-1.42195700	-1.85843600	3.22774600
35	1	H	-2.62767400	-1.03251200	2.78688100
36	8	O	-0.49919300	0.32160000	-0.09489400
37	1	H	0.49270700	-1.45424500	-0.28080000
38	1	H	1.45571500	0.93322000	-0.09289300
39	8	O	4.60910700	-0.95749900	-0.04194300
40	1	H	3.79345800	0.14692400	-0.01020000
41	1	H	2.37968900	-0.02835500	-0.08801700
42	8	O	1.82376800	-1.40729100	-0.19862000
43	1	H	2.71905000	-2.51709300	-0.22961400
44	1	H	4.07175500	-2.29026000	-0.15269200

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.49223500	0.39013500	-0.10416200
2	7	N	0.38770700	-1.44668000	-0.33797000
3	7	N	1.49349900	0.87956800	-0.09361300
4	6	C	4.52503600	-1.20106400	-0.05288000
5	6	C	3.77571000	-0.05017900	-0.00521200
6	6	C	2.35546000	-0.13852900	-0.10082900
7	6	C	1.71981300	-1.47856000	-0.24528200
8	6	C	2.54529900	-2.63812000	-0.29287600
9	6	C	3.90971500	-2.49520300	-0.19829400
10	1	H	5.61395700	-1.14316100	0.02194700
11	1	H	4.26232800	0.91950700	0.10852600
12	1	H	2.10140900	-3.62885500	-0.39995300
13	1	H	4.55057600	-3.38016800	-0.23012800
14	6	C	-1.52868400	3.39989800	-0.19129600
15	6	C	0.58462900	2.99496300	-0.07634300
16	6	C	0.34368800	4.43759100	-0.06861600
17	7	N	-0.93969700	4.65589000	-0.14022700
18	1	H	-2.61258100	3.27963500	-0.25533200
19	1	H	1.08960400	5.23512400	-0.01597900
20	6	C	-3.09121100	-2.75990900	-0.71677600
21	6	C	-1.82095200	-2.04864900	-0.57933200
22	6	C	-3.46450900	-0.65742900	-0.53924000
23	7	N	-4.06857500	-1.89732100	-0.68761500
24	1	H	-3.24019300	-3.83748200	-0.82481400
25	1	H	-4.05193300	0.26227900	-0.48727100
26	6	C	1.72165500	2.21059400	-0.04073900
27	6	C	-0.50047100	-2.44876400	-0.51950200
28	1	H	-0.20449800	-3.49886000	-0.61377900
29	1	H	2.72623600	2.64346300	0.01191300
30	7	N	-0.68151400	2.39082300	-0.15638700
31	7	N	-2.14855200	-0.68873900	-0.46993700
32	8	O	-0.25762000	-0.25826600	1.98307400
33	8	O	-1.91600200	-1.71604000	2.41564900
34	1	H	-0.82659300	-1.13336700	2.42184100
35	1	H	-2.49567400	-1.25220100	3.05748400
36	8	O	-0.49223500	0.39013500	-0.10416200
37	1	H	0.38770700	-1.44668000	-0.33797000
38	1	H	1.49349900	0.87956800	-0.09361300
39	8	O	4.52503600	-1.20106400	-0.05288000
40	1	H	3.77571000	-0.05017900	-0.00521200
41	1	H	2.35546000	-0.13852900	-0.10082900
42	8	O	1.71981300	-1.47856000	-0.24528200
43	1	H	2.54529900	-2.63812000	-0.29287600
44	1	H	3.90971500	-2.49520300	-0.19829400

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-1.21047300	-0.61528600	-0.30701000
2	7	N	0.27662700	0.52429900	-1.07743200
3	7	N	-2.04101800	1.22757400	-0.21421400
4	6	C	-0.46750100	4.57129100	-0.52633700
5	6	C	-1.46307000	3.63805500	-0.28201700
6	6	C	-1.18884900	2.26805900	-0.46457800
7	6	C	0.12229600	1.86499500	-0.93017500
8	6	C	1.13018900	2.83926900	-1.13585700
9	6	C	0.82929700	4.17233900	-0.94008800
10	1	H	-0.67720900	5.63295300	-0.37579500
11	1	H	-2.44467600	3.96004200	0.06908900
12	1	H	2.14086000	2.52390600	-1.39079000
13	1	H	1.60341100	4.92892100	-1.08382400
14	6	C	-3.87138600	-2.20040100	0.47653500
15	6	C	-3.86614200	-0.04691300	0.40326200
16	6	C	-5.14250500	-0.51950900	0.81581400
17	7	N	-5.13321900	-1.84993100	0.85556200
18	1	H	-3.54370700	-3.23931000	0.41230500
19	1	H	-6.02404700	0.07201700	1.07007700
20	6	C	2.16478500	-2.64187500	-1.48270300
21	6	C	1.23657200	-1.54907300	-1.33427000
22	6	C	0.27739000	-3.40622200	-0.83575400
23	7	N	1.55512400	-3.77330500	-1.18358000
24	1	H	3.22088900	-2.55671700	-1.73879700
25	1	H	-0.47344500	-4.13325300	-0.52103000
26	6	C	-3.29664400	1.21967000	0.18687700
27	6	C	1.35124100	-0.15964400	-1.45157900
28	1	H	2.28532500	0.30238600	-1.78026200
29	1	H	-3.87722200	2.13803700	0.34200600
30	7	N	-3.07487800	-1.17715400	0.19299600
31	7	N	0.03104800	-2.10654800	-0.90812900
32	8	O	-0.00116000	-0.75077100	1.55132000
33	15	P	3.56184700	-0.11542300	0.86393400
34	8	O	4.89392700	0.08412200	1.63701800
35	8	O	2.76430500	-1.38102800	1.52209400
36	1	H	1.82302900	-1.17852900	1.68580700
37	8	O	2.57799100	1.06909200	0.86291900
38	8	O	4.08900800	-0.51251800	-0.53104600
39	8	O	0.37451900	1.31352200	1.97803500
40	1	H	0.53781600	1.09572400	2.90836500
41	1	H	1.32646000	1.23432200	1.53319600

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.99974100	-0.68649400	0.25269900
2	7	N	0.13156600	0.96899300	1.05253500
3	7	N	2.47785800	0.70653400	0.03814400
4	6	C	2.22989800	4.41081000	-0.00397200
5	6	C	2.79834400	3.15742200	-0.17509900
6	6	C	2.06612300	2.00438600	0.17699100
7	6	C	0.73766600	2.14900500	0.72874900
8	6	C	0.17673700	3.43719000	0.86828100
9	6	C	0.91919700	4.55018200	0.51111000
10	1	H	2.79416000	5.30284500	-0.28566300
11	1	H	3.79976100	3.06030500	-0.59815700
12	1	H	-0.84462300	3.54665600	1.23558100
13	1	H	0.48450300	5.54696700	0.61309400
14	6	C	2.94659300	-3.21149700	-0.19055400
15	6	C	3.70957300	-1.20788600	-0.35735000
16	6	C	4.73490100	-2.15121900	-0.66437800
17	7	N	4.25158900	-3.38429900	-0.55575500
18	1	H	2.26708500	-4.04921400	-0.02524900
19	1	H	5.76918300	-1.94469000	-0.94660700
20	6	C	-2.69549700	-1.21447200	1.93792300
21	6	C	-1.44769500	-0.59533500	1.64456300
22	6	C	-1.44525200	-2.61669800	0.91064100
23	7	N	-2.69327200	-2.45530900	1.45066000
24	1	H	-3.57043900	-0.75711600	2.39853200
25	1	H	-1.13028100	-3.54130200	0.42549700
26	6	C	3.64150600	0.19636300	-0.30885500
27	6	C	-1.02906500	0.74799200	1.62869800

28	1	H	-1.67444700	1.54080600	2.02061600
29	1	H	4.52033400	0.81497800	-0.53409200
30	7	N	2.57025600	-1.94566300	-0.05429500
31	7	N	-0.66184100	-1.55251400	1.01254600
32	8	O	0.61837100	-0.30856100	-1.80042700
33	15	P	-3.84725400	0.01761500	-0.86379600
34	8	O	-4.64075000	0.89203700	-1.84456500
35	8	O	-4.69978500	-1.29110800	-0.49681100
36	1	H	-4.18027800	-1.96010400	-0.00888000
37	8	O	-2.48947700	-0.58203100	-1.40632900
38	8	O	-3.63569400	0.96920600	0.33371900
39	8	O	-0.63233400	1.11799000	-1.70065600
40	1	H	-0.53238200	1.27865700	-2.65241700
41	1	H	-1.74014900	0.12341300	-1.54037500

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.60786300	0.08736100	-0.16775200
2	7	N	0.90140900	-1.25564100	-0.29969600
3	7	N	0.99966000	1.31997400	-0.18050900
4	6	C	4.63293800	0.60003300	-0.13099400
5	6	C	3.47642400	1.35569300	-0.12059500
6	6	C	2.21709400	0.71008700	-0.17609000
7	6	C	2.16179900	-0.74258900	-0.24272500
8	6	C	3.36837800	-1.48344200	-0.25081200
9	6	C	4.57887700	-0.81933300	-0.19616800
10	1	H	5.60482000	1.09642400	-0.08810900
11	1	H	3.53263600	2.44403100	-0.06897500
12	1	H	3.34235900	-2.57301600	-0.30034900
13	1	H	5.51027300	-1.38968700	-0.20274300
14	6	C	-2.78802700	2.41039100	-0.24410500
15	6	C	-0.68876900	2.89204600	-0.19238000
16	6	C	-1.47343200	4.09463600	-0.19394900
17	7	N	-2.75572800	3.78175200	-0.22549500
18	1	H	-3.72416600	1.85008800	-0.27224300
19	1	H	-1.11376600	5.12536600	-0.17361400
20	6	C	-1.77248000	-3.82548400	-0.52835700
21	6	C	-0.90045400	-2.68983200	-0.43625100
22	6	C	-2.95799000	-2.04993400	-0.43120700
23	7	N	-3.02866300	-3.41622000	-0.52253300
24	1	H	-1.49162000	-4.87849400	-0.59504700
25	1	H	-3.84917700	-1.42036600	-0.40678100
26	6	C	0.67992000	2.60962500	-0.17074100
27	6	C	0.48568700	-2.51304300	-0.39730600
28	1	H	1.17217500	-3.36633900	-0.44942800
29	1	H	1.42868400	3.41034700	-0.15390900
30	7	N	-1.59811600	1.83021800	-0.22621200
31	7	N	-1.72726500	-1.56396900	-0.37686100
32	8	O	-0.65069500	-0.01708900	2.21408200
33	8	O	-0.34252800	-1.20991500	2.66460200
34	1	H	-0.49729700	-1.18173100	3.63575000

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.74609400	0.59928200	0.62546400
2	7	N	-1.00163300	-1.41164100	0.78843200
3	7	N	-2.60792400	0.41187800	-0.10324800
4	6	C	-4.67397500	-2.60897400	-0.80553800
5	6	C	-4.32432500	-1.26341800	-0.75264200
6	6	C	-3.08432400	-0.88016200	-0.20968600
7	6	C	-2.19351100	-1.89333700	0.28296000
8	6	C	-2.56939200	-3.24859400	0.21766600
9	6	C	-3.79999100	-3.60151600	-0.32181000
10	1	H	-5.63853300	-2.89800100	-1.22929500
11	1	H	-5.01061700	-0.50566900	-1.13469000
12	1	H	-1.89456800	-4.01984400	0.59355600
13	1	H	-4.09021700	-4.65307900	-0.37162700
14	6	C	-0.56775000	3.75958000	0.38290600
15	6	C	-2.33839000	2.70389600	-0.26045100
16	6	C	-2.48095800	4.08977100	-0.50553600
17	7	N	-1.37953300	4.73193300	-0.10153900
18	1	H	0.42594700	3.96221200	0.78585300
19	1	H	-3.33177200	4.60751500	-0.95211000
20	6	C	2.51994600	-1.45104500	1.92488300

21	6	C	1.16320700	-1.21008300	1.55996900
22	6	C	2.18058100	0.66246600	1.87672400
23	7	N	3.13215900	-0.28153200	2.12609100
24	1	H	3.03153000	-2.40945400	2.00696500
25	1	H	2.38236800	1.73142900	1.92773900
26	6	C	-3.12829100	1.55647800	-0.48290000
27	6	C	0.07593000	-2.03966300	1.17857900
28	1	H	0.17461300	-3.13204000	1.17590500
29	1	H	-4.11686600	1.63278500	-0.95427600
30	7	N	-1.08204700	2.53273800	0.32126300
31	7	N	0.99131900	0.16195000	1.54573200
32	8	O	0.39611800	0.15379500	-1.44036800
33	15	P	3.78914400	-0.32050200	-1.11640800
34	8	O	4.34231100	-0.36372300	-2.51400600
35	8	O	4.93891500	-0.29159700	-0.00886800
36	1	H	4.56369700	-0.19538600	0.89857500
37	8	O	2.95795400	1.04169300	-0.78310100
38	8	O	2.79611200	-1.50160600	-0.83393600
39	8	O	0.52978600	-1.12811100	-1.69638200
40	1	H	1.55430400	-1.36777200	-1.40296400
41	1	H	2.02116500	0.92237600	-1.07052900

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.87439900	0.51940100	0.64110000
2	7	N	-1.36154600	-1.44898200	0.67280900
3	7	N	-2.69305800	0.59391600	-0.19730500
4	6	C	-5.12230000	-2.11046700	-1.05789900
5	6	C	-4.59451800	-0.82419800	-0.95251500
6	6	C	-3.33375900	-0.62742200	-0.36560000
7	6	C	-2.60445700	-1.75839400	0.11479800
8	6	C	-3.15282500	-3.04394700	0.00409400
9	6	C	-4.40637900	-3.21863500	-0.58088400
10	1	H	-6.10398500	-2.25358100	-1.51543400
11	1	H	-5.16170300	0.03006900	-1.32687800
12	1	H	-2.60122200	-3.90773200	0.38075800
13	1	H	-4.83079300	-4.22136200	-0.66517300
14	6	C	-0.29963100	3.64248900	0.57707900
15	6	C	-2.14833600	2.84425100	-0.20462300
16	6	C	-2.11348200	4.24412100	-0.37370300
17	7	N	-0.96177100	4.72742200	0.11558600
18	1	H	0.68807100	3.70003800	1.03791600
19	1	H	-2.87258000	4.88519300	-0.82555200
20	6	C	2.11272100	-1.95912100	1.68241900
21	6	C	0.79366300	-1.55423300	1.51381900
22	6	C	2.01144900	0.21039500	1.82200000
23	7	N	2.86513200	-0.84062800	1.88106900
24	1	H	2.55698900	-2.95042700	1.61929200
25	1	H	2.34445200	1.24413400	1.88295800
26	6	C	-3.05901800	1.80929500	-0.52185100
27	6	C	-0.39530300	-2.21974800	1.05948500
28	1	H	-0.43582100	-3.31559300	0.99947000
29	1	H	-4.01526000	2.02943000	-1.01502100
30	7	N	-0.95361000	2.49012400	0.41955500
31	7	N	0.76073200	-0.16533000	1.60817100
32	8	O	0.74831400	0.14295000	-1.26290000
33	15	P	4.23004000	-0.27547900	-0.88845300
34	8	O	5.33547300	-0.01085800	-1.98095400
35	8	O	4.86590500	-0.60015800	0.47525100
36	1	H	3.99160400	-0.72039800	1.34863500
37	8	O	3.32511100	1.04950300	-0.66898100
38	8	O	3.35268200	-1.35859500	-1.54763700
39	8	O	0.90309600	-1.12430400	-1.55333900
40	1	H	1.96446800	-1.27513800	-1.63677100
41	1	H	2.42001300	0.93464800	-1.03975100

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.72030900	0.40287400	0.54383500
2	7	N	-1.56326100	-1.44457500	0.49789500
3	7	N	-2.57230400	0.88101500	-0.05200800
4	6	C	-5.46115300	-1.26974300	-1.03451900
5	6	C	-4.72139700	-0.10807000	-0.82095100
6	6	C	-3.41603200	-0.18894500	-0.30593300

7	6	C	-2.86379000	-1.47492100	-0.01384100
8	6	C	-3.62440600	-2.63235000	-0.23331800
9	6	C	-4.91787400	-2.53034200	-0.74206200
10	1	H	-6.47511300	-1.19542000	-1.43463200
11	1	H	-5.15487700	0.86559600	-1.05659100
12	1	H	-3.20599800	-3.61367000	-0.00044400
13	1	H	-5.50795500	-3.43334400	-0.91216400
14	6	C	0.41438800	3.35971300	0.67471200
15	6	C	-1.64188600	2.99391100	0.11649800
16	6	C	-1.35987300	4.37660700	0.05676600
17	7	N	-0.08422700	4.59036100	0.40513900
18	1	H	1.45262700	3.18490000	0.96178400
19	1	H	-2.03308200	5.18719000	-0.22841400
20	6	C	1.76136200	-2.67474900	1.38018000
21	6	C	0.55446800	-2.01116000	1.25664900
22	6	C	2.03833300	-0.51719500	1.78790000
23	7	N	2.67327200	-1.71667500	1.72986800
24	1	H	2.03623000	-3.71169300	1.20908500
25	1	H	2.56297900	0.41752600	1.96736300
26	6	C	-2.74895800	2.17319900	-0.19356000
27	6	C	-0.73974800	-2.40617600	0.74649200
28	1	H	-0.96526200	-3.46505700	0.56397500
29	1	H	-3.69495600	2.60776700	-0.54354900
30	7	N	-0.46645100	2.36988000	0.53237900
31	7	N	0.75922500	-0.66133500	1.52453600
32	8	O	0.60657200	-0.01551700	-1.22226000
33	15	P	4.06590500	-0.14335900	-0.88725300
34	8	O	5.28655400	0.35033500	-1.70927700
35	8	O	4.71772400	-0.46512600	0.46266200
36	1	H	3.69351700	-1.77961700	1.67092500
37	8	O	2.94236100	0.98141000	-0.74944700
38	8	O	3.37151900	-1.39950700	-1.55949700
39	8	O	0.82204000	-1.27336900	-1.53469100
40	1	H	2.34815000	-1.38756400	-1.65282000
41	1	H	-1.33863600	-0.35980100	1.66079700

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.79005700	-0.92011800	-0.23499500
2	7	N	2.69321300	0.62402000	0.00550300
3	7	N	0.29000300	1.27031500	-0.80429200
4	6	C	1.65161600	4.67598300	-0.12051100
5	6	C	0.74087700	3.69111900	-0.49267700
6	6	C	1.11005100	2.33107500	-0.47466100
7	6	C	2.43285600	1.98308500	-0.04519900
8	6	C	3.33491200	2.99515800	0.33074700
9	6	C	2.95032800	4.33232900	0.29018300
10	1	H	1.34687200	5.72535200	-0.13525600
11	1	H	-0.27453200	3.97057500	-0.77997900
12	1	H	4.33481700	2.72594900	0.67926900
13	1	H	3.65282400	5.11226500	0.59288500
14	6	C	-2.00185900	-1.99927000	-1.29651400
15	6	C	-1.55173400	0.07869700	-1.58310200
16	6	C	-2.84780200	-0.20704800	-2.08448300
17	7	N	-3.11763500	-1.51228000	-1.88572100
18	1	H	-1.90683800	-3.04034500	-0.98565400
19	1	H	-3.55714500	0.48182800	-2.53840100
20	6	C	4.72148000	-2.40483400	0.31659000
21	6	C	3.73691300	-1.45185400	0.14534900
22	6	C	2.75157300	-3.38112600	0.05183400
23	7	N	4.07583600	-3.61843200	0.25625400
24	1	H	5.79266600	-2.31678400	0.47671200
25	1	H	2.00741800	-4.17087700	-0.03830900
26	6	C	-0.84512800	1.31387500	-1.42161500
27	6	C	3.80516800	0.00685100	0.11040800
28	1	H	4.79956800	0.48557200	0.15499500
29	1	H	-1.30417600	2.23394300	-1.81377700
30	7	N	-1.02840200	-1.09847800	-1.10197600
31	7	N	2.51641400	-2.09010500	-0.02025300
32	8	O	0.51500500	-0.75464600	1.82497200
33	15	P	-4.17239100	0.07230700	0.87893300
34	8	O	-4.90417800	0.75204100	1.99592600
35	8	O	-3.02225300	-0.98609500	1.35948600
36	1	H	4.50845500	-4.53089500	0.34887600
37	8	O	-5.11875400	-0.90516000	0.02922000
38	8	O	-3.46259300	1.12903300	-0.03246300

39	8	O	-0.35929100	0.01151400	2.22299800
40	1	H	-2.22953700	-0.51182100	1.66016600
41	1	H	-4.62115800	-1.34894100	-0.69648600

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	-0.43514100	0.14146600	-1.11331000
2	7	N	-2.52664100	1.05442400	-0.22060100
3	7	N	-1.91599200	-1.49162400	-0.23062600
4	6	C	-5.51069700	-1.73164200	0.73070100
5	6	C	-4.21255800	-2.14317100	0.43040300
6	6	C	-3.21699400	-1.19786500	0.12104800
7	6	C	-3.56251500	0.19427400	0.11389200
8	6	C	-4.87777700	0.58604800	0.41476800
9	6	C	-5.84615500	-0.36950100	0.72134300
10	1	H	-6.27454800	-2.47825300	0.96213300
11	1	H	-3.96266800	-3.20639000	0.40870200
12	1	H	-5.14280100	1.64574900	0.38305400
13	1	H	-6.86926600	-0.05647200	0.94255300
14	6	C	1.85499600	-1.69269000	-1.46690500
15	6	C	0.17231900	-2.51536800	-0.39752100
16	6	C	1.32881300	-3.17262500	0.02422800
17	7	N	2.38147400	-2.64206300	-0.65813400
18	1	H	2.47441900	-1.04918400	-2.08870300
19	1	H	1.45628400	-3.94170900	0.78411700
20	6	C	-0.51112800	4.09953500	0.10022000
21	6	C	-1.06588400	2.87567500	-0.22005900
22	6	C	1.02210400	2.79184800	-0.83552300
23	7	N	0.80355100	4.02435900	-0.29985800
24	1	H	-0.93020000	4.98193800	0.57640800
25	1	H	2.00013000	2.41537500	-1.13943500
26	6	C	-1.17876500	-2.48845800	0.11731900
27	6	C	-2.34968000	2.27132700	0.12799700
28	1	H	-3.04900900	2.85138700	0.75660800
29	1	H	-1.49751000	-3.26315900	0.83716800
30	7	N	0.54251600	-1.56921100	-1.34454900
31	7	N	-0.09044400	2.08972100	-0.81496700
32	8	O	0.14662000	0.08410200	1.41949100
33	15	P	4.13572700	-0.21160900	0.52024500
34	8	O	3.33645100	0.73008900	-0.41089400
35	8	O	3.23111600	-0.54439800	1.83689700
36	1	H	1.50630300	4.74623800	-0.18438900
37	8	O	4.51512800	-1.60760000	-0.01336300
38	8	O	5.33064100	0.70748100	0.88523900
39	8	O	0.67212100	1.02584200	1.96349700
40	1	H	2.81344700	0.26087400	2.17497400
41	1	H	3.56428200	-2.30246400	-0.28812000

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Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	29	Cu	0.64208900	0.00000000	-0.20738600
2	7	N	-0.89506300	1.30068100	-0.28297600
3	7	N	-0.89506300	-1.30068200	-0.28297600
4	6	C	-4.58246500	-0.70233000	-0.33097800
5	6	C	-3.38254900	-1.41189500	-0.31575600
6	6	C	-2.16811000	-0.71194300	-0.30210200
7	6	C	-2.16811100	0.71194200	-0.30210200
8	6	C	-3.38254900	1.41189200	-0.31575600
9	6	C	-4.58246500	0.70232700	-0.33097800
10	1	H	-5.52991200	-1.24530300	-0.34189200
11	1	H	-3.39964200	-2.50310400	-0.31390500
12	1	H	-3.39964400	2.50310200	-0.31390400
13	1	H	-5.52991200	1.24530000	-0.34189100
14	6	C	2.95560800	-2.19867800	-0.18296900
15	6	C	0.86555100	-2.80933900	-0.25151000
16	6	C	1.61669200	-3.96846700	-0.24317200
17	7	N	2.92122700	-3.55491400	-0.19995300
18	1	H	3.73650500	-4.16586200	-0.18406400
19	1	H	3.87999100	-1.62442600	-0.14861400
20	1	H	1.32990600	-5.01799600	-0.26455400
21	6	C	1.61668900	3.96846800	-0.24317200
22	6	C	0.86554900	2.80934000	-0.25151000
23	6	C	2.95560600	2.19868000	-0.18296900
24	7	N	2.92122500	3.55491600	-0.19995400

25	1	H	3.73650200	4.16586400	-0.18406500
26	1	H	1.32990200	5.01799700	-0.26455500
27	1	H	3.87999000	1.62442900	-0.14861400
28	6	C	-0.55469600	-2.54785900	-0.28929800
29	6	C	-0.55469800	2.54785800	-0.28929800
30	1	H	-1.27592800	3.37387300	-0.32108200
31	1	H	-1.27592500	-3.37387400	-0.32108200
32	7	N	1.72927900	-1.71466200	-0.21333100
33	7	N	1.72927800	1.71466300	-0.21333100
34	8	O	0.20377800	-0.00000100	2.39986900
35	8	O	-0.91364100	0.00000100	2.83756800