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Theoretical investigations on the chiral transition of Cu(II) chelated by bis-α-alanine in the aqueous-liquid phase

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1. Data related to the reaction potential energy surface

Table S1. Pathways a and b Gibbs free energy thermal corrections(Gtc), single point energies(Esp(a.u)), total free energies(E_{total}) and relative free energies of stationary point species(ΔG_{total}) of *S*-A_2-Cu(II) to *R*-allo-α-Ala-Cu(II) enantiomers transition in under the implicit aqueous solvent model

Species	Gtc	Esp(a.u)	E_{total} (a.u)	ΔG_{total}(kcal/mol)
Pathway a and b				
S-A_2·Cu(II)	0.176190	-2287.668597	-2287.492407	0.0
S-T1[a(b)]	0.175939	-2287.664012	-2287.488073	2.7
S-I1[a(b)]	0.172623	-2287.662711	-2287.490088	1.5
T2[a(b)]	0.167132	-2287.556375	-2287.389243	64.8
I2[a(b)]	0.167554	-2287.625705	-2287.458151	21.5
T3[a]	0.167201	-2287.556114	-2287.388913	65.0
R-allo-I3[a]	0.174311	-2287.663167	-2287.488856	2.2
R-all-T4[a]	0.175835	-2287.664974	-2287.489139	2.1
R-all-ACu(II)[a]	0.176004	-2287.668031	-2287.492027	0.2
Pathway b				
I2[a(b)]	0.167554	-2287.625705	-2287.458151	21.5
T3[b]	0.165055	-2287.550689	-2287.385634	67.1
R-allo-I3[b]	0.171632	-2287.639883	-2287.468251	15.2
R-allo-T4[b]	0.170352	-2287.632812	-2287.46246	18.8
R-allo-I4[b]	0.172294	-2287.638155	-2287.465861	16.7
R-allo-T5[b]	0.173665	-2287.636278	-2287.462613	18.7
R-allo-I5[b]	0.173087	-2287.645483	-2287.472396	12.6
R-allo-T6[b]	0.169918	-2287.643396	-2287.473478	11.9
R-allo-I6[b]	0.172682	-2287.663310	-2287.490628	1.1
R-allo-T7[b]	0.174571	-2287.664631	-2287.49006	1.5
R-allo- A·Cu(II)[b]	0.175467	-2287.667679	-2287.492212	0.1

Table S2. Pathway c Gibbs free energy thermal corrections(Gtc), single point energies(Esp(a.u)), total free energies(E_{total}) and relative free energies of stationary point species(ΔG_{total}) of *S*-A_2-Cu(II) to *R*-allo-α-Ala-Cu(II) enantiomers transition in under the implicit aqueous solvent model

Species	Gtc	Esp(a.u)	E_{total} (a.u)	ΔG_{total}(kcal/mol)
Pathway c				
S-A_2·Cu(II)	0.176190	-2287.668597	-2287.492407	0.0
S-TS1[c]	0.173984	-2287.663571	-2287.489587	1.8
S-INT1[c]	0.173306	-2287.663453	-2287.490147	1.4
S-T2[c]	0.169024	-2287.643052	-2287.474028	11.6
S-I2[c]	0.171082	-2287.644190	-2287.473108	12.1
S-T3m[c]	0.169384	-2287.618581	-2287.449197	27.2
S-T3n[c]	0.171472	-2287.618823	-2287.447351	28.3
S-I3[c]	0.176689	-2287.636331	-2287.459642	17.4
S-T4[c]	0.170233	-2287.548429	-2287.378196	71.7
I4[c]	0.172430	-2287.628047	-2287.455617	23.1

R-allo-T5[c]	0.167393	-2287.548847	-2287.381454	69.7
R-allo-I5[c]	0.174782	-2287.635623	-2287.460841	19.8
R-allo-T6m[c]	0.170378	-2287.619056	-2287.448678	27.5
R-allo-T6n[c]	0.170060	-2287.618465	-2287.448405	27.6
R-allo-I6[c]	0.170073	-2287.644168	-2287.474095	11.5
R-allo-T7[c]	0.168847	-2287.642817	-2287.47397	11.6
R-allo-I7[c]	0.174404	-2287.663141	-2287.488737	2.3
R-allo-T8[c]	0.175835	-2287.664974	-2287.489139	2.1
R-allo-Ala[c(a)]	0.176004	-2287.668031	-2287.492027	0.2

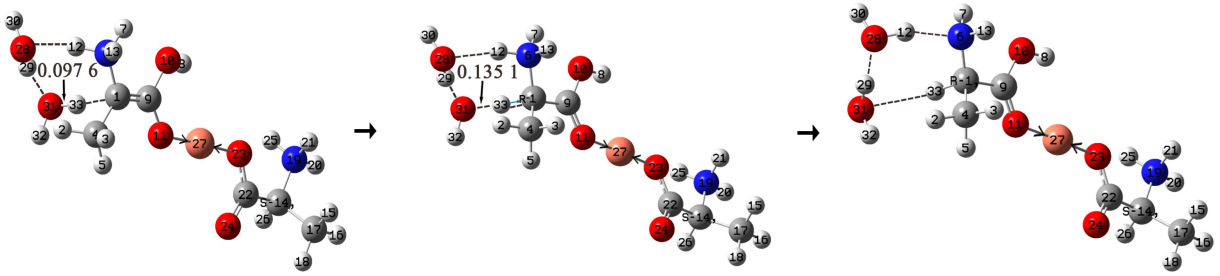
Table S3. Pathways a and b Gibbs free energy thermal corrections(Gtc), single point energies(Esp(a.u)), total free energies(E_{total}) and relative free energies of stationary point species(ΔG_{total}) of S-A_2-Cu(II) to R-allo-α-Ala-Cu(II) enantiomers transition in water solvent effect

Species	Gtc	Esp(a.u)	E_{total} (a.u)	ΔG_{total}(kcal/mol)
S-I1·$(H_2O)_2$[a(b)]	0.217101	-2440.463293	-2440.246192	0.0
S-T2$(H_2O)_2$[a(b)]	0.213294	-2440.400426	-2440.187132	37.1
I2·$(H_2O)_2$[a(b)]	0.215927	-2440.425945	-2440.210018	22.7
S-I1·$(H_2O)_2$·(H_2O)[a(b)]	0.242325	-2516.875280	-2516.632955	0.0
S-T2·$(H_2O)_2$·(H_2O)[a(b)]	0.239750	-2516.813573	-2516.573823	37.2
I2·$(H_2O)_2$·(H_2O)[a(b)]	0.239307	-2516.837076	-2516.597769	22.1
S-I1·$(H_2O)_2$·$(H_2O)_2$[a(b)]	0.264534	-2593.286801	-2593.022267	0.0
S-T2·$(H_2O)_2$·$(H_2O)_2$[a(b)]	0.262682	-2593.222444	-2592.959762	39.3
I2·$(H_2O)_2$·$(H_2O)_2$[a(b)]	0.268164	-2593.250083	-2592.981919	25.3
S-I1·$(H_2O)_2$·$(H_2O)_3$[a(b)]	0.284157	-2669.685799	-2669.401642	0.0
S-T2·$(H_2O)_2$·$(H_2O)_3$[a(b)]	0.282692	-2669.621711	-2669.339019	39.3
I2·$(H_2O)_2$·$(H_2O)_2$[a(b)]	0.283091	-2669.643097	-2669.360006	26.1
S-I1·$(H_2O)_2$·$(H_2O)_4$[a(b)]	0.307076	-2746.089221	-2745.782145	0.0
S-T2·$(H_2O)_2$·$(H_2O)_4$[a(b)]	0.307275	-2746.025218	-2745.717943	40.3
I2·$(H_2O)_2$·$(H_2O)_4$[a(b)]	0.306009	-2746.046181	-2745.740172	26.4

Table S4. Pathway c Gibbs free energy thermal corrections(Gtc), single point energies(Esp(a.u)), total free energies(E_{total}) and relative free energies of stationary point species(ΔG_{total}) of S-A_2-Cu(II) to R-allo-α-Ala-Cu(II) enantiomers transition in water solvent effect

Species	Gtc	Esp(a.u)	E_{total} (a.u)	ΔG_{total}(kcal/mol)
Pathway c				
Second step				
S-I1·H_2O[c]	0.194801	-2364.063590	-2363.868789	0.0
S-T2·H_2O[c]	0.192402	-2364.037853	-2363.845451	14.7
S-I2·H_2O[c]	0.192165	-2364.041871	-2363.849706	12.0

Fourth step				
S-I3·$(H_2O)_2m^c$	0.216817	-2440.438020	-2440.221203	0.0
S-T4·$(H_2O)_2m^c$	0.214886	-2440.394194	-2440.179308	26.3
I4·$(H_2O)_2m^c$	0.215429	-2440.423554	-2440.208125	8.2
Fifth step				
I4·$(H_2O)_2n^c$	0.215190	-2440.413019	-2440.197829	0.0
R-all-T5·$(H_2O)_2n^c$	0.215329	-2440.394600	-2440.179271	11.7
R-all-I5·$(H_2O)_2n^c$	0.216794	-2440.438134	-2440.22134	-14.8



I4·$(H_2O)_2n^c$ R-all-T5·$(H_2O)_2n^c$ R-all-I5·$(H_2O)_2n^c$

Fig. S1 The fifth reaction step of *S*-A_2·Cu(II) isomerization into *R*-allo-α-Ala·Cu(II) in the c channel under the action of water molecules (clusters)

Table S5. Pathway d Gibbs free energy thermal corrections(Gtc), single point energies(Esp(a.u)), total free energies(E_{total}) and relative free energies of stationary point species(ΔG_{total}) of R-allo-α-Ala-Cu(II) to R-A_2-Cu(II) enantiomers transition in under the implicit aqueous solvent model

Species	Gtc	Esp(a.u)	E_{total} (a.u)	ΔG_{total}(kcal/mol)
Pathway d				
R-allo-Ala$^{c(a)}$	0.176004	-2287.668031	-2287.492027	0.2
R-allo-T1^d	0.175835	-2287.664974	-2287.489139	2.1
R-allo-I1^d	0.174404	-2287.663141	-2287.488737	2.3
R-allo-T2^d	0.168847	-2287.642817	-2287.47397	11.6
R-allo-I2^d	0.170073	-2287.644168	-2287.474095	11.5
R-allo-T3m^d	0.170378	-2287.619056	-2287.448678	27.5
R-allo-T3n^d	0.170060	-2287.618465	-2287.448405	27.6
R-allo-I3^d	0.174782	-2287.635623	-2287.460841	19.8
T4^d	0.167393	-2287.548847	-2287.381454	69.7
I4^d	0.172430	-2287.628047	-2287.455617	23.1
T5^d	0.170233	-2287.548429	-2287.378196	71.7
R-I5^d	0.170671	-2287.635425	-2287.459642	17.4
R-T6m^d	0.169384	-2287.618581	-2287.449197	27.2
R-T6n^d	0.171472	-2287.618823	-2287.447351	28.3
R-I6^d	0.171082	-2287.644190	-2287.473108	12.1
R-T7^d	0.169024	-2287.643052	-2287.474028	11.6
R-I7^d	0.173306	-2287.663453	-2287.490147	1.4

R-T8[d]	0.173984	-2287.663571	-2287.489587	1.8
R-A_2·Cu(II)[d]	0.176190	-2287.668597	-2287.492407	0.0

Table S6. Pathway d Gibbs free energy thermal corrections(Gtc), single point energies(Esp(a.u)), total free energies(E_{total}) and relative free energies of stationary point species(ΔG_{total}) of R-allo-α-Ala-Cu(II) to R-A_2-Cu(II) enantiomers transition in water solvent effect

Species	Gtc	Esp(a.u)	E_{total} (a.u)	ΔG_{total}(kcal/mol)
Pathway d Fourth step				
R-allo-I3·$(H_2O)_2$[d]	0.212243	-2440.436559	-2440.224316	0.0
R-allo-T4·$(H_2O)_2$[d]	0.212213	-2440.393394	-2440.181181	27.1
I4·$(H_2O)_2$[d]	0.210177	-2440.423537	-2440.21336	6.9

2. The Cartesian coordinates of the stagnation points on the potential energy surface

2.1 Coordinates of the relevant stationary points under the hidden water solvent effect

Pathway a

_S_-A_2·Cu(II)

C	-3.73327800	-0.22925800	-0.18241400
H	-3.99332500	0.20290300	1.91878200
H	-5.19671600	0.96676300	0.84563200
C	-4.14305400	0.69056900	0.94884300
H	-3.54175900	1.60201900	0.91693100
N	-4.59702000	-1.44659000	-0.18409300
H	-5.57992200	-1.18236300	-0.30729200
H	-4.51772600	-1.95268900	0.70565300
C	-2.29347900	-0.65350000	-0.07267800
O	-1.97815400	-1.87932800	-0.01703100
O	-1.38475300	0.22378300	-0.01361800
H	-4.34131200	-2.09576300	-0.93506800
H	-3.87162300	0.25931900	-1.15321400
C	3.65771500	-2.34157300	0.66505100
H	4.07235600	-2.28714800	-1.45525000
H	5.51291300	-2.15870100	-0.41006200
C	4.46553400	-1.86310100	-0.52436500
H	4.41777100	-0.77340200	-0.58603000
N	3.76598000	-3.82511900	0.78572200
H	4.74845900	-4.10024900	0.88696800

H	3.39311900	-4.28799600	-0.05149100
C	2.20734800	-1.96248500	0.53679000
O	1.30004700	-2.84177600	0.46473300
O	1.89206900	-0.73819000	0.47388100
H	3.24757300	-4.18284800	1.59433900
H	4.04385100	-1.91614400	1.59705600
Cu	-0.04188800	-1.30621800	0.22374000

T1[a(b)]

C	-3.83467200	-0.37271300	-0.17361800
H	-4.27211300	0.02697200	1.90387400
H	-5.57393400	0.47354300	0.76905100
C	-4.48976600	0.44830400	0.91575900
H	-4.11283300	1.47291000	0.88004900
N	-4.40362000	-1.75456100	-0.17240100
H	-5.41251000	-1.72111600	-0.35074600
H	-4.25982900	-2.20826700	0.73658900
C	-2.33336200	-0.43851400	-0.01873600
O	-1.77053500	-1.59063000	0.00350000
O	-1.67529800	0.61241400	0.08355900
H	-3.96977100	-2.34703900	-0.88699400
H	-4.04814000	0.05067100	-1.16148000
C	3.70243400	-2.38227800	0.65086000
H	4.06940000	-2.39560700	-1.47838600
H	5.53598700	-2.26675100	-0.47051600
C	4.49240200	-1.95268200	-0.56931300
H	4.46463500	-0.86435600	-0.66161200
N	3.78168200	-3.86444300	0.80392000
H	4.75924400	-4.15900000	0.89670300
H	3.38475600	-4.33678700	-0.01679800
C	2.25557200	-1.98203600	0.53739600
O	1.34238700	-2.83434900	0.40800900
O	1.97224900	-0.73932400	0.54403700
H	3.26744700	-4.19206600	1.62783100
H	4.11732800	-1.94249000	1.56314200
Cu	0.06023100	-1.06044500	0.27669600

I1[a(b)]

C	-4.08965000	-0.34435500	-0.18431600

H	-4.67220500	0.10096200	1.84768200
H	-5.90232000	0.49451800	0.61807200
C	-4.82969600	0.49117600	0.83559800
H	-4.46843500	1.52116000	0.79744600
N	-4.64310200	-1.73319700	-0.19406000
H	-5.63493800	-1.71903200	-0.45175500
H	-4.56662700	-2.16409800	0.73377900
C	-2.59054500	-0.37668300	0.05523200
O	-2.03613700	-1.53906400	0.01937400
O	-1.99494100	0.68989300	0.23873000
H	-4.14435400	-2.33454600	-0.85655600
H	-4.24400200	0.05198400	-1.19460100
C	3.81219100	-2.50364500	0.66421900
H	4.20926900	-2.42211200	-1.45709900
H	5.52995300	-1.80009000	-0.43299100
C	4.44284900	-1.85212000	-0.54973600
H	4.05841600	-0.83581400	-0.66493000
N	4.38280400	-3.87166800	0.84441400
H	5.39946400	-3.82376700	0.96214000
H	4.17871400	-4.45729100	0.02676000
C	2.30854600	-2.62746400	0.50292200
O	1.78612000	-3.72389500	0.27296900
O	1.68587900	-1.50630300	0.60136400
H	3.98526600	-4.34129400	1.66391400
H	4.03571400	-1.94302900	1.57675600
Cu	-0.17002400	-1.54319100	0.30680800

T2[a(b)]

C	-4.01032700	-0.01433500	-0.18639500
H	-4.36885800	0.14502300	1.96382000
H	-5.43390700	1.14143200	0.94391300
C	-4.41116600	0.76096600	1.04966500
H	-3.75167000	1.62318700	1.19057800
N	-4.86149800	-1.23778100	-0.28408500
H	-5.84597000	-0.96882500	-0.37080800
H	-4.78734600	-1.84317000	0.54659100
C	-2.57262600	-0.33219100	-0.22379600
O	-1.95788600	-1.33224700	0.21395100
O	-2.02982900	0.66231500	-0.86824100
H	-4.63014400	-1.80386700	-1.10474600
H	-3.18165800	0.89356700	-1.08953600
C	3.89790500	-2.38240700	0.63550500

H	4.17807000	-3.40513000	-1.24619900
H	5.58618400	-2.45782400	-0.69970500
C	4.49301600	-2.47806600	-0.75291000
H	4.16218300	-1.62971300	-1.35620300
N	4.42601000	-3.49365500	1.48186900
H	5.44212900	-3.41380200	1.58484200
H	4.21935300	-4.40325100	1.05468600
C	2.38173200	-2.45975100	0.63748200
O	1.79326400	-3.35197400	1.25839300
O	1.81513400	-1.52927600	-0.04708100
H	4.00217900	-3.49075900	2.41475600
H	4.19429900	-1.44854300	1.12528200
Cu	-0.06656300	-1.51461500	-0.02031300

I2[a(b)]

C	4.12094400	0.14905600	-0.03812700
H	5.81525200	0.77972500	-1.13678800
H	6.03152300	0.75960900	0.61625800
C	5.31258400	0.99010400	-0.17946900
H	5.08553600	2.05761300	-0.14088300
N	4.34160200	-1.23752800	0.31826800
H	4.81264300	-1.31478000	1.23189400
H	4.95134900	-1.70519500	-0.36911900
C	2.73902900	0.48718700	-0.24723700
O	1.85814800	-0.37183500	-0.06197700
O	2.38577200	1.70096300	-0.63092500
H	3.45192900	-1.75417500	0.36790900
H	3.13450700	2.30359100	-0.77774100
C	-4.16432100	-0.13723800	-0.20075200
H	-4.26892100	0.80246400	1.74142000
H	-5.52354300	1.33974400	0.59435100
C	-4.47299800	1.04701700	0.69181000
H	-3.85069100	1.89791800	0.40418500
N	-5.06362700	-1.27298300	0.16466400
H	-6.04721300	-1.00096500	0.07442800
H	-4.89677600	-1.56192500	1.13489200
C	-2.71766400	-0.58679000	-0.04927500
O	-2.46452400	-1.65028800	0.54064200
O	-1.87484700	0.23304900	-0.54556400
H	-4.89782400	-2.09107900	-0.42874600
H	-4.36315600	0.09722200	-1.25072800
Cu	-0.01083300	-0.07546300	-0.30673200

T3[a]

C	4.04340400	0.15803000	-0.25051400
H	6.02566600	1.00135400	-0.18965000
H	4.98746500	1.54575900	1.15002300
C	5.00074200	1.28364500	0.07838000
H	4.74602600	2.18165000	-0.49346700
N	4.35605600	-1.00829600	0.62922300
H	5.32040000	-1.31364400	0.46856800
H	3.75050600	-1.81083700	0.43796700
C	2.63364100	0.57250300	-0.14287200
O	1.86272500	0.55030500	0.84434900
O	2.31048300	0.96569900	-1.34189000
H	4.27573700	-0.78452700	1.63202500
H	3.35942600	0.45588800	-1.58688100
C	-3.86107500	2.16191100	1.33725200
H	-3.45783400	4.27877500	1.49116500
H	-4.98657700	3.87259500	0.66833000
C	-3.94167000	3.57592200	0.80286400
H	-3.44069400	3.63309800	-0.16610300
N	-4.61127600	2.07258900	2.62534000
H	-5.59345600	2.33022400	2.48832400
H	-4.20970900	2.70801200	3.32353700
C	-2.43248500	1.70816700	1.58090700
O	-2.04860800	1.40062100	2.71457900
O	-1.71295700	1.68682000	0.51518300
H	-4.57699600	1.12705900	3.01831300
H	-4.33671300	1.45588500	0.64841900
Cu	0.06334600	1.11684800	0.68345800

R-allo-I3[a]

C	4.02910600	0.00312400	-0.17390300
H	6.05485600	0.71879100	-0.35249300
H	4.90395300	1.92552700	0.28049800
C	5.03429300	1.10554300	-0.43580100
H	4.89442400	1.49698900	-1.44653500
N	4.25488700	-0.55898200	1.19268100

H	5.20923800	-0.92352900	1.27412400
H	3.60252300	-1.32086100	1.40204700
C	2.60885200	0.52111000	-0.30568800
O	1.95923200	0.66616900	0.79656600
O	2.18338800	0.79754000	-1.43170200
H	4.12628400	0.16406100	1.90913700
H	4.15949600	-0.82353100	-0.87849100
C	-3.69713100	2.44943600	1.36649100
H	-3.16395700	4.43198000	2.03833200
H	-4.65213300	4.35792100	1.05914300
C	-3.64250600	3.95169400	1.17633100
H	-3.06775800	4.19017800	0.27817200
N	-4.53095700	2.13365100	2.56382600
H	-5.46864600	2.53451600	2.46591300
H	-4.10197000	2.52373100	3.41096800
C	-2.31144100	1.86768700	1.57885700
O	-1.95693000	1.46992800	2.69406700
O	-1.58583700	1.86986600	0.51745500
H	-4.62597400	1.12344500	2.70591500
H	-4.16969100	1.95890800	0.51053500
Cu	0.18324600	1.27220800	0.66427700

R-allo-T4[a]

C	-2.59398400	2.37453200	1.90384600
H	-3.05824400	4.33682700	1.15565000
H	-2.34552100	3.24212900	-0.05919600
C	-2.31543900	3.55045800	0.99185000
H	-1.32603900	3.95829500	1.21128500
N	-3.97243600	1.85744200	1.65540900
H	-4.66363100	2.59142500	1.84274000
H	-4.19278000	1.04951900	2.24645100
C	-1.60328000	1.25836200	1.71051700
O	-1.99785200	0.08863100	1.40149600
O	-0.37185800	1.48263300	1.85068600
H	-4.08245200	1.56625500	0.67699400
H	-2.55516100	2.67815300	2.95564600
C	2.86174400	-3.12738400	1.44890800
H	3.71315200	-2.68228200	-0.48666500
H	4.87466100	-3.30762000	0.71392700
C	4.00181100	-2.66347700	0.57005700
H	4.28041000	-1.64240400	0.84030800

N	2.52527100	-4.54971000	1.14580500
H	3.33111200	-5.15358100	1.33637100
H	2.27331200	-4.66260200	0.15719600
C	1.61218200	-2.29347600	1.30812100
O	0.48838500	-2.80960200	1.13144700
O	1.74454600	-1.02608200	1.42224900
H	1.73286800	-4.87788600	1.70688800
H	3.15106300	-3.09527800	2.50586800
Cu	-0.12207600	-0.55556700	1.37046700

R-allo-A·Cu(II)[a]

C	-2.40249100	2.52456000	1.93561900
H	-2.84095900	4.51203500	1.24288100
H	-2.20212400	3.42380700	-0.01845800
C	-2.12570200	3.71025200	1.03640000
H	-1.11840800	4.08771100	1.22719200
N	-3.80036700	2.04496300	1.72518200
H	-4.46712600	2.79092600	1.94967000
H	-4.01927500	1.23167900	2.30943300
C	-1.45114400	1.38488000	1.69034600
O	-1.88086600	0.23551300	1.37032500
O	-0.20676300	1.57256100	1.80714600
H	-3.94933600	1.77367500	0.74627200
H	-2.32061500	2.80671500	2.99103700
C	2.45388900	-3.43313000	1.38327500
H	3.33396600	-3.10670300	-0.56374400
H	4.32346100	-4.09051700	0.54813900
C	3.64967400	-3.23140800	0.47795800
H	4.19708900	-2.33868100	0.78902200
N	1.73404200	-4.68714300	1.01468200
H	2.35199300	-5.49702200	1.12898100
H	1.43029500	-4.66040000	0.03435800
C	1.48477700	-2.28272900	1.33736500
O	0.24891300	-2.46631800	1.14230000
O	1.91689700	-1.10484000	1.51393400
H	0.90110500	-4.83232700	1.59451500
H	2.77180000	-3.54931100	2.42590100
Cu	0.03147800	-0.42297600	1.35608400

Pathway b

Follow I2[a(b)]

T3[b]

C	4.10177600	0.10375600	-0.33911700
H	6.17214100	0.40021500	-0.75977000
H	5.56538800	1.37909200	0.59047700
C	5.31088500	0.97253400	-0.39824600
H	5.18357500	1.80741900	-1.09447900
N	4.31540300	-1.26552200	0.29396200
H	5.27225600	-1.37538900	0.61708100
H	4.10912000	-1.02847200	-0.92036100
C	2.77103200	0.52900800	-0.30543000
O	1.83724800	-0.21733500	0.12838900
O	2.40529800	1.72973200	-0.77149700
H	3.59701100	-1.52444200	0.96738400
H	3.16725300	2.25944500	-1.05838800
C	-4.12404900	-0.01861500	-0.20972700
H	-4.32002600	0.85772200	1.75572200
H	-5.54849600	1.39374200	0.58007300
C	-4.49420900	1.12832100	0.70762500
H	-3.88787900	2.00436800	0.46634200
N	-5.00853700	-1.18701600	0.07393000
H	-5.99087600	-0.93861000	-0.07861300
H	-4.90468300	-1.48921900	1.04909800
C	-2.67910900	-0.45166800	-0.03323500
O	-2.39622600	-1.57732300	0.38883800
O	-1.83718000	0.46672100	-0.35293600
H	-4.77984800	-1.98907900	-0.52094300
H	-4.28388400	0.25095500	-1.25869000
Cu	-0.00671100	0.13050100	-0.13758200

R-allo-I3[b]

C	4.10177600	0.10375600	-0.33911700
H	6.17214100	0.40021500	-0.75977000
H	5.56538800	1.37909200	0.59047700
C	5.31088500	0.97253400	-0.39824600
H	5.18357500	1.80741900	-1.09447900
N	4.31540300	-1.26552200	0.29396200
H	5.27225600	-1.37538900	0.61708100

H	4.10912000	-1.02847200	-0.92036100
C	2.77103200	0.52900800	-0.30543000
O	1.83724800	-0.21733500	0.12838900
O	2.40529800	1.72973200	-0.77149700
H	3.59701100	-1.52444200	0.96738400
H	3.16725300	2.25944500	-1.05838800
C	-4.12404900	-0.01861500	-0.20972700
H	-4.32002600	0.85772200	1.75572200
H	-5.54849600	1.39374200	0.58007300
C	-4.49420900	1.12832100	0.70762500
H	-3.88787900	2.00436800	0.46634200
N	-5.00853700	-1.18701600	0.07393000
H	-5.99087600	-0.93861000	-0.07861300
H	-4.90468300	-1.48921900	1.04909800
C	-2.67910900	-0.45166800	-0.03323500
O	-2.39622600	-1.57732300	0.38883800
O	-1.83718000	0.46672100	-0.35293600
H	-4.77984800	-1.98907900	-0.52094300
H	-4.28388400	0.25095500	-1.25869000
Cu	-0.00671100	0.13050100	-0.13758200

R-allo-T4[b]

C	4.26632100	-0.05501400	-0.55420800
H	5.96759300	1.16661600	-0.07047800
H	4.57145400	1.40700600	1.00862100
C	4.87714500	1.24422200	-0.03234500
H	4.56550800	2.10818400	-0.62763900
N	4.63600900	-1.15449100	0.26307500
H	4.60652800	-2.09481800	-0.09330100
H	4.59324100	-0.20679800	-1.59424000
C	2.76632300	0.17381500	-0.62118800
O	2.00049400	-0.18742000	0.28272900
O	2.25731300	0.81500100	-1.64843700
H	5.01654500	-0.99021300	1.18068300
H	2.92662500	1.03358700	-2.32280700
C	-3.94573200	0.47093200	0.77016800
H	-3.80897200	2.15933100	2.11125000
H	-5.17071700	2.23472800	0.96233500
C	-4.12283600	1.94247700	1.08334200
H	-3.51740400	2.54061300	0.39813300
N	-4.82101000	-0.33827400	1.66818400
H	-5.80167200	-0.06177300	1.55886300

H	-4.55729400	-0.20206700	2.65057500
C	-2.50875900	0.02249900	0.96711900
O	-2.19537400	-0.73611000	1.88887700
O	-1.70092600	0.52912900	0.10316200
H	-4.74439500	-1.34004200	1.46673900
H	-4.25223700	0.24743400	-0.25638200
Cu	0.11143100	0.14198300	0.23391800

R-allo-I4[b]

C	4.26123800	-0.07499400	-0.63440400
H	5.99361000	1.07320000	-0.09093300
H	4.55489100	1.43408500	0.89266100
C	4.90868300	1.21467700	-0.12247700
H	4.68912900	2.07231200	-0.76847600
N	4.53281900	-1.25272300	0.17146200
H	5.53557800	-1.42323500	0.13737300
H	4.60452400	-0.26452700	-1.65932000
C	2.78284100	0.16893100	-0.70213000
O	2.02368000	-0.20483400	0.20306400
O	2.27542600	0.85130800	-1.70109100
H	4.31519500	-1.04239600	1.14527100
H	2.93480500	1.07134100	-2.38434400
C	-3.91389400	0.47837000	0.78219400
H	-3.74107400	2.10955900	2.18851400
H	-5.11731600	2.24497700	1.06273500
C	-4.07097400	1.93787700	1.15700200
H	-3.46819400	2.55742200	0.48853400
N	-4.78218600	-0.35704200	1.66251400
H	-5.76003400	-0.05917300	1.59028200
H	-4.49155800	-0.27166200	2.64312800
C	-2.47810700	0.01263800	0.94258800
O	-2.15154700	-0.74942300	1.85681000
O	-1.68407400	0.51296400	0.06160500
H	-4.72945500	-1.34942000	1.41261500
H	-4.23817800	0.29893500	-0.24729200
Cu	0.13107100	0.12825900	0.17112200

R-allo-T5[b]

C	4.33069900	0.15262300	-0.69481000

H	6.06752800	1.09223200	0.12250300
H	4.66729300	1.09937500	1.21734700
C	4.98018400	1.20941900	0.17262200
H	4.72563800	2.22085400	-0.16401800
N	4.57215400	-1.23089400	-0.27870800
H	5.53740100	-1.46615700	-0.49770300
H	4.67975300	0.25270000	-1.72990100
C	2.82917800	0.30021700	-0.72854000
O	2.20508800	0.75848100	0.23823100
O	2.15373700	-0.10327600	-1.77667600
H	4.48249300	-1.28388300	0.73569400
H	2.73135400	-0.44579700	-2.48330600
C	-3.61370600	1.75455300	1.19443400
H	-3.90584000	3.41779800	-0.15340500
H	-5.31907800	2.34563100	0.02489500
C	-4.22677600	2.37606000	-0.03999200
H	-3.92041300	1.81604900	-0.92627000
N	-4.11192400	2.45551200	2.41526100
H	-5.12702800	2.34927700	2.50294400
H	-3.89859500	3.45826200	2.37139200
C	-2.09554400	1.78570500	1.22155400
O	-1.48911800	2.21218900	2.20915100
O	-1.54565700	1.30726900	0.15954900
H	-3.66872000	2.08536300	3.26214000
H	-3.92074900	0.70695700	1.29394400
Cu	0.30620500	1.04485200	0.21182800

R-allo-I5[b]

C	4.31248300	0.45584100	-0.59705600
H	6.12695900	0.59120800	0.53656500
H	4.91264700	-0.49727500	1.24723800
C	5.05804900	0.45572900	0.72516400
H	4.71472900	1.26652300	1.37407000
N	4.68917700	-0.61638300	-1.51351600
H	5.28195000	-0.27072800	-2.26088500
H	4.45895800	1.42408000	-1.09677600
C	2.81780600	0.36952900	-0.39126800
O	2.21299500	1.09117200	0.42083400
O	2.18204800	-0.48379000	-1.13735500
H	5.19683500	-1.34790200	-1.02109400
H	2.91264500	-0.92327000	-1.67284600
C	-3.65902100	1.82594000	1.28890600

H	-4.03593900	2.83812200	-0.58199900
H	-5.39069300	1.84184300	0.01059800
C	-4.30137500	1.90122600	-0.07885200
H	-3.96144600	1.06411900	-0.69253400
N	-4.19814000	2.91427200	2.15761100
H	-5.20820000	2.80158800	2.28687600
H	-4.03305000	3.83353300	1.73319900
C	-2.14606700	1.94847700	1.25428700
O	-1.55976400	2.79824300	1.93172000
O	-1.57607500	1.08958300	0.48097400
H	-3.74949000	2.91706100	3.07902800
H	-3.90802000	0.88101900	1.78509600
Cu	0.29555900	1.10161000	0.46217400

R-allo-**T6**[b]

C	4.31135000	0.17939300	-0.38640500
H	6.10549500	1.23852100	0.13434400
H	4.67473700	1.73038200	1.07257400
C	5.03006300	1.43037400	0.07951700
H	4.85930200	2.25631100	-0.61664200
N	4.42265800	-0.95313400	0.54325500
H	4.89737800	-1.74944400	0.12757900
H	4.66594900	-0.11247600	-1.38231600
C	2.81595800	0.40824400	-0.50976800
O	2.33564600	1.31709600	-1.21727400
O	2.10988100	-0.42124900	0.17514400
H	4.90785000	-0.69253500	1.39920400
H	2.93607200	-0.99206400	0.60791900
C	-3.50058900	2.52306100	-2.08310900
H	-3.81410400	1.16505800	-3.73362500
H	-5.21638800	1.35077600	-2.64818500
C	-4.12462900	1.28396700	-2.68892300
H	-3.81185300	0.40082900	-2.12685100
N	-3.98900600	3.73406000	-2.80722600
H	-5.00788100	3.81072700	-2.73236800
H	-3.74227200	3.68603900	-3.80214600
C	-1.98518200	2.50667300	-2.15518700
O	-1.37288300	3.32735000	-2.84541700
O	-1.44313700	1.57793100	-1.44558000
H	-3.57185700	4.59067900	-2.42956200
H	-3.79966700	2.64139700	-1.03665100
Cu	0.42934600	1.53069200	-1.40562200

R-allo-**I6**[b]

C	4.20721300	0.17257400	-0.40925500
H	6.03597400	1.16483800	0.14766700
H	4.60203000	1.71125000	1.05551300
C	4.96724700	1.38956000	0.07318300
H	4.83704600	2.21049200	-0.63561800
N	4.46384500	-0.97449300	0.51146600
H	5.46061300	-1.21125700	0.52366900
H	4.55508600	-0.13824200	-1.40015700
C	2.70853300	0.40062900	-0.47821700
O	2.36143400	1.34501000	-1.28088600
O	1.92989100	-0.28570500	0.19387700
H	4.17999200	-0.74158500	1.46985100
H	3.93534700	-1.80630800	0.23142300
C	-3.45847000	2.55640100	-2.07074200
H	-3.81760900	1.10239000	-3.62848200
H	-5.18637600	1.34938500	-2.51293600
C	-4.09605900	1.28284700	-2.58363600
H	-3.76327000	0.43501800	-1.98019600
N	-3.97539200	3.72172600	-2.84811200
H	-4.99084400	3.80420000	-2.74016000
H	-3.76699700	3.61173900	-3.84689500
C	-1.94464600	2.54079600	-2.18135600
O	-1.35508300	3.33407400	-2.92318600
O	-1.38418600	1.64778600	-1.44449100
H	-3.54409600	4.59908100	-2.54128400
H	-3.72810800	2.73367800	-1.02448100
Cu	0.49511700	1.59575200	-1.41906600

R-allo-T7[b]

C	4.30866800	0.09096000	-0.36926200
H	6.04780500	1.29818200	0.00707300
H	4.56647000	1.88239300	0.81066100
C	4.96677700	1.42728900	-0.10224200
H	4.78270900	2.10194500	-0.94136100
N	4.62068700	-0.86040500	0.73808400
H	5.63308500	-1.00271900	0.81185100
H	4.69786600	-0.35952900	-1.28927200

C	2.81169200	0.19453600	-0.50618900
O	2.33486200	1.02919800	-1.34142400
O	2.03938400	-0.52364800	0.17698000
H	4.28752700	-0.49400700	1.63753000
H	4.17631500	-1.77239400	0.59269000
C	-3.45844200	0.68626200	-0.72550300
H	-3.74730200	-0.51733800	-2.49631000
H	-5.07397400	-0.61426400	-1.30722700
C	-3.98837700	-0.54794300	-1.42737900
H	-3.53708000	-1.44173200	-0.98991800
N	-4.11109100	1.90426700	-1.29024800
H	-5.12723600	1.85104300	-1.16730400
H	-3.91477700	1.98999100	-2.29424600
C	-1.96452600	0.81194200	-0.88810500
O	-1.44698600	1.70829700	-1.58447100
O	-1.24475200	-0.06679900	-0.29806100
H	-3.77595400	2.75985800	-0.83594700
H	-3.69559800	0.66389700	0.34273200
Cu	0.47930500	0.54681800	-0.89720100

R-allo-A·Cu(II)[b]

C	4.43295500	0.30663200	-0.50622600
H	6.10392200	1.63848200	-0.27127200
H	4.74165700	1.97498500	0.83054700
C	5.01356100	1.66673600	-0.18525200
H	4.63023400	2.40586400	-0.89249500
N	4.99294500	-0.71952700	0.42140400
H	6.00735300	-0.79482600	0.29407100
H	4.70672700	-0.00370200	-1.52109200
C	2.93113700	0.27966300	-0.41891400
O	2.25497800	1.10794000	-1.09570300
O	2.32872200	-0.56502200	0.30612400
H	4.81695800	-0.46589600	1.40049900
H	4.57993900	-1.64382200	0.26101500
C	-3.27692800	0.08105200	-0.26435400
H	-3.49532100	-1.36327800	-1.85689300
H	-4.88850100	-1.26063900	-0.74679400
C	-3.79668700	-1.23229300	-0.81149800
H	-3.39426500	-2.05957300	-0.22200900
N	-3.86049300	1.21953500	-1.03268500
H	-4.88141600	1.22082400	-0.94048200
H	-3.63182600	1.14508500	-2.03074700

C	-1.77611800	0.15778100	-0.32799000
O	-1.18518300	1.01998300	-1.04090000
O	-1.08968600	-0.66914800	0.34100800
H	-3.50820900	2.12296500	-0.69913300
H	-3.57819500	0.21566400	0.77989800
Cu	0.57763600	0.22704200	-0.37438600

Pathway c

***S*-A_2·Cu(II)**

C	-3.73327800	-0.22925800	-0.18241400
H	-3.99332500	0.20290300	1.91878200
H	-5.19671600	0.96676300	0.84563200
C	-4.14305400	0.69056900	0.94884300
H	-3.54175900	1.60201900	0.91693100
N	-4.59702000	-1.44659000	-0.18409300
H	-5.57992200	-1.18236300	-0.30729200
H	-4.51772600	-1.95268900	0.70565300
C	-2.29347900	-0.65350000	-0.07267800
O	-1.97815400	-1.87932800	-0.01703100
O	-1.38475300	0.22378300	-0.01361800
H	-4.34131200	-2.09576300	-0.93506800
H	-3.87162300	0.25931900	-1.15321400
C	3.65771500	-2.34157300	0.66505100
H	4.07235600	-2.28714800	-1.45525000
H	5.51291300	-2.15870100	-0.41006200
C	4.46553400	-1.86310100	-0.52436500
H	4.41777100	-0.77340200	-0.58603000
N	3.76598000	-3.82511900	0.78572200
H	4.74845900	-4.10024900	0.88696800
H	3.39311900	-4.28799600	-0.05149100
C	2.20734800	-1.96248500	0.53679000
O	1.30004700	-2.84177600	0.46473300
O	1.89206900	-0.73819000	0.47388100
H	3.24757300	-4.18284800	1.59433900
H	4.04385100	-1.91614400	1.59705600
Cu	-0.04188800	-1.30621800	0.22374000

S-T1[c]

C	-3.64397500	-0.25350400	-0.16971300
H	-3.85443600	0.22005400	1.92755700
H	-5.11228800	0.92349200	0.87641100
C	-4.04774900	0.68119200	0.95200500
H	-3.47568400	1.60926700	0.88208700
N	-4.47394000	-1.49261700	-0.11335800
H	-5.46728300	-1.25976300	-0.21120200
H	-4.34831000	-1.97401800	0.78427600
C	-2.18982300	-0.64659500	-0.08305600
O	-1.84206500	-1.82955200	0.10479400
O	-1.32731000	0.29427400	-0.18880100
H	-4.22187700	-2.15299100	-0.85556500
H	-3.82452500	0.20569900	-1.14728400
C	4.11858700	-0.51325800	0.62563000
H	4.63133400	-0.32076600	-1.46516700
H	5.90977100	0.19527700	-0.33289600
C	4.83077000	0.18526700	-0.51382400
H	4.48274700	1.21824700	-0.58510500
N	4.63656400	-1.90535000	0.77249400
H	5.64209300	-1.88760000	0.97202600
H	4.49579500	-2.44364000	-0.09008600
C	2.62792100	-0.55363400	0.42030300
O	2.00096200	-1.66218900	0.42340600
O	1.99797600	0.51859000	0.23300000
H	4.16828300	-2.40812900	1.53334900
H	4.31155600	-0.00345500	1.57621000
Cu	0.27625400	-0.74266600	0.08728600

S-I1[c]

C	-4.09149700	-0.10533700	-0.19521900
H	-4.37286900	0.32287300	1.90417100
H	-5.59602900	1.04813600	0.82838500
C	-4.53409400	0.80352200	0.93208500
H	-3.96243000	1.73383100	0.90232800
N	-4.93340000	-1.33785400	-0.20244000
H	-5.92083400	-1.09638400	-0.33102800
H	-4.84252800	-1.84390400	0.68553200
C	-2.63518500	-0.52012700	-0.07752700
O	-2.32000200	-1.70937800	0.03777800
O	-1.81972000	0.47220300	-0.10581100

H	-4.65480800	-1.97968300	-0.95077500
H	-4.23671400	0.37926300	-1.16666100
C	4.13858900	0.41924600	0.20718500
H	4.57783800	-0.19955700	-1.81558400
H	6.00436800	0.28190800	-0.85990900
C	4.95290000	0.50670700	-1.06567000
H	4.89005500	1.51796300	-1.47396200
N	4.28825500	-0.94625100	0.79871700
H	5.27366400	-1.13903600	1.00430600
H	3.95419300	-1.66483200	0.14758300
C	2.66979900	0.73030900	-0.02789500
O	1.84797000	-0.20563100	0.29164500
O	2.36282000	1.83123700	-0.49530100
H	3.75154600	-1.04421600	1.66562600
H	4.51211000	1.12383200	0.95783100
Cu	0.00874000	0.11283000	0.05284900

***S*-T2[c]**

C	-4.52640800	0.36020800	-0.24700200
H	-4.46267700	1.18051200	1.75038300
H	-5.55327900	2.03078700	0.62959300
C	-4.58575000	1.52838100	0.71783900
H	-3.79648100	2.25257900	0.49741200
N	-5.49910300	-0.70195600	0.04427400
H	-6.15945600	-0.83996000	-0.71534900
H	-6.01798200	-0.51358400	0.89938900
C	-3.18302700	-0.34421300	-0.18642400
O	-3.27265500	-1.60264300	0.06733100
O	-2.10657500	0.25624900	-0.37150400
H	-4.36070700	-1.65667000	0.15319400
H	-4.64837100	0.71301700	-1.27814400
C	3.41121400	-2.20115400	-0.30252400
H	3.97273300	-1.53475600	-2.27950800
H	5.28165400	-2.32900300	-1.36440800
C	4.42335300	-1.65424200	-1.28726300
H	4.78010300	-0.68014800	-0.94429800
N	2.96904900	-3.55811500	-0.74626400
H	3.77094200	-4.19448200	-0.79651400
H	2.53936300	-3.51725900	-1.67698500
C	2.21673400	-1.27745100	-0.15478100
O	1.08441300	-1.75844100	-0.54177100
O	2.39303300	-0.14668400	0.30518600
H	2.27834300	-3.96040000	-0.10589100

H	3.85932200	-2.32891300	0.68823500
Cu	-0.43395700	-0.69150600	-0.37452800

***S*-I2[c]**

C	-4.17543100	-0.09381000	-0.19979400
H	-4.49408200	0.37268000	1.88727900
H	-5.63345900	1.15155800	0.76440600
C	-4.58928200	0.85971900	0.90949500
H	-3.97190000	1.76240500	0.90653400
N	-4.92584700	-1.34570300	-0.21628200
H	-5.52931500	-1.41827400	0.59874500
H	-3.31029200	-2.16195200	-0.11562400
C	-2.70892500	-0.44241700	-0.07856600
O	-2.41399200	-1.70768700	-0.05228300
O	-1.82961900	0.43202600	-0.01719600
H	-5.50485400	-1.42098900	-1.04609800
H	-4.26658800	0.41429200	-1.16932500
C	4.15835300	0.41519400	0.21112500
H	4.54010200	-0.21644700	-1.81980800
H	5.98991500	0.29677200	-0.91684600
C	4.92873600	0.50258100	-1.08924100
H	4.83580600	1.50910300	-1.50389300
N	4.33697000	-0.94570900	0.80434400
H	5.33139600	-1.13504500	0.96580300
H	3.97502200	-1.66970300	0.17447700
C	2.68277100	0.71397700	0.01377900
O	1.87984700	-0.25802400	0.27879800
O	2.34741400	1.83293400	-0.38265700
H	3.84313000	-1.03837400	1.69703000
H	4.54860400	1.12788600	0.94495300
Cu	0.04971300	0.06621700	0.09171600

***S*-T3m[c]**

C	-4.15397000	0.02680100	-0.30692200
H	-4.58292200	-0.11722600	1.81745800
H	-5.65642500	0.96846400	0.90361600
C	-4.62005100	0.63489200	1.01950500
H	-4.00640700	1.49466900	1.31040700
N	-4.93936100	-1.10768200	-0.76680800
H	-5.09263200	-1.74232200	0.01637500
H	-2.25655700	-2.24391200	-0.33948000
C	-2.72184000	-0.36641900	-0.12532300

O	-2.46576700	-1.58805500	0.34876100
O	-1.81615800	0.45376800	-0.27944100
H	-5.85782000	-0.75957300	-1.03290800
H	-4.16460000	0.80484600	-1.07796200
C	4.17127000	0.44889700	0.16421700
H	4.46159800	-0.40349100	-1.79962500
H	5.95396900	0.17917600	-1.01612300
C	4.88942400	0.38390000	-1.16784600
H	4.79201700	1.34130300	-1.68506200
N	4.35899400	-0.84422900	0.89117700
H	5.35697900	-1.02944200	1.03449900
H	3.96620100	-1.62487100	0.35382800
C	2.69347800	0.74569800	-0.01856100
O	1.89056500	-0.20026300	0.32913600
O	2.35643400	1.83351300	-0.49210900
H	3.89963800	-0.83758100	1.80700200
H	4.59767000	1.23022600	0.80132200
Cu	0.06373600	0.09764100	0.04337000

***S*-T3n[c]**

C	-4.20600500	-0.27589000	-0.15016500
H	-4.23921800	1.31306800	1.31314200
H	-5.58125200	1.33337500	0.14918400
C	-4.50817200	1.14930400	0.26269800
H	-3.96765200	1.87599100	-0.35273500
N	-4.92504700	-1.30482600	0.59501400
H	-4.93924100	-1.04195900	1.57942500
H	-2.24665700	-2.44917800	0.20010500
C	-2.73734800	-0.59071400	-0.10817900
O	-2.36196300	-1.80648800	-0.52028300
O	-1.89149300	0.25398200	0.18683600
H	-5.89292400	-1.30662800	0.28462700
H	-4.45337100	-0.41238900	-1.21510400
C	4.10810600	0.31158200	0.37299200
H	4.48330300	0.40750500	-1.75227800
H	5.92290700	0.66515800	-0.73168600
C	4.85061300	0.86333100	-0.82550900
H	4.70299800	1.94421700	-0.88305500
N	4.35859100	-1.15827700	0.48073700
H	5.36253200	-1.34181700	0.57649900
H	4.02575500	-1.64849500	-0.35675100
C	2.61916600	0.59193400	0.29166600
O	1.85199000	-0.44363500	0.26079500

O	2.23351100	1.76288700	0.25640900
H	3.87974500	-1.56799100	1.28858000
H	4.47946400	0.75911100	1.30079800
Cu	0.02206800	-0.09555500	0.17859800

***S*-I3[c]**

C	-4.14998900	-0.05535100	-0.29748400
H	-4.58153800	-0.00338600	1.82788800
H	-5.59675200	1.06448700	0.83028300
C	-4.58022200	0.68381200	0.97228900
H	-3.91960800	1.52866700	1.19577900
N	-5.00474900	-1.17171500	-0.66860000
H	-5.15740300	-1.75897500	0.15094800
H	-1.62861300	-1.94009600	0.46040600
C	-2.73219800	-0.49343600	-0.08980600
O	-2.56779400	-1.73356800	0.29029600
O	-1.80163800	0.31704200	-0.21648400
H	-5.91592300	-0.78927700	-0.91192400
H	-4.12047200	0.65715300	-1.12953900
C	4.18047600	0.45326800	0.17338500
H	4.48771100	-0.36316800	-1.80316800
H	5.96668200	0.24477900	-1.01334800
C	4.89720200	0.42526300	-1.16070500
H	4.77532400	1.38744300	-1.66370500
N	4.40284700	-0.84454500	0.88169300
H	5.40527900	-1.00426900	1.02460200
H	4.03296300	-1.62785000	0.33216800
C	2.69518000	0.71468400	-0.00123900
O	1.91557600	-0.25134000	0.34378400
O	2.32910100	1.79717100	-0.46568400
H	3.94183400	-0.86334900	1.79651000
H	4.58829700	1.23633300	0.82054800
Cu	0.08252700	0.01539800	0.07019500

***S*-T4[c]**

C	-4.05132600	0.05034800	-0.00627000
H	-4.98957700	-0.60822700	-1.82247900
H	-5.33714200	-1.61422400	-0.40196700
C	-4.55971500	-1.02518700	-0.90039700
H	-3.75067500	-1.70735400	-1.17480400
N	-5.11372400	0.89858700	0.67762000

H	-6.04723800	0.62423000	0.38434900
H	-4.93389700	1.90050000	0.65983500
C	-2.78758100	0.63208200	-0.12716700
O	-2.59938000	1.79056500	0.52247600
O	-1.84928500	0.09047900	-0.79304500
H	-1.68617700	2.10150600	0.40470900
H	-4.37088700	0.04969200	1.22773300
C	4.17314600	0.20786200	-0.51429500
H	4.45414500	-1.22094100	1.08195100
H	5.96078500	-0.67399200	0.29972900
C	4.91461000	-0.94527800	0.12611300
H	4.88955500	-1.81201200	-0.53836100
N	4.27503000	1.41400700	0.36325100
H	5.25748700	1.67152200	0.50066300
H	3.86374900	1.23111300	1.28482200
C	2.71632000	-0.12579800	-0.78787400
O	2.45491200	-1.08906400	-1.51427200
O	1.85399900	0.64842400	-0.22744800
H	3.78363800	2.21779000	-0.03890500
H	4.63367900	0.48252400	-1.46949700
Cu	0.00758500	0.35221900	-0.50862100

I4[c]

C	-3.62831600	-0.46972500	0.27992400
H	-4.49748300	1.40279600	0.73253600
H	-2.96598900	1.49095900	-0.13757400
C	-3.50343400	0.94008800	0.64816200
H	-2.97244400	1.05165800	1.59388600
N	-4.29578500	-0.76445700	-0.97260500
H	-4.40580200	-1.77317200	-1.13806500
H	-2.92909900	-3.46880100	1.06301300
C	-3.12336400	-1.57488000	1.04634400
O	-3.30734000	-2.76693700	0.49626900
O	-2.55944200	-1.38831800	2.13539400
H	-5.23279900	-0.33461800	-0.99489200
H	-3.77511700	-0.36900000	-1.77076200
C	-0.13408200	-5.09886500	6.25085200
H	1.87274800	-5.03655900	5.45447100
H	1.72059400	-5.90505000	7.00417600
C	1.36820400	-5.04335700	6.42806900
H	1.64075000	-4.13389100	6.96887200
N	-0.50104900	-6.37607700	5.56392100
H	-0.18876700	-7.18281300	6.11275000
H	-0.05924700	-6.42700500	4.63982100

C	-0.65625600	-3.90888000	5.45740900
O	-1.17771000	-4.17922600	4.32286100
O	-0.52718000	-2.78416200	5.96597600
H	-1.51242400	-6.45200300	5.42259800
H	-0.64078800	-5.11257400	7.22103700
Cu	-1.86168000	-2.75163400	3.26864600

R-allo-T5[c]

C	-3.71904600	-0.46712900	0.43648700
H	-3.95593000	1.65736800	0.31442800
H	-2.36175000	1.07039400	-0.20046600
C	-3.17666600	0.91604300	0.52169300
H	-2.79015200	1.11354100	1.52512000
N	-4.52506700	-0.78278200	-0.81782300
H	-4.27935200	-1.65807200	-1.27574900
H	-3.15200400	-3.47962500	1.20889000
C	-3.16092700	-1.56314700	1.09757100
O	-3.51832600	-2.77526400	0.64866700
O	-2.37906500	-1.42464200	2.09160700
H	-4.97839500	-0.66561300	0.33927200
H	-4.56457600	0.02447100	-1.43343700
C	-0.60125800	-4.86537500	6.63330100
H	1.49394000	-4.36726400	6.47278400
H	1.06736700	-5.32100900	7.91817600
C	0.73692100	-4.51824200	7.25142200
H	0.64514900	-3.59935100	7.83537200
N	-0.47851000	-6.14856700	5.87650000
H	-0.17055300	-6.90236200	6.49881600
H	0.20967200	-6.05919100	5.12108200
C	-1.09407000	-3.76013900	5.71716800
O	-1.15846600	-4.06170000	4.46693300
O	-1.37932200	-2.66351300	6.20589900
H	-1.36791700	-6.42611400	5.45062800
H	-1.35916700	-5.02829400	7.40592100
Cu	-1.79664900	-2.75411500	3.29512700

R-allo-I5[c]

C	-4.11280600	-0.37244200	0.57909700
H	-4.66816400	1.51195400	-0.29129200
H	-3.33836300	0.69274900	-1.14382700
C	-3.75618600	0.92186500	-0.15532700

H	-3.03232400	1.52287500	0.40597600
N	-5.09037600	-1.20797500	-0.10028200
H	-4.82111400	-1.30551100	-1.07891200
H	-1.67372200	-2.45652100	0.12290000
C	-2.83113800	-1.11171700	0.81474300
O	-2.54287900	-2.04598800	-0.05404800
O	-2.08360600	-0.79191500	1.75174200
H	-4.49602800	-0.12202800	1.57449100
H	-5.97455700	-0.70407100	-0.10175700
C	3.20277100	-2.45906900	4.05184700
H	4.31206800	-1.14687100	2.74198300
H	5.28925600	-1.92045600	4.01757200
C	4.31858900	-1.46862300	3.79020200
H	4.18834500	-0.59059800	4.42738900
N	3.42423400	-3.67962000	3.21764200
H	4.32473000	-4.11106800	3.44867200
H	3.43424200	-3.43973800	2.22008800
C	1.84616200	-1.84954000	3.74708800
O	1.23586400	-2.34268800	2.72471500
O	1.43185700	-0.92800100	4.45379300
H	2.68856000	-4.37839100	3.35963500
H	3.20436700	-2.78687700	5.09580600
Cu	-0.39676900	-1.58324100	2.23961200

R-allo-T6m[c]

C	-4.10345800	-0.20111900	0.72762300
H	-4.63222500	1.45790600	-0.52942700
H	-3.52986300	0.29835700	-1.30740200
C	-3.76131200	0.81457000	-0.36707100
H	-2.90924900	1.44470100	-0.08721600
N	-5.22802900	-1.07276500	0.41979100
H	-5.11396700	-1.43652200	-0.52576700
H	-2.13796100	-1.83663100	-0.65203500
C	-2.86629100	-1.01124500	0.94974200
O	-2.65319600	-2.05728900	0.14430600
O	-2.06058700	-0.73220100	1.83891300
H	-4.30740100	0.32919400	1.66323700
H	-6.06670300	-0.49631100	0.40255900
C	3.16276700	-2.56448600	3.94827800
H	4.36725800	-0.90841100	3.25709200
H	5.16544700	-1.95949800	4.45637500
C	4.21522000	-1.49918500	4.16780400
H	3.89871000	-0.83043100	4.97144900

N	3.62726800	-3.51774400	2.89461400
H	4.50258400	-3.96604400	3.18376900
H	3.79980000	-3.03026100	2.00868700
C	1.81772800	-1.97153900	3.57345800
O	1.31861900	-2.36120500	2.44922700
O	1.27969800	-1.17343300	4.34589600
H	2.93503600	-4.25151300	2.71442200
H	3.01543600	-3.15745200	4.85747900
Cu	-0.35694700	-1.62259600	2.08608300

R-allo-T6n[c]

C	-4.13697600	-0.30007000	0.67654900
H	-4.67705100	1.45701700	-0.43262700
H	-3.37036400	0.51304300	-1.18563700
C	-3.77017600	0.87756800	-0.23123500
H	-3.03034300	1.53664800	0.23664500
N	-5.12649400	-1.21138900	0.12276000
H	-4.88979900	-1.40585200	-0.84973800
H	-2.70851100	-2.86601200	0.34591100
C	-2.86549500	-1.03016600	0.97305500
O	-2.46301200	-1.95713400	0.09981300
O	-2.14388800	-0.69626300	1.91413600
H	-4.50311300	0.08660400	1.63330300
H	-6.02014400	-0.72502200	0.10532600
C	3.17867000	-2.52620900	3.98770000
H	4.35606700	-1.01709200	2.98638600
H	5.26047900	-2.00515000	4.16430800
C	4.30368100	-1.51313600	3.96259600
H	4.13551200	-0.75677500	4.73278700
N	3.44784200	-3.58997300	2.97287700
H	4.33391700	-4.06259700	3.17706300
H	3.51359100	-3.18622400	2.03211500
C	1.83116800	-1.87883000	3.72428400
O	1.23249500	-2.26686400	2.65006600
O	1.40233200	-1.03912000	4.51866800
H	2.70438700	-4.29421500	2.95408100
H	3.12524900	-3.02802300	4.95927000
Cu	-0.42389500	-1.50289100	2.29786400

R-allo-I6[c]

C	-4.09912100	-0.19165200	0.70316200

H	-4.77257900	1.41462300	-0.55282100
H	-3.59800100	0.33090500	-1.33425600
C	-3.85971200	0.83302100	-0.39493800
H	-3.05069800	1.51851800	-0.12791900
N	-5.12560100	-1.17347500	0.36487500
H	-5.48230700	-1.01900600	-0.57435300
H	-3.83815000	-2.40948200	0.59532000
C	-2.82159400	-0.95061400	0.98415000
O	-2.87798200	-2.24193600	0.85398500
O	-1.77305200	-0.37417200	1.31661100
H	-4.34824100	0.32543300	1.63912300
H	-5.90686500	-1.13457600	1.01125400
C	3.83027500	-2.01636100	2.45083800
H	4.72313700	-1.08136700	0.71990400
H	5.89151100	-1.66884100	1.93290600
C	4.91618500	-1.19228100	1.79325000
H	4.94935100	-0.19948500	2.24803900
N	3.82661900	-3.39289800	1.86834100
H	4.73799800	-3.84032800	2.00688400
H	3.63908200	-3.36113400	0.86014900
C	2.46296700	-1.37685100	2.30017300
O	1.58027500	-2.07452600	1.67143600
O	2.27391400	-0.25349800	2.77477100
H	3.10846800	-3.98489100	2.29620800
H	4.02460300	-2.13260500	3.52240900
Cu	-0.09293700	-1.26316100	1.53575300

R-allo-T7[c]

C	-4.09827400	-0.17101400	0.71650700
H	-4.85126200	1.40664000	-0.53432500
H	-3.61534000	0.38978100	-1.31329800
C	-3.91249400	0.86909400	-0.37264000
H	-3.14127400	1.59134000	-0.09073200
N	-5.05066600	-1.22954700	0.35412500
H	-5.43725700	-1.08830600	-0.57642600
H	-3.94334500	-2.21520100	0.49475300
C	-2.80087500	-0.91586200	0.97295200
O	-2.88567400	-2.18332600	0.77115000
O	-1.76054100	-0.33149500	1.33335000
H	-4.38949200	0.30974700	1.65759700
H	-5.81600400	-1.30413000	1.01831500
C	3.83266300	-2.01395500	2.45442200
H	4.73244400	-1.14118100	0.69513700

H	5.89677800	-1.71877300	1.91660500
C	4.92982800	-1.22731900	1.77001600
H	4.98444500	-0.22378100	2.19830500
N	3.79997200	-3.40417700	1.90588800
H	4.70242700	-3.86656100	2.05339700
H	3.60927300	-3.39429000	0.89787200
C	2.47659100	-1.35264100	2.29472700
O	1.58098100	-2.04603100	1.68075400
O	2.30921400	-0.21727900	2.74868700
H	3.07127600	-3.97032900	2.35085200
H	4.03156300	-2.10758200	3.52729200
Cu	-0.08574300	-1.22037200	1.53983600

R-allo-I7[c]

C	-4.01391600	-0.26295100	0.71857500
H	-4.85823700	1.35462000	-0.43083400
H	-3.54239000	0.47790800	-1.25500100
C	-3.89089300	0.86234100	-0.28892100
H	-3.17518400	1.60461400	0.07236800
N	-5.03670700	-1.24257700	0.24612100
H	-5.93819100	-0.77941500	0.09727300
H	-4.74240900	-1.66970800	-0.63951500
C	-2.69690000	-0.99512700	0.89858200
O	-2.54849500	-2.14653200	0.47339500
O	-1.79366100	-0.29662800	1.48858500
H	-4.35495400	0.11152400	1.68832800
H	-5.17185300	-2.00185200	0.92075100
C	3.82054600	-1.95147900	2.46714400
H	4.62355000	-1.36758400	0.54854800
H	5.85211400	-1.81560500	1.76151900
C	4.89235400	-1.31165400	1.61003700
H	5.00656600	-0.26118500	1.88816800
N	3.70432600	-3.40032800	2.11783300
H	4.59604800	-3.87889300	2.27834600
H	3.45401400	-3.51718500	1.12981900
C	2.48012200	-1.26022100	2.29673400
O	1.55152900	-1.96192000	1.74905600
O	2.36539400	-0.08949700	2.67311400
H	2.98299900	-3.86759700	2.67537600
H	4.08926000	-1.90654400	3.52733000
Cu	-0.11792200	-1.12142300	1.61119600

R-allo-T8[c]

C	-2.18499300	2.67718000	1.97097800
H	-2.41961500	4.68001700	1.22432900
H	-1.91402200	3.49488000	-0.00981400
C	-1.79588100	3.80102300	1.03569300
H	-0.75252900	4.07590000	1.20600900
N	-3.62862900	2.34154400	1.79192200
H	-4.21164600	3.15330300	2.01909800
H	-3.82273100	2.07691600	0.81912100
C	-1.36890600	1.42906400	1.76060000
O	-1.91066800	0.30695500	1.59244600
O	-0.09894600	1.52452900	1.76537200
H	-2.06051500	2.97978200	3.01705300
H	-3.91558800	1.55932800	2.38894600
C	2.01681500	-3.82059000	0.80805800
H	2.35260600	-3.63175200	-1.31799000
H	3.31088500	-4.90832100	-0.52130800
C	2.90863100	-3.89657800	-0.41162700
H	3.74521400	-3.20342400	-0.29752000
N	0.90854600	-4.81554500	0.69020000
H	1.29049400	-5.76449300	0.62623300
H	0.34902900	-4.64342200	-0.15271100
C	1.43938300	-2.44340700	1.02474600
O	0.17243900	-2.31668500	1.16278000
O	2.19635500	-1.45384500	1.09192200
H	0.27573800	-4.77620100	1.49538400
H	2.57506400	-4.08427600	1.71387700
Cu	0.13061800	-0.40440300	1.46960800

R-allo-A·Cu(II)[c(a)]

C	-2.40249100	2.52456100	1.93562000
H	-2.84096100	4.51203600	1.24288100
H	-2.20212400	3.42380800	-0.01845800
C	-2.12570300	3.71025400	1.03640000
H	-1.11840900	4.08771300	1.22719400
N	-3.80036600	2.04496200	1.72518100
H	-4.46712600	2.79092400	1.94967000
H	-3.94933500	1.77367500	0.74627100
C	-1.45114200	1.38488200	1.69034700
O	-1.88086300	0.23551400	1.37032500

O	-0.20676100	1.57256400	1.80714700
H	-2.32061500	2.80671500	2.99103700
H	-4.01927300	1.23167800	2.30943200
C	2.45388800	-3.43313000	1.38327500
H	3.33396600	-3.10670300	-0.56374400
H	4.32346100	-4.09051500	0.54813900
C	3.64967400	-3.23140800	0.47795800
H	4.19708700	-2.33868000	0.78902200
N	1.73404300	-4.68714500	1.01468200
H	2.35199500	-5.49702300	1.12898200
H	1.43029700	-4.66040300	0.03435800
C	1.48477500	-2.28273100	1.33736400
O	0.24891100	-2.46632200	1.14230200
O	1.91689400	-1.10484100	1.51393000
H	0.90110600	-4.83232900	1.59451500
H	2.77179900	-3.54931000	2.42590100
Cu	0.03147800	-0.42297500	1.35608300

Pathway d

R-allo-A·Cu(II)[c(a)]

C	-2.40249100	2.52456100	1.93562000
H	-2.84096100	4.51203600	1.24288100
H	-2.20212400	3.42380800	-0.01845800
C	-2.12570300	3.71025400	1.03640000
H	-1.11840900	4.08771300	1.22719400
N	-3.80036600	2.04496200	1.72518100
H	-4.46712600	2.79092400	1.94967000
H	-3.94933500	1.77367500	0.74627100
C	-1.45114200	1.38488200	1.69034700
O	-1.88086300	0.23551400	1.37032500
O	-0.20676100	1.57256400	1.80714700
H	-2.32061500	2.80671500	2.99103700
H	-4.01927300	1.23167800	2.30943200
C	2.45388800	-3.43313000	1.38327500
H	3.33396600	-3.10670300	-0.56374400
H	4.32346100	-4.09051500	0.54813900
C	3.64967400	-3.23140800	0.47795800
H	4.19708700	-2.33868000	0.78902200
N	1.73404300	-4.68714500	1.01468200
H	2.35199500	-5.49702300	1.12898200

H	1.43029700	-4.66040300	0.03435800
C	1.48477500	-2.28273100	1.33736400
O	0.24891100	-2.46632200	1.14230200
O	1.91689400	-1.10484100	1.51393000
H	0.90110600	-4.83232900	1.59451500
H	2.77179900	-3.54931000	2.42590100
Cu	0.03147800	-0.42297500	1.35608300

R-allo-T1[d]

C	-2.59398400	2.37453200	1.90384600
H	-3.05824400	4.33682700	1.15565000
H	-2.34552100	3.24212900	-0.05919600
C	-2.31543900	3.55045800	0.99185000
H	-1.32603900	3.95829500	1.21128500
N	-3.97243600	1.85744200	1.65540900
H	-4.66363100	2.59142500	1.84274000
H	-4.08245200	1.56625500	0.67699400
C	-1.60328000	1.25836200	1.71051700
O	-1.99785200	0.08863100	1.40149600
O	-0.37185800	1.48263300	1.85068600
H	-2.55516100	2.67815300	2.95564600
H	-4.19278000	1.04951900	2.24645100
C	2.86174400	-3.12738400	1.44890800
H	3.71315200	-2.68228200	-0.48666500
H	4.87466100	-3.30762000	0.71392700
C	4.00181100	-2.66347700	0.57005700
H	4.28041000	-1.64240400	0.84030800
N	2.52527100	-4.54971000	1.14580500
H	3.33111200	-5.15358100	1.33637100
H	2.27331200	-4.66260200	0.15719600
C	1.61218200	-2.29347600	1.30812100
O	0.48838500	-2.80960200	1.13144700
O	1.74454600	-1.02608200	1.42224900
H	1.73286800	-4.87788600	1.70688800
H	3.15106300	-3.09527800	2.50586800
Cu	-0.12207600	-0.55556700	1.37046700

R-allo-I1[d]

C	-2.55490800	2.80277600	1.09616800

H	-3.22212000	4.41057000	-0.17624500
H	-2.06397200	3.29604200	-0.94912700
C	-2.32380000	3.80666700	-0.01426200
H	-1.50379700	4.47464900	0.26012000
N	-3.71233500	1.92725700	0.74029800
H	-4.55648100	2.49160000	0.60084800
H	-3.52633000	1.41422600	-0.12833100
C	-1.31517100	1.96429200	1.34667000
O	-1.41473600	0.71207300	1.06038700
O	-0.30201000	2.52163300	1.78000400
H	-2.81898100	3.30698300	2.03126700
H	-3.90471400	1.23558600	1.47131300
C	2.84299600	-3.41900800	1.43290500
H	3.58936900	-3.09187100	-0.56776500
H	4.83103900	-3.57895200	0.61566300
C	3.92636700	-2.98037700	0.46968000
H	4.17511000	-1.93139700	0.64651600
N	2.55705600	-4.87061400	1.23074500
H	3.39931800	-5.42951200	1.39767400
H	2.24223100	-5.04485900	0.26973900
C	1.55113000	-2.64750600	1.23630300
O	0.52969200	-3.21445300	0.83314800
O	1.65053300	-1.39458700	1.51495400
H	1.81823600	-5.20158400	1.85845700
H	3.16899900	-3.30322100	2.47140600
Cu	0.11833500	-0.34238100	1.29155000

R-allo-T2[d]

C	-2.56760000	2.80364600	1.08538300
H	-3.35733400	4.45989600	-0.04354100
H	-2.20561500	3.44050800	-0.94714500
C	-2.43130300	3.88122900	0.03093700
H	-1.62096700	4.56116200	0.30439500
N	-3.71431000	1.91006300	0.73913600
H	-4.58440200	2.45008500	0.69095700
H	-3.56829000	1.46320700	-0.17244300
C	-1.29147700	1.99627800	1.23295000
O	-1.38254900	0.74284000	0.94118800
O	-0.26550400	2.56978000	1.60767700
H	-2.79861000	3.24121900	2.06228100
H	-3.83639100	1.16481100	1.43135900
C	2.90804000	-3.47810500	1.46821200

H	3.70497900	-3.16270200	-0.51454000
H	4.90590200	-3.66191100	0.70078200
C	4.01827500	-3.04608400	0.52985000
H	4.28350000	-1.99880100	0.69952300
N	2.43575900	-4.84906600	1.23404700
H	2.89835900	-5.27546100	0.43383900
H	1.06787200	-4.29091000	0.99712600
C	1.66784000	-2.62388200	1.28193200
O	0.61295000	-3.30000500	0.99257600
O	1.69326000	-1.38171800	1.39991100
H	2.56763800	-5.44685900	2.04477600
H	3.22279300	-3.35527200	2.51137800
Cu	0.14796900	-0.30226100	1.15645200

R-allo-I2[d]

C	-2.57651700	2.78927700	1.08049000
H	-3.34961100	4.50579800	0.03313600
H	-2.14179700	3.56966500	-0.88669200
C	-2.41659200	3.93857500	0.10830500
H	-1.63204700	4.61146100	0.46209400
N	-3.69304600	1.90350500	0.62947500
H	-4.57293500	2.42840600	0.59445300
H	-3.50946500	1.53266500	-0.30918600
C	-1.29559000	1.98937300	1.23095600
O	-1.37485000	0.74018100	0.91734600
O	-0.27985600	2.56033000	1.63539400
H	-2.85393100	3.15624900	2.07442300
H	-3.81952300	1.10385800	1.25721300
C	2.90411600	-3.48415700	1.45002700
H	3.60210000	-3.20423300	-0.57739000
H	4.86853900	-3.62791600	0.59771900
C	3.95736200	-3.04178200	0.44725000
H	4.20065500	-1.98258500	0.56884300
N	2.49662100	-4.87889800	1.30536800
H	2.89765800	-5.28878100	0.46548600
H	0.81793000	-4.24093400	1.16761300
C	1.66000700	-2.63460900	1.32093200
O	0.53863000	-3.27214500	1.16846400
O	1.70148000	-1.39259800	1.36294600
H	2.79063700	-5.43646000	2.10046600
H	3.26990900	-3.30176100	2.46944500
Cu	0.15464500	-0.30149200	1.13944600

R-allo-T3m[d]

C	-2.62347500	2.77125700	1.11525300
H	-3.09617800	4.48996700	-0.09609300
H	-1.82139600	3.44322700	-0.77476000
C	-2.22854800	3.86962600	0.14966800
H	-1.46772000	4.50585000	0.60819900
N	-3.70070000	1.93699200	0.50167700
H	-4.51276700	2.51784300	0.27014000
H	-3.36961100	1.49406400	-0.36257000
C	-1.43057300	1.90974400	1.48210400
O	-1.46874700	0.68768000	1.06557900
O	-0.50283900	2.41390500	2.11940900
H	-3.03679900	3.19011800	2.03795900
H	-4.01043000	1.19077000	1.13147100
C	2.99017300	-3.34245600	1.53434500
H	3.21215100	-3.54654600	-0.61547300
H	4.72853400	-3.64010200	0.31066700
C	3.76600900	-3.12424000	0.23205500
H	3.95286000	-2.06134700	0.04192300
N	2.70695100	-4.73565800	1.84773200
H	2.38448100	-5.20552600	1.00219400
H	0.06266800	-3.60887100	1.32100800
C	1.71063700	-2.57960900	1.40866900
O	0.71027700	-3.16625400	0.74506900
O	1.61465000	-1.40729400	1.77792900
H	3.58522800	-5.18159500	2.10270300
H	3.54414400	-2.89336200	2.36477500
Cu	0.03956900	-0.34754200	1.43831700

R-allo-T3n[d]

C	-2.65642000	2.74470400	1.11984800
H	-3.12307800	4.52577900	0.00005400
H	-1.81917100	3.53613500	-0.70851900
C	-2.25354000	3.90183200	0.22936100
H	-1.51162100	4.51876100	0.74214100
N	-3.70703300	1.93324000	0.43373200
H	-4.51671400	2.51818300	0.20416000
H	-3.34490700	1.53247300	-0.43873900

C	-1.46106100	1.87781000	1.46535900
O	-1.46418400	0.68776900	0.96505600
O	-0.56240200	2.35064100	2.16524500
H	-3.09734700	3.10423100	2.05471700
H	-4.02907200	1.15638100	1.01865500
C	2.98757400	-3.34757300	1.49963400
H	3.21826900	-3.71887800	-0.62739200
H	4.72650000	-3.77050700	0.31420600
C	3.77451800	-3.24393700	0.19058700
H	3.98449300	-2.20238000	-0.07846800
N	2.66718100	-4.70688800	1.91262900
H	2.29897200	-5.21720000	1.11057000
H	0.68271000	-3.06732000	-0.25947400
C	1.72854600	-2.56435700	1.30477900
O	0.70289000	-3.17908400	0.70765900
O	1.62355400	-1.39672300	1.68478800
H	3.53998600	-5.16538800	2.16497500
H	3.54692100	-2.85369600	2.30028400
Cu	0.04811800	-0.33926200	1.33858500

R-allo-I3[d]

C	-2.64083700	2.78982300	1.10778700
H	-3.11553500	4.57776000	0.00336800
H	-1.80251600	3.60408500	-0.71034200
C	-2.24267300	3.95731400	0.22947600
H	-1.50693100	4.57450900	0.75048900
N	-3.69015800	1.98191600	0.41525500
H	-4.50240800	2.56666100	0.19444100
H	-3.32950400	1.59278800	-0.46303700
C	-1.44559800	1.92159000	1.45209700
O	-1.48380300	0.70805500	1.01260700
O	-0.51986600	2.41304800	2.10202800
H	-3.08384000	3.13974400	2.04575700
H	-4.00725500	1.19712100	0.99208900
C	2.98013600	-3.37213300	1.50247600
H	3.20332800	-3.59944400	-0.64267500
H	4.72920300	-3.58563900	0.27255200
C	3.73663000	-3.13063200	0.19389500
H	3.85878300	-2.06212800	-0.01637200
N	2.79279000	-4.77438300	1.84343100
H	2.43912800	-5.26977000	1.02520300

H	-0.13328400	-2.87148000	0.78267600
C	1.66531200	-2.66604400	1.37779400
O	0.68584400	-3.38972600	0.90048100
O	1.55862600	-1.45835600	1.64848500
H	3.71204400	-5.16811400	2.03204700
H	3.51227500	-2.87696700	2.32135600
Cu	0.01432900	-0.35061400	1.36171100

T4[d]

C	-2.52285600	2.74170200	0.91413800
H	-3.51928900	4.18622700	-0.33699700
H	-2.47752200	3.04219500	-1.22433300
C	-2.57384700	3.63541400	-0.30724200
H	-1.75467700	4.35764800	-0.26851100
N	-3.67321400	1.78707000	0.87661500
H	-4.56220400	2.29740500	0.85929700
H	-3.62925500	1.19629000	0.03899300
C	-1.21013500	1.98206900	0.99010400
O	-1.29346800	0.71492000	0.77261000
O	-0.17351200	2.60708200	1.22647200
H	-2.63155100	3.32556700	1.83324500
H	-3.67671900	1.16596300	1.69136300
C	2.69632400	-3.67200500	1.08392900
H	4.38608000	-3.22239300	-0.16404400
H	4.79965800	-3.79540100	1.46421100
C	4.09002200	-3.18569200	0.89450200
H	4.18563800	-2.15406600	1.24359000
N	2.48872800	-5.17072000	0.90300600
H	1.69869500	-5.42517100	0.31362900
H	-0.34700400	-2.89702600	0.71605400
C	1.56502300	-2.87327000	0.90272300
O	0.39884400	-3.51875000	0.75369500
O	1.63281300	-1.60444100	0.90293700
H	3.36365800	-5.63120200	0.66946200
H	2.42250300	-4.54327200	1.98009100
Cu	0.21849900	-0.36432900	0.90558900

I4[d]

C	-2.47200800	2.81220100	0.86169900

H	-3.61938400	4.07438000	-0.46011400
H	-2.73193100	2.76421200	-1.28201200
C	-2.68746800	3.49990800	-0.46992600
H	-1.86149700	4.18759000	-0.66647700
N	-3.64085000	1.92429800	1.15034800
H	-4.50984300	2.46707500	1.17408900
H	-3.73355300	1.20292600	0.42746900
C	-1.18502600	1.99884400	0.87611400
O	-1.32627500	0.73514400	0.99831800
O	-0.11578000	2.61711500	0.75467500
H	-2.42917600	3.54195400	1.67673900
H	-3.53535100	1.44360400	2.04824300
C	2.71681100	-3.69776900	0.91185700
H	4.65277300	-3.58562000	0.07423800
H	4.61576400	-3.61227700	1.83730000
C	4.09808800	-3.21905700	0.95022200
H	4.13252100	-2.12936900	0.96804900
N	2.51681300	-5.13272000	0.87088100
H	2.97062800	-5.54507600	0.04120100
H	-0.35310100	-2.88843600	0.83968700
C	1.54863800	-2.86209300	0.90897400
O	0.39699400	-3.51578600	0.84630100
O	1.64994700	-1.62779900	0.96012500
H	2.94635900	-5.58590600	1.69206000
H	1.52305700	-5.39546200	0.84924600
Cu	0.21684900	-0.37693900	0.97104900

T5[d]

C	-2.82009200	2.28194200	-0.03557500
H	-4.08594400	3.09356500	-1.58397800
H	-3.25629300	1.58009500	-2.03147600
C	-3.15241000	2.52919700	-1.49194800
H	-2.35260300	3.10949600	-1.95806700
N	-3.95014200	1.54142500	0.60675900
H	-4.82135000	2.07580400	0.53167900
H	-4.09131500	0.63389800	0.15087200
C	-1.52469400	1.49748100	0.12257500
O	-1.63405800	0.33769400	0.64802600
O	-0.48036700	2.03475700	-0.27840400
H	-2.71976500	3.22659600	0.50835400
H	-3.76646800	1.35944700	1.59762200
C	2.90148200	-3.65023700	1.22875200

H	4.95622400	-3.66494700	0.67272700
H	4.45530900	-2.30141900	1.70051500
C	4.15284500	-2.95016800	0.86746400
H	3.99604200	-2.32804500	-0.01605100
N	2.98860300	-4.89196700	1.92314900
H	2.72903200	-4.77167000	0.63097000
H	-0.18984800	-3.10938100	1.82962100
C	1.61807100	-2.94120400	1.29509000
O	0.64116000	-3.62679300	1.84766100
O	1.51855400	-1.80333900	0.83833100
H	3.90659600	-5.32875900	2.03198300
H	2.16949400	-5.29766900	2.38295700
Cu	-0.06747000	-0.72560200	0.80002800

R-I5[d]

C	-2.35178300	2.87718200	0.96013200
H	-4.09446600	3.67598500	-0.02177500
H	-3.76765600	1.96228300	-0.39173400
C	-3.30659900	2.94066600	-0.21280400
H	-2.76431200	3.24230500	-1.11195000
N	-3.11035500	2.53066500	2.19996500
H	-3.83442400	3.23342900	2.38139200
H	-3.57150700	1.61934600	2.10459500
C	-1.23294200	1.87854000	0.72609400
O	-1.16289600	0.90793100	1.57347200
O	-0.47746100	2.04455300	-0.23440500
H	-1.89105500	3.85418600	1.14133700
H	-2.49717800	2.48088800	3.01914200
C	3.17753900	-3.38055300	1.24932200
H	5.12004100	-3.39085800	2.16406400
H	3.77677300	-3.30579300	3.32779400
C	4.13678900	-2.95053800	2.35392700
H	4.24112900	-1.86188600	2.39348200
N	3.07641800	-4.82302300	1.19930500
H	3.54621600	-3.00619700	0.28720500
H	0.18325600	-2.76841900	2.33683500
C	1.87963900	-2.65309800	1.49134700
O	0.97675200	-3.31198500	2.16973300
O	1.72461700	-1.48539500	1.09945700
H	2.77496400	-5.17762000	2.10537700
H	2.37647100	-5.10827200	0.51854500
Cu	0.20814100	-0.34413700	1.34652700

R-T6m[d]

C	-2.53575800	2.64360000	1.18893400
H	-3.90263500	3.68023900	-0.11419400
H	-3.15643400	2.23185700	-0.83972000
C	-2.98076800	3.09474400	-0.18666800
H	-2.20752700	3.72285300	-0.63507800
N	-3.62303100	1.83784500	1.82359300
H	-4.47820700	2.39739500	1.90421000
H	-3.84069300	1.00896100	1.25954400
C	-1.24994200	1.84126500	1.12298100
O	-1.32691700	0.62074300	1.53256600
O	-0.23255500	2.38027200	0.68131800
H	-2.36172400	3.50325800	1.84422400
H	-3.36145000	1.51474600	2.76008900
C	2.89392500	-3.65662900	1.35817300
H	4.99951300	-3.61234900	0.98911800
H	4.42432300	-2.28226100	2.01635600
C	4.18566100	-2.89597200	1.13929200
H	4.13433100	-2.24408400	0.26126700
N	2.90829300	-4.59166100	2.47803800
H	2.65023900	-4.23640600	0.45258500
H	0.23984500	-3.35213700	2.61385100
C	1.70552100	-2.74702900	1.49020200
O	0.51167900	-3.31887100	1.68039600
O	1.79057100	-1.52874800	1.32494900
H	3.47460000	-5.39404700	2.21619000
H	3.38340100	-4.14944100	3.26367600
Cu	0.21332400	-0.39985600	1.38297800

R-T6n[d]

C	-2.49380500	2.67013400	0.89420200
H	-4.30826500	3.29916000	-0.08390100
H	-3.87155500	1.59389200	-0.37433100
C	-3.47609300	2.60969900	-0.25693000
H	-2.97375900	2.89981700	-1.18309200
N	-3.19442400	2.31465300	2.16460000
H	-3.97200200	2.96082800	2.33428500

H	-3.57640400	1.36355500	2.11872300
C	-1.31752600	1.74311500	0.66064600
O	-1.25039100	0.70559800	1.42460700
O	-0.51779600	2.01122700	-0.24035700
H	-2.10393500	3.68451800	1.02358000
H	-2.56373400	2.35587900	2.97105300
C	3.08215800	-3.44101900	1.11990200
H	4.96403300	-3.61581100	2.13759000
H	3.60223600	-3.23676200	3.21835700
C	4.04580400	-3.02790300	2.23681000
H	4.30211000	-1.96422400	2.17958700
N	2.71454800	-4.84885500	1.12293400
H	3.52586200	-3.18784000	0.15135300
H	0.17516700	-3.48714900	1.64283400
C	1.86221200	-2.59046100	1.26706400
O	0.90429300	-3.02366000	2.09174600
O	1.78830900	-1.46809600	0.76157600
H	3.53913600	-5.38498000	0.86223800
H	2.48525900	-5.12728600	2.07675000
Cu	0.23814700	-0.36917300	1.08670300

R-I6[d]

C	-2.53601500	2.64837800	1.10172400
H	-4.00434200	3.65492100	-0.11208200
H	-3.41901000	2.11557400	-0.79712200
C	-3.12608700	3.01524100	-0.24349000
H	-2.38584500	3.56305600	-0.83127800
N	-3.56974700	1.95624000	1.93049000
H	-4.37761300	2.57014100	2.07562000
H	-3.90099300	1.10372500	1.46567200
C	-1.30335900	1.77649500	0.95742800
O	-1.36578900	0.61123300	1.50613100
O	-0.33293000	2.21779700	0.33574100
H	-2.24373100	3.54636900	1.65666100
H	-3.20183600	1.68617400	2.84769400
C	2.94267300	-3.59795500	1.16059800
H	5.08709400	-3.55546200	1.13939000
H	4.36124100	-2.65526700	2.49076300
C	4.26302500	-2.89553600	1.42540500
H	4.34257600	-1.96956900	0.84893500
N	2.74633000	-4.82343300	1.93035300
H	2.85595600	-3.81980500	0.08792800

H	1.16932200	-4.10783100	2.42353900
C	1.77278700	-2.68707700	1.45615800
O	0.83228300	-3.18402300	2.20249000
O	1.69651300	-1.53411000	0.99897400
H	2.82264600	-5.64666800	1.34215100
H	3.43939200	-4.89886000	2.67113200
Cu	0.15613400	-0.44121900	1.28499200

R-T7[d]

C	-2.52534400	2.62710300	1.08992600
H	-4.03282400	3.68090500	-0.03100100
H	-3.52472600	2.13537400	-0.76208300
C	-3.17934900	3.02142900	-0.21702500
H	-2.45986700	3.55772200	-0.83989300
N	-3.52978000	1.95798300	1.97291000
H	-4.30543000	2.59646700	2.17625600
H	-3.91971900	1.12462800	1.51877200
C	-1.32297700	1.72542200	0.88236200
O	-1.33849700	0.60093500	1.51318000
O	-0.41038700	2.10946600	0.14515200
H	-2.17886700	3.51316300	1.63368600
H	-3.11420900	1.66026800	2.86068800
C	2.99477100	-3.57338000	1.12803500
H	5.13304800	-3.56499000	1.32566000
H	4.28369800	-2.65280500	2.59663200
C	4.29132000	-2.89634800	1.52753800
H	4.43640500	-1.97292300	0.95994200
N	2.68621500	-4.77924500	1.90865000
H	3.00400600	-3.80898500	0.05698100
H	1.39032400	-4.14442500	2.29801200
C	1.80011200	-2.66742800	1.36197300
O	0.89462900	-3.19136700	2.11088500
O	1.71704500	-1.52538200	0.86645300
H	2.65215300	-5.61512200	1.33222700
H	3.35847500	-4.92542400	2.65904700
Cu	0.17567900	-0.45191900	1.19394200

R-I7[d]

C	-2.50089400	2.61891000	1.10496600

H	-3.99678700	3.71579900	0.00949200
H	-3.49183700	2.19162000	-0.76739300
C	-3.14551300	3.05799300	-0.19208600
H	-2.41953200	3.61010100	-0.79326200
N	-3.51491700	1.93236600	1.96342500
H	-4.28295000	2.57212700	2.18981700
H	-3.91415100	1.12054800	1.47954000
C	-1.30459400	1.71261300	0.87877000
O	-1.32150800	0.58152600	1.49439500
O	-0.39363700	2.10516500	0.14229600
H	-2.15025200	3.48565000	1.67663500
H	-3.10290600	1.59605700	2.83907500
C	2.88197500	-3.55079800	1.14372600
H	5.03363200	-3.61217400	1.22344200
H	4.28375600	-2.59290400	2.47908700
C	4.22184300	-2.90781500	1.43081400
H	4.35498000	-2.03115000	0.79302700
N	2.74068200	-4.79547100	1.95770500
H	2.81041300	-3.85393700	0.09361200
H	1.83373600	-5.24612900	1.80363200
C	1.70723300	-2.64336900	1.45841800
O	0.84615400	-2.98648800	2.27730300
O	1.70539200	-1.53580800	0.80382100
H	3.48113900	-5.46371700	1.72279200
H	2.80905900	-4.58195200	2.95908300
Cu	0.19824200	-0.47295700	1.15645300

R-T8[d]

C	-3.64398200	-0.25351200	0.16971200
H	-5.11227000	0.92354300	-0.87638000
H	-3.85444600	0.22009000	-1.92754700
C	-4.04773800	0.68121500	-0.95198500
H	-3.47564800	1.60927300	-0.88205400
N	-4.47398200	-1.49260100	0.11334100
H	-5.46731800	-1.25972200	0.21120100
H	-4.34837500	-1.97398700	-0.78430400
C	-2.18984100	-0.64664800	0.08304300
O	-1.84212700	-1.82961900	-0.10478500
O	-1.32730000	0.29419900	0.18876600
H	-3.82451200	0.20567800	1.14729300
H	-4.22192800	-2.15299700	0.85553100
C	4.11859600	-0.51325600	-0.62563000

H	5.90977800	0.19531900	0.33286800
H	4.63136200	-0.32073000	1.46515900
C	4.83078000	0.18529500	0.51380800
H	4.48274100	1.21827100	0.58508000
N	4.63659000	-1.90534200	-0.77248000
H	4.31154800	-0.00346300	-1.57621900
H	4.16830500	-2.40814100	-1.53331900
C	2.62793100	-0.55364700	-0.42029100
O	2.00099200	-1.66221400	-0.42334700
O	1.99797100	0.51857200	-0.23302700
H	5.64211600	-1.88758000	-0.97202900
H	4.49584400	-2.44362000	0.09011100
Cu	0.27626000	-0.74274200	-0.08729300

R-A_2·Cu(II)[d]

C	-2.47705200	2.62746600	1.13087100
H	-3.93699300	3.67655900	-0.05224900
H	-3.41372800	2.11986200	-0.74918900
C	-3.08214200	3.01072200	-0.20379800
H	-2.33783600	3.53557200	-0.80696000
N	-3.51116100	1.97354400	1.98762600
H	-4.28490200	2.62252800	2.16454700
H	-3.89896700	1.14276100	1.52551300
C	-1.30898800	1.69126700	0.97192300
O	-1.29943500	0.56006700	1.54622400
O	-0.33728100	2.02433600	0.23804100
H	-2.13105600	3.51395900	1.67392100
H	-3.12688200	1.67557200	2.89008500
C	3.42961600	-2.26771100	0.14911800
H	5.56767900	-2.23730900	0.38939800
H	4.68816500	-1.20336300	1.54629700
C	4.71839500	-1.55804100	0.50980600
H	4.86429700	-0.70089500	-0.15125900
N	3.26577700	-3.48141600	1.00280800
H	3.45040000	-2.61171500	-0.89064300
H	2.39963700	-3.98644500	0.78998500
C	2.22669000	-1.37993400	0.32588800
O	1.26247800	-1.71796500	1.06908500
O	2.19801800	-0.25737300	-0.26263200
H	4.05414200	-4.12130000	0.86139100
H	3.24118300	-3.22741800	1.99728400
Cu	0.45481900	0.15150500	0.64585200

2.2 The stagnation coordinates of the main elementary reaction under the dominant aqueous solvent effect

2.2.1 Coordinates of stationary point of a and b channel speed step

S-I1·$(H_2O)_2$[a(b)]

C	4.06983700	0.55120500	0.17227000
H	4.50673600	0.12282500	-1.90040100
H	5.93364700	0.52546700	-0.90883600
C	4.87944100	0.76106600	-1.09036500
H	4.80730800	1.80528400	-1.40653100
N	4.21977400	-0.86382200	0.62646300
H	5.20700700	-1.07903000	0.79926300
H	3.87300300	-1.51319000	-0.08793200
C	2.60485700	0.87793100	-0.04611400
O	1.79765400	-0.11488600	-0.00158800
O	2.28715300	2.05497500	-0.26773600
H	3.69533100	-1.04475100	1.48765000
H	4.44611300	1.18539000	0.98373500
C	-4.13815400	-0.20083000	-0.31371500
H	-4.39824700	0.98046400	1.47604500
H	-5.67488300	1.19903200	0.25037400
C	-4.60075500	1.05147200	0.40081700
H	-4.07428700	1.92121300	0.00135600
N	-4.91982500	-1.37222000	0.18187800
H	-5.92106300	-1.23233600	0.01488700
H	-4.77885000	-1.50083500	1.19008500
C	-2.66254000	-0.48439600	-0.09573800
O	-2.28998200	-1.51712300	0.47266200
O	-1.88976800	0.44112000	-0.54183100
H	-4.63217900	-2.24012600	-0.28027600
H	-4.32644300	-0.12961900	-1.39005300
Cu	-0.04467400	0.18951200	-0.25792200
O	6.49681900	2.75212300	1.29997900
H	6.86965800	2.25851400	0.55950000
H	5.70536600	3.19512700	0.92814000

O	4.22188400	4.03257300	0.24235000
H	3.52865500	3.36461800	0.05710800
H	3.83752000	4.61704600	0.90738200

***S*-T2·$(H_2O)_2$[a(b)]**

C	4.19734800	0.52810100	0.03206600
H	5.03225800	0.05060600	-1.92427300
H	6.19035700	0.71441600	-0.74331700
C	5.15944800	0.77820400	-1.11145700
H	5.02012800	1.78131600	-1.52350400
N	4.37240800	-0.86421400	0.53839900
H	5.33743600	-0.99111300	0.85831300
H	4.19037100	-1.57323600	-0.18290400
C	2.79289300	0.78310600	-0.22776100
O	1.91130800	-0.08346100	0.01009700
O	2.41288500	1.95594200	-0.66602900
H	3.75398000	-1.06318700	1.33040300
H	4.58082300	1.35661600	0.96471800
C	-4.04299800	-0.04082000	-0.22807200
H	-4.37745200	0.82239800	1.72416400
H	-5.59876600	1.25701200	0.49982200
C	-4.53242400	1.07603000	0.66892600
H	-3.98721100	1.99580700	0.44519100
N	-4.85105400	-1.27083200	0.02233400
H	-5.84096300	-1.09759100	-0.17749000
H	-4.77083600	-1.56233300	1.00296700
C	-2.57864100	-0.37738200	-0.01101300
O	-2.23027800	-1.50380300	0.35695400
O	-1.78762600	0.60837400	-0.25247900
H	-4.53473400	-2.05459600	-0.55655100
H	-4.18302000	0.21673900	-1.28332500
Cu	0.04414000	0.28089200	-0.09777600
O	5.05477200	2.28229100	1.77366200
H	6.01608500	2.21038700	1.72284300
H	4.55289100	3.39988100	0.63466500
O	4.13048700	3.86168800	-0.15062800
H	3.11226700	2.68648500	-0.57117900
H	3.63256700	4.60492500	0.21284500

I2·$(H_2O)_2$[a(b)]

C	4.19399200	0.34418300	-0.61380800

H	6.13088300	1.06399500	-1.16687400
H	5.70140300	1.40517000	0.51628900
C	5.29611400	1.33548600	-0.50396300
H	4.95818700	2.33293500	-0.79631600
N	4.61851200	-1.05722600	-0.48722800
H	5.07960800	-1.23519500	0.41180400
H	5.28141000	-1.33399600	-1.22231900
C	2.90787100	0.51592100	-1.03489900
O	2.14491900	-0.48898400	-1.36158400
O	2.33181100	1.73091300	-1.16617700
H	3.80418900	-1.67902700	-0.55759100
H	3.47000400	0.76821400	1.49319400
C	-3.75620100	-1.09421400	-0.96339800
H	-3.91896000	-0.58467800	1.13074800
H	-5.29798700	-0.05882300	0.13049400
C	-4.21019400	-0.17942300	0.15459900
H	-3.75318000	0.80533100	0.03349500
N	-4.45080400	-2.41066300	-0.84336200
H	-5.46503700	-2.28881400	-0.92165700
H	-4.25073600	-2.84578700	0.06380600
C	-2.25525000	-1.33565300	-0.95314600
O	-1.79619100	-2.47587800	-0.81815500
O	-1.56959200	-0.25955200	-1.09227600
H	-4.14476700	-3.06403500	-1.57060900
H	-4.03277600	-0.68306900	-1.93998200
Cu	0.30557800	-0.37911800	-1.10956600
O	3.27392300	1.27449900	2.30273500
H	4.09078100	1.23590400	2.81766300
H	3.21263300	2.89414200	1.40464600
O	3.17621100	3.55266300	0.67798300
H	2.74010100	2.41912800	-0.57958700
H	2.41851200	4.11539200	0.88249700

***S*-I1←$H_2O\cdot(H_2O)_2$[a(b)]**

C	4.23682000	0.54819700	0.02992500
H	4.50820700	0.71058500	-2.10790300
H	5.94445000	1.14382800	-1.14263200
C	4.85178400	1.20180000	-1.18982800
H	4.56363100	2.25567400	-1.22790200
N	4.66637000	-0.88087900	0.10080500

H	5.68689100	-0.94593700	0.16858100
H	4.36920700	-1.39450100	-0.73597400
C	2.72212400	0.63913300	0.01161100
O	2.09300400	-0.46857600	-0.10189400
O	2.19845200	1.76111700	0.09658100
H	4.26041500	-1.35654900	0.91242900
H	4.59457700	1.02897400	0.94845300
C	-4.00873600	-0.27222500	-0.45999300
H	-4.18039300	1.51429300	0.74340200
H	-5.24946500	1.47221600	-0.68270800
C	-4.25438700	1.21251300	-0.30781600
H	-3.51420300	1.77069500	-0.88524900
N	-5.08040900	-1.03127200	0.25056600
H	-5.99646900	-0.82602300	-0.15929200
H	-5.11117800	-0.77421800	1.24340100
C	-2.65790100	-0.72497100	0.07236600
O	-2.60181300	-1.64688100	0.90399300
O	-1.67228300	-0.08762300	-0.42998500
H	-4.91877200	-2.04183000	0.20040000
H	-4.06615700	-0.56840600	-1.51339200
Cu	0.18795800	-0.39977600	-0.11780700
O	6.32049300	2.77517100	1.69677700
H	6.65075200	2.36553200	0.88779400
H	5.45427100	3.15924800	1.44524900
O	3.81880400	3.87419900	1.00657900
H	3.23105500	3.15650400	0.68906600
H	3.39238000	4.21368700	1.80324000
O	0.05266700	-2.16508400	0.93279700
H	0.50633700	-2.03600600	1.77860700
H	-0.91499900	-2.14599100	1.12964600

***S*-T2←$H_2O\cdot(H_2O)_2$[a(b)]**

C	4.28601800	0.53840900	-0.11493600
H	5.14490200	0.69830000	-2.11181300
H	6.17884100	1.29541600	-0.78858500
C	5.14612000	1.23190800	-1.15173000
H	4.79681100	2.25334800	-1.32572100
N	4.75274500	-0.86803600	0.05639300
H	5.73460800	-0.86988400	0.34888700
H	4.68762100	-1.41430500	-0.81150200

C	2.85110000	0.55090500	-0.33400700
O	2.17556100	-0.50869400	-0.31852300
O	2.22315600	1.69024500	-0.49519900
H	4.21474400	-1.36354500	0.77346600
H	4.52168900	1.19589000	0.99079500
C	-3.93774000	-0.17535600	-0.30844100
H	-3.93507000	1.58243800	0.94914000
H	-5.12268100	1.62199100	-0.37996300
C	-4.11049500	1.31407800	-0.09926400
H	-3.39972500	1.85922800	-0.72457700
N	-4.96228200	-0.91263100	0.48896600
H	-5.90731800	-0.64257900	0.19907500
H	-4.86327700	-0.70237900	1.48843700
C	-2.55867700	-0.66632600	0.10037800
O	-2.44351200	-1.48124600	1.03044300
O	-1.61353700	-0.15954100	-0.59563100
H	-4.86659700	-1.92664700	0.37845500
H	-4.10224600	-0.44490900	-1.35687100
Cu	0.25471900	-0.45231700	-0.33069400
O	4.82158300	1.99510800	1.99049400
H	5.77719500	2.12339400	1.94348400
H	4.07972100	3.20749000	1.11926200
O	3.55126800	3.74309300	0.45366000
H	2.76060600	2.50915700	-0.22976600
H	2.93190500	4.27397100	0.97027200
O	0.13339800	-2.21563100	0.69920700
H	0.73783100	-2.15865200	1.45389200
H	-0.78127500	-2.11596200	1.05800900

I2←$H_2O\cdot(H_2O)_2$[a(b)]

C	4.28479600	0.33763400	-0.42240000
H	6.00305600	0.97716200	-1.53278800
H	5.89831000	1.68672600	0.08624500
C	5.30074100	1.36521400	-0.77926800
H	4.82909900	2.25588000	-1.20253400
N	4.85541600	-0.96585800	-0.04732700
H	5.46052600	-0.89526500	0.77781500
H	5.42418900	-1.37342600	-0.80021800
C	2.94423800	0.31452800	-0.68658500
O	2.23794000	-0.77362800	-0.61335600

O	2.25258000	1.41877800	-1.04966900
H	4.10507900	-1.63334200	0.16531300
H	3.87165000	1.34577100	1.49303100
C	-3.76200900	-0.00412700	-0.13883800
H	-3.36353500	1.63367400	1.21386600
H	-4.68088200	1.93619100	0.05155800
C	-3.69667100	1.47494800	0.18130800
H	-2.99348000	1.96802600	-0.49381900
N	-4.77677400	-0.65686700	0.74076500
H	-5.69416300	-0.21765900	0.61868300
H	-4.50851200	-0.56924900	1.72738100
C	-2.42290300	-0.69140600	0.07063300
O	-2.30245500	-1.54360600	0.96721000
O	-1.51159900	-0.28876800	-0.72978500
H	-4.86668200	-1.65679700	0.53673400
H	-4.08597300	-0.16852000	-1.17137100
Cu	0.35484700	-0.66491800	-0.58631800
O	3.75072300	2.05382300	2.15522900
H	4.63250800	2.19830200	2.52280500
H	3.39036200	3.34748200	0.88097800
O	3.17176400	3.76114500	0.01823500
H	2.67749300	2.26504500	-0.75525400
H	2.39211200	4.30561400	0.18634300
O	0.20290000	-2.43408400	0.45092900
H	0.84676200	-2.40329300	1.17357600
H	-0.68515400	-2.29265000	0.85757900

***S*-I1←$(H_2O)_2$·$(H_2O)_2$[a(b)]**

C	3.64467100	0.23519700	0.18392700
H	4.32807800	-0.37197400	-1.77413300
H	5.62174400	0.16159100	-0.66904600
C	4.59187000	0.34920200	-0.99153900
H	4.54026900	1.35619100	-1.41305600
N	3.77376900	-1.12128100	0.79536400
H	4.73347400	-1.27422000	1.12052900
H	3.55058100	-1.85250400	0.11099700
C	2.19906100	0.49423100	-0.20954100
O	1.37654200	-0.44518500	0.01482700
O	1.94129100	1.60577000	-0.71969400
H	3.13855300	-1.24080700	1.58990300
H	3.91223700	0.95581000	0.96673300

C	-4.85054900	-0.76150000	-0.37417900
H	-5.20477700	0.81451900	1.05968200
H	-6.30227100	0.83380700	-0.34543800
C	-5.27240900	0.65038900	-0.02261100
H	-4.62002700	1.36712300	-0.52725100
N	-5.78375300	-1.73099700	0.27362000
H	-6.74752500	-1.56628500	-0.03278500
H	-5.74901000	-1.63271100	1.29432100
C	-3.43449900	-1.05357900	0.09963100
O	-3.26740700	-1.81947600	1.06919600
O	-2.53864400	-0.43685200	-0.55914900
H	-5.53622600	-2.70018700	0.05198100
H	-4.91125100	-0.93603100	-1.45248400
Cu	-0.58901200	-0.41184100	-0.24796900
O	5.82126100	2.58220600	1.48910500
H	6.26289100	1.95271800	0.90595800
H	5.10040500	2.96182500	0.94423800
O	3.72981300	3.70011300	-0.04379000
H	3.08792000	3.00658600	-0.29982200
H	3.23076300	4.31214700	0.51131100
O	-0.60320000	-1.83592300	1.16579900
H	-0.19312600	-1.47874400	1.96671400
H	-1.57028500	-1.94095700	1.35399700
O	-0.54138200	1.05006500	-1.64170300
H	-0.54318500	0.64928800	-2.52314800
H	0.36251100	1.42355000	-1.50619400

***S*-T2←$(H_2O)_2$·$(H_2O)_2$[a(b)]**

C	-4.13566000	-0.65067100	-0.32987500
H	-4.51377800	1.26727900	0.58934500
H	-5.62428800	0.85261800	-0.74227700
C	-4.58737700	0.79285000	-0.39654300
H	-3.95738800	1.34444300	-1.09833100
N	-5.04625000	-1.41229100	0.57690900
H	-6.01032600	-1.37476700	0.23209400
H	-5.02857500	-1.01506200	1.52266800
C	-2.71044500	-0.77989000	0.18644500
O	-2.51773400	-1.30163900	1.30216600
O	-1.83407600	-0.30874700	-0.60652600
H	-4.76792400	-2.39525700	0.65306300

H	-4.19840300	-1.12841400	-1.31241300
C	4.36996300	0.29393000	-0.11734300
H	5.27989800	0.06251200	-2.08633000
H	6.36630800	0.67396500	-0.81356500
C	5.34157900	0.71240000	-1.20256000
H	5.15224700	1.74121500	-1.52071400
N	4.62641700	-1.12800800	0.25523600
H	5.58595000	-1.22423100	0.60043600
H	4.51725500	-1.77009300	-0.53945300
C	2.95602200	0.47039500	-0.40079800
O	2.13113400	-0.46281500	-0.28653400
O	2.51966400	1.66696500	-0.74117400
H	3.99466900	-1.44551800	0.99605200
H	4.67768100	1.05710800	0.90814500
Cu	0.12468200	-0.28442700	-0.35790800
O	5.06982800	1.91882700	1.80748800
H	6.03472200	1.90480900	1.77998100
H	4.53724000	3.11727700	0.75475400
O	4.11728600	3.62294000	-0.00248300
H	3.16953200	2.42173000	-0.55847800
H	3.56495500	4.30246600	0.40434600
O	0.12707900	-1.44988100	1.26455700
H	0.61224800	-1.00263700	1.97329900
H	-0.83029000	-1.45505500	1.52284700
O	0.10882300	0.92270700	-1.99481100
H	0.09750000	0.37411500	-2.79322100
H	0.97275000	1.37161500	-1.99065900

I2←$(H_2O)_2 \cdot (H_2O)_2$[a(b)]

C	3.71632100	-0.20067600	-0.51655400
H	5.82118800	0.16794200	-0.37699700
H	4.85517200	1.05454800	0.81239900
C	4.86552800	0.68977700	-0.22645500
H	4.85525700	1.56116800	-0.88690500
N	3.72657000	-1.48386600	0.19519000
H	3.75459700	-1.35508800	1.21411800
H	4.53517200	-2.06446900	-0.05602500
C	2.64686200	-0.00843000	-1.32689000
O	1.74639800	-0.91708500	-1.56664800
O	2.47262900	1.18796100	-1.98158200

H	2.87315300	-2.00839100	-0.03739800
H	2.61426700	0.57564500	2.17728700
C	-4.19565600	-0.40030100	0.13701600
H	-4.12428600	1.59920000	0.95105900
H	-5.58380800	1.24321200	-0.00853300
C	-4.50364300	1.08003500	0.06273400
H	-4.03166700	1.51141800	-0.82296100
N	-4.90668500	-0.99322800	1.30994500
H	-5.91878100	-0.86271600	1.21920300
H	-4.60218400	-0.54344100	2.18027300
C	-2.70451400	-0.67423500	0.27452200
O	-2.28205600	-1.20879000	1.31850700
O	-2.02135000	-0.30152700	-0.73159500
H	-4.71397000	-1.99515400	1.40128000
H	-4.56593700	-0.92384000	-0.75025900
Cu	-0.08160700	-0.52608200	-1.00277000
O	1.73032300	0.81640200	1.86458800
H	1.26829800	1.12458100	2.65688500
H	2.08649000	2.27424100	0.74571200
O	2.35364800	2.93980600	0.07772400
H	2.53622700	1.93189800	-1.32827700
H	1.58310300	3.51144400	-0.03290500
O	0.35470900	-1.38098200	0.78228800
H	0.87041800	-0.67849100	1.23955500
H	-0.53972900	-1.38182400	1.20052800
O	-0.24502100	0.85167400	-2.54723000
H	-0.47801400	0.38121700	-3.36061900
H	0.69831300	1.10090700	-2.64272400

2.2.2 Coordinates of stationary points of the second, fourth, fifth primitive reactions in channel c

S-I1·H_2O[c]

C	-3.62463800	1.16127900	0.07300300
H	-3.51243700	2.19985900	1.96432000
H	-4.57575000	2.96878700	0.75818200
C	-3.63259400	2.43108700	0.89923600
H	-2.81376200	3.08378200	0.58776500
N	-4.78847800	0.30711500	0.44127900
H	-5.66255000	0.82333700	0.31086400

H	-4.73082400	0.02450500	1.42489600
C	-2.34829500	0.35906100	0.26539400
O	-2.37215600	-0.77427500	0.76048900
O	-1.29173800	0.98011400	-0.12120400
H	-4.80720500	-0.55374900	-0.14711200
H	-3.72910500	1.39027700	-0.99347100
C	4.43218200	-0.49791200	0.02100600
H	4.63938500	-0.81877400	-2.10580800
H	6.17903800	-0.78621600	-1.20670500
C	5.18313100	-0.33897400	-1.28366700
H	5.29957900	0.72266500	-1.51331000
N	4.32808200	-1.95006200	0.36095300
H	5.26167400	-2.36573500	0.43719800
H	3.81496000	-2.45825600	-0.36778400
C	3.04993500	0.12714400	-0.03787100
O	2.06290000	-0.66875800	0.18992200
O	2.95103400	1.33082800	-0.29530700
H	3.83487500	-2.09926600	1.24595600
H	4.97793800	-0.02511200	0.84434700
Cu	0.36308900	0.12048500	0.06534900
O	-4.30703300	-1.87787000	-1.29176200
H	-4.88811500	-2.64927500	-1.26698900
H	-3.52089200	-2.13929100	-0.78965800

***S*-T2·H_2O[c]**

C	-4.50524500	0.12108600	-0.04952500
H	-3.97144500	1.37330900	1.63031200
H	-5.19637100	2.05862300	0.53960600
C	-4.26866800	1.47817100	0.58024600
H	-3.49209900	2.03804600	0.05174000
N	-5.63315200	-0.60100500	0.57204400
H	-6.46164300	-0.01328800	0.48876400
H	-5.45574200	-0.70179400	1.57239100
C	-3.25489200	-0.74951700	-0.08603700
O	-3.30470300	-1.97277700	-0.42156400
O	-2.15538700	-0.18735400	0.17928100
H	-5.82550200	-1.94043100	-0.14011400
H	-4.76550200	0.25227800	-1.11158800
C	3.50979000	-2.01972600	-0.30016200
H	3.62077100	-1.73930300	-2.44017300
H	5.17849700	-2.11892600	-1.65978000
C	4.23770500	-1.57050000	-1.54965700

H	4.46627500	-0.50456000	-1.47824900
N	3.25662900	-3.49150900	-0.37798600
H	4.14260500	-3.99939400	-0.46583800
H	2.67868100	-3.71979300	-1.19427900
C	2.20606900	-1.26427300	-0.11357700
O	1.13393900	-1.97380900	-0.17860500
O	2.24894100	-0.04448000	0.07009700
H	2.76826100	-3.84056100	0.45205800
H	4.12459900	-1.85631400	0.59082900
Cu	-0.50752300	-1.09026700	-0.00132100
O	-5.53911200	-2.76488300	-0.74816700
H	-5.72359700	-3.58650800	-0.26864000
H	-4.41143200	-2.47851700	-0.64603300

***S*-I2·H_2O[c]**

C	-4.59071100	0.07103300	-0.08653100
H	-3.84828100	1.74512700	1.06294100
H	-5.30058300	2.07733000	0.09369900
C	-4.33963200	1.55283500	0.10210200
H	-3.71719400	1.96423200	-0.69871300
N	-5.48183200	-0.51894500	0.92128200
H	-6.35681800	0.00211800	0.89242900
H	-5.08875100	-0.35402300	1.84781300
C	-3.30347300	-0.72364000	-0.15233500
O	-3.32557800	-2.01272200	-0.30722100
O	-2.20483900	-0.14301200	-0.08729000
H	-5.95750700	-2.23441100	0.30455800
H	-5.06107100	-0.09869800	-1.06862500
C	3.46415400	-2.14758300	-0.25209200
H	4.11433700	-1.22297400	-2.09321200
H	5.40604200	-2.04064400	-1.17490700
C	4.50095000	-1.43133600	-1.08889500
H	4.76752100	-0.48486300	-0.61299700
N	3.15457300	-3.47300600	-0.87031600
H	3.99786700	-4.05454100	-0.90655000
H	2.81040900	-3.35805700	-1.82980800
C	2.19132300	-1.33573100	-0.08416000
O	1.10690000	-1.92581100	-0.45220700
O	2.26376600	-0.19955600	0.39026900
H	2.43475200	-3.97780200	-0.34440100
H	3.85180900	-2.35799800	0.75087300
Cu	-0.51911700	-1.03374400	-0.24446800

O	-5.76678400	-2.96668100	-0.33118300
H	-5.83306400	-3.78792200	0.17373800
H	-4.24908500	-2.42636200	-0.36690300

S-I3^{c}·$(H_2O)_2m^{c}$

C	-3.64446800	0.26885900	0.61519200
H	-4.66191200	-0.18010800	-1.24079600
H	-4.94177900	-1.34930500	0.06890400
C	-4.18840600	-0.71530700	-0.40901000
H	-3.39661000	-1.35524500	-0.80702300
N	-4.72484500	1.03181000	1.21521700
H	-5.24709000	1.51964400	0.48883100
H	-4.36081200	1.73910800	1.84944300
C	-2.53742600	1.09620200	0.01070800
O	-2.60752700	2.38480800	0.21896800
O	-1.61183500	0.55152700	-0.61181300
H	-1.84672300	2.86015300	-0.16750500
H	-3.13836800	-0.29997900	1.41328100
C	3.65189500	2.09018700	-3.01893600
H	4.86398200	1.82960200	-1.24916400
H	5.78875400	2.11168800	-2.74771400
C	4.91022400	1.61571100	-2.32335400
H	5.02204400	0.53788800	-2.46235600
N	3.53521300	3.57400800	-2.88119100
H	4.35149600	4.03334500	-3.29801800
H	3.48884800	3.84753600	-1.89349000
C	2.41273800	1.40602300	-2.47223300
O	2.31369700	0.18106800	-2.57628600
O	1.53853700	2.17997200	-1.92561800
H	2.69443500	3.93547200	-3.34178000
H	3.69844900	1.88040000	-4.09279800
Cu	-0.00822200	1.37710300	-1.27755300
O	-3.64450700	-2.69115000	2.58687300
H	-3.44067200	-2.75295100	1.64564300
H	-4.44975100	-2.13251200	2.62915400
O	-5.93409900	-1.05144400	2.68376200
H	-5.60806400	-0.25090500	2.20082600
H	-6.09199400	-0.75734000	3.58922200

S-T4·$(H_2O)_2$m^c

C	-3.76768900	0.21605300	0.42096200
H	-4.83434200	-0.11293400	-1.44980000
H	-5.12742600	-1.32685500	-0.17981300
C	-4.36743000	-0.68120200	-0.63449500
H	-3.59452100	-1.32896100	-1.05742400
N	-4.82691200	1.01818200	1.09602400
H	-5.44102200	1.49496500	0.42674600
H	-4.43185400	1.72780200	1.71925900
C	-2.63727900	1.01798800	0.01595900
O	-2.50506400	2.18943200	0.61695000
O	-1.79252700	0.58021100	-0.79685400
H	-1.67854000	2.63533700	0.35875200
H	-3.34769200	-0.59560500	1.32435300
C	3.58117500	2.07323500	-2.95354700
H	4.71080600	1.59561500	-1.17484700
H	5.70446200	1.97372300	-2.60661800
C	4.79034700	1.48021200	-2.26204100
H	4.86340500	0.41593200	-2.49753700
N	3.52915800	3.54320700	-2.68697000
H	4.36942500	4.00029200	-3.05550800
H	3.48272600	3.73205600	-1.67958400
C	2.29352000	1.40716000	-2.50523500
O	2.14881700	0.19780300	-2.70145600
O	1.43278100	2.17714400	-1.93323900
H	2.70953400	3.97933000	-3.12035200
H	3.65679000	1.95717100	-4.03980400
Cu	-0.14520500	1.38395100	-1.33735700
O	-3.17135300	-1.54112500	2.26974300
H	-3.07014600	-2.35627600	1.76216400
H	-4.81934700	-1.38916700	2.65556100
O	-5.77802400	-1.10983000	2.70487600
H	-5.39821800	0.36974000	1.68264400
H	-5.93408600	-0.86523800	3.62501200

I4·$(H_2O)_2$m^c

C	-4.10933800	0.46967700	-0.06183600
H	-5.36112200	-0.91546000	-1.13316400
H	-4.55208100	-1.60063600	0.28311200
C	-4.42815800	-0.89525500	-0.55048900
H	-3.62411200	-1.26924200	-1.19042400

N	-5.01999800	0.99367900	0.95901000
H	-5.99938200	0.91128500	0.66262800
H	-4.84067400	1.98386900	1.15134600
C	-3.15039700	1.30153900	-0.54883000
O	-3.00675100	2.52822600	0.04010200
O	-2.37023900	0.99964100	-1.54093700
H	-2.42148500	3.07289300	-0.50963400
H	-2.29827600	-0.43406300	1.07077900
C	3.19383900	2.35727200	-3.05088800
H	4.02648500	0.39777600	-2.68460300
H	5.13130600	1.53051800	-3.50581400
C	4.09089900	1.19865600	-3.43068300
H	3.78582800	0.79900200	-4.40056000
N	3.65863600	2.93577700	-1.75256900
H	4.63363400	3.24288900	-1.82587800
H	3.60071800	2.23751400	-1.00354600
C	1.73766500	1.93534400	-2.94472400
O	1.17738300	1.49078300	-3.95255400
O	1.20197900	2.07161900	-1.78456200
H	3.08817500	3.73741800	-1.46844700
H	3.25970900	3.16177700	-3.79090200
Cu	-0.59069300	1.51284000	-1.58817500
O	-1.92096000	-1.01823400	1.75133000
H	-1.94378900	-1.89750100	1.34998200
H	-3.45410600	-0.86762900	2.80161200
O	-4.35220600	-0.66855300	3.14109100
H	-4.90832400	0.46174000	1.85448100
H	-4.21319500	-0.20846300	3.97847300

$I4\cdot(H_2O)_2n^c$

C	0.05704200	1.68060000	-2.55454600
H	-0.21264000	3.81243800	-2.59355300
H	1.14436800	3.27544900	-1.59223000
C	0.12247600	3.01911700	-1.91048100
H	-0.52063900	3.04770400	-1.02618300
N	0.76561800	1.57831800	-3.83469500
H	0.71908400	0.62776800	-4.21312900
H	-0.88069600	-1.30192200	-2.40299200
C	-0.44414000	0.54095500	-2.00897700
O	-0.25181600	-0.62587700	-2.69689900
O	-1.08257600	0.51161400	-0.87751800
H	0.33214200	2.22261000	-4.53364700

H	1.75829700	1.82358000	-3.74581600
C	-3.92169500	-3.24790700	2.68636400
H	-2.19092100	-3.81756400	3.84681700
H	-3.74581600	-4.39397800	4.50268500
C	-3.24453400	-3.55842000	4.00442000
H	-3.29627200	-2.68547100	4.65926300
N	-3.90172500	-4.46590400	1.82048700
H	-4.38998800	-5.24064300	2.28092300
H	-2.93763900	-4.76489700	1.63704300
C	-3.25931300	-2.08414500	1.97149800
O	-2.74819600	-2.34938600	0.81902900
O	-3.24169800	-0.97950200	2.52299800
H	-4.34925900	-4.29584800	0.91514400
H	-4.97526000	-2.99178000	2.83939100
Cu	-1.90459200	-0.93121500	-0.05911100
O	-0.83373000	3.34099400	-5.37836400
H	-1.64547000	3.14420200	-4.86625000
H	-1.01974400	3.04737300	-6.27907200
O	-2.81254800	2.57266200	-3.50105700
H	-2.93774900	3.33456500	-2.91969100
H	-2.07610300	2.07876700	-3.09428900

R-all-T5·$(H_2O)_2$n[c]

C	-4.03025100	-0.60906200	1.08417200
H	-3.90353300	1.51669700	0.85749100
H	-2.41283900	0.78817400	1.50535900
C	-3.50953400	0.73765500	1.52025400
H	-3.85583100	0.96136000	2.53316800
N	-3.68347200	-0.87658100	-0.34041700
H	-3.90627000	-1.83713700	-0.61619700
H	-3.56020900	-3.63106300	2.01007300
C	-3.73734700	-1.72856400	1.94776400
O	-3.67161200	-2.91345200	1.36089700
O	-3.64535200	-1.58722200	3.18848300
H	-4.25395600	-0.23938500	-0.94045900
H	-2.68831700	-0.71913500	-0.53381200
C	-3.31130800	-4.85971000	8.17320000
H	-1.16986200	-5.15248900	8.17412800
H	-1.99178300	-5.67167100	9.66932700
C	-1.97358700	-4.91348000	8.88008600
H	-1.76165200	-3.94465900	9.33816000
N	-3.63865900	-6.20877300	7.61743000

H	-3.68574800	-6.90097200	8.37169000
H	-2.91961800	-6.51517300	6.95289200
C	-3.33244200	-3.81451300	7.07308000
O	-3.61372500	-4.24628900	5.88972200
O	-3.08749200	-2.64032400	7.36095600
H	-4.53678500	-6.20839800	7.12440100
H	-4.11297500	-4.61266900	8.87726800
Cu	-3.62506100	-2.95402500	4.53638300
O	-5.67762400	0.79834800	-1.43979000
H	-6.16623300	0.51040300	-0.61610900
H	-6.14969200	0.39811800	-2.18000500
O	-6.59997400	-0.13414200	0.89267000
H	-6.72921200	0.61821400	1.48385700
H	-5.30699400	-0.47791900	1.08110100

R-all-I5·$(H_2O)_2$n[c]

C	-0.15033800	1.75948100	-2.84560400
H	0.37011800	3.83301400	-3.00281400
H	1.68688800	2.80705100	-2.39324600
C	0.60510800	2.98272700	-2.35527800
H	0.32702100	3.23977400	-1.32997900
N	0.12733800	1.51307000	-4.25092100
H	-0.31639500	0.65259500	-4.56351800
H	0.29255100	-1.30791100	-1.88717100
C	0.07989300	0.57970800	-1.93464500
O	0.19876400	-0.57896200	-2.52992800
O	0.10072100	0.72004200	-0.70248200
H	-0.78469200	2.92533600	-5.02521800
H	1.13069200	1.40271900	-4.38972800
C	0.40196800	-2.56917200	4.28718300
H	2.54641100	-2.80576000	4.40810000
H	1.65583200	-3.34695500	5.85530000
C	1.69838800	-2.58820700	5.06761600
H	1.85925500	-1.61475300	5.53634900
N	0.14407100	-3.92503700	3.71287200
H	0.06123300	-4.61882600	4.46259100
H	0.91423300	-4.21498700	3.10016100
C	0.40585000	-1.52171600	3.18847000
O	0.13748500	-1.95131600	2.00087700
O	0.64734200	-0.34821800	3.48051600
H	-0.71672400	-3.94484100	3.15754700
H	-0.44506400	-2.34682000	4.94559200

Cu	0.13143800	-0.65568300	0.65274900
O	-1.36839300	3.69347900	-5.24475900
H	-2.37335600	3.86718500	-3.71125700
H	-1.92210100	3.39114700	-5.97524800
O	-2.89167300	3.94121600	-2.88189300
H	-2.22786400	4.04890300	-2.18949000
H	-1.23311700	1.95028500	-2.74027000

2.2.3 Coordinates of stationary points of the fourth primitive reactions in channel d

R-allo-I3·$(H_2O)_2$[d]

C	-3.18690600	3.89669100	-0.57007000
H	-3.50832000	5.75418400	-1.61230200
H	-2.07883400	4.84244300	-2.16561700
C	-2.67232400	5.12620300	-1.28866300
H	-2.04332000	5.71031900	-0.61280300
N	-4.09514000	3.13593500	-1.48150700
H	-4.87422100	3.72918700	-1.78385500
H	-3.59132700	2.82375800	-2.31884200
C	-2.04920300	3.01013900	-0.09627700
O	-2.01098500	1.83018300	-0.61624500
O	-1.24361800	3.45867800	0.72171500
H	-3.78353900	4.17499700	0.30481200
H	-4.48350400	2.30407800	-1.02683200
C	1.83057600	-2.75775200	0.40778100
H	2.93278500	-2.38372400	-1.41703700
H	3.92567400	-2.89481000	-0.03380000
C	3.07050600	-2.28122700	-0.33380900
H	3.29528200	-1.23652900	-0.10464400
N	1.61217800	-4.17589200	0.18059100
H	0.74977100	-4.48505600	0.62326700
H	-1.18711300	-1.85483900	-0.38369400
C	0.65502800	-1.86778100	0.08688800
O	-0.45484300	-2.48150800	-0.23094800
O	0.76472600	-0.63404100	0.16188200
H	1.51829300	-4.35572200	-0.81795300
H	1.98944100	-2.60222800	1.48775900
Cu	-0.61521900	0.68611000	-0.16256000

O	3.83201200	-2.73604800	3.19297500
H	4.16320700	-2.92043600	4.07974300
H	3.83212400	-3.60396200	2.73587900
O	3.74784000	-5.15056000	1.74497600
H	4.55584800	-5.18112500	1.21770900
H	3.03041600	-4.91104100	1.10640600

R-allo-T4·$(H_2O)_2$[d]

C	-2.64150700	2.82537200	0.75737100
H	-3.36135300	4.54106800	-0.32813100
H	-2.11021200	3.60381600	-1.18644000
C	-2.43338000	3.97361100	-0.20640700
H	-1.66718500	4.64690300	0.18454300
N	-3.74369100	1.94898200	0.25575400
H	-4.61709700	2.48079100	0.18395000
H	-3.52272000	1.58082700	-0.67606700
C	-1.37328100	2.01589100	0.96353900
O	-1.46431400	0.75870000	0.69037500
O	-0.36042600	2.58785200	1.37198100
H	-2.96076900	3.19347100	1.73826400
H	-3.90355400	1.14742300	0.87329900
C	2.41003900	-3.71651500	1.48744100
H	3.85037500	-3.36505000	-0.10860000
H	4.54144700	-3.91296100	1.43873200
C	3.76512100	-3.28721300	0.98331200
H	3.96229300	-2.25237300	1.27611700
N	2.17760900	-5.16235600	1.21437100
H	1.22947700	-5.45415700	1.46770900
H	-0.61713300	-2.86615500	0.90950700
C	1.28632100	-2.88692900	1.12148800
O	0.10994000	-3.49284300	1.07524400
O	1.41983900	-1.65316200	0.95517200
H	2.32625900	-5.40267300	0.22819100
H	2.50556900	-3.65388700	2.76482300
Cu	0.02779400	-0.33784200	0.89212200
O	2.88924600	-3.75849300	4.05737300
H	2.07563900	-3.89957700	4.55672900
H	3.56470200	-5.26912800	3.70088400
O	3.84464300	-6.13455900	3.28413700
H	4.78095900	-6.02911800	3.07482800
H	2.84257300	-5.71087300	1.80463700

I4·$(H_2O)_2$[d]

C	-2.63180800	3.61825500	-0.13524500
H	-3.52577900	5.37966200	-0.99864400
H	-2.72752300	4.30852900	-2.18039600
C	-2.66519900	4.72488500	-1.16806800
H	-1.75547700	5.32516500	-1.09248800
N	-3.90462200	2.83765200	-0.20450400
H	-4.70865800	3.44839800	-0.02885200
H	-4.02221300	2.41694600	-1.13236900
C	-1.44066200	2.69660500	-0.33112500
O	-1.71312600	1.46459400	-0.57929300
O	-0.30558300	3.18030800	-0.24966900
H	-2.57510800	4.03116200	0.87730800
H	-3.92175400	2.07786900	0.48181700
C	2.20783600	-2.75240600	-0.43685600
H	4.28842200	-2.63466300	-0.96349800
H	3.95827500	-2.45922800	0.76545700
C	3.57629600	-2.21685700	-0.23653400
H	3.58108000	-1.12911800	-0.34593700
N	2.05451900	-4.18131500	-0.15483000
H	1.13717100	-4.52976900	-0.44952800
H	-0.67620100	-2.21618900	-1.53376800
C	1.13293900	-2.07934200	-0.92389400
O	-0.05891200	-2.75069800	-1.00902400
O	1.16086200	-0.84048900	-1.31619200
H	2.76609800	-4.73505600	-0.64529000
H	1.60390100	-1.51686800	1.58161600
Cu	-0.23142400	0.31349800	-0.87077600
O	1.73706100	-1.47146500	2.54205300
H	0.86060200	-1.28429900	2.90318900
H	2.11975600	-3.26338600	2.75883400
O	2.26883000	-4.22738600	2.65255500
H	3.18518600	-4.37355600	2.92010800
H	2.15729600	-4.36219300	0.87323100