Electronic Supplementary Information

Mechanistic Insights into Artificial Metalloenzyme towards Imine Reduction

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Contents

Selection of basis sets and methods

The active site was sensitive to basis sets and methods. Especially for biosystem, the non-bonded interaction is important for the part of catalytic active site. Therefore, an appropriate functional method and basis sets need to be chose to calculate our study systems. In 2006, Truhlar group developed M06 series of functional [1] including M06、M06-L、M06-2X [2]. The testing result indicate that those functional methods can perfectly describe the non-bonded interaction. In addition, our previous works found that the results of ωB97X-D [3] is also reliable [4-6]. In order to find an appropriate method and basis set for our research system, we calculated the key bonds length of active site models using different methods and basis sets, and then compared those bonds with crystal structure.

We tested the basis sets on the base of the M06 method, and chose LANL2DZ， SDD [7,8] and def2-TZVP [9] basis sets for transition metal (Rh atom), the 6-31G(d,p) basis set for the other atoms. We calculated the key bond lengths which included the rhodium with carbon on Cp* ring, nitrogen of H112 as well as nitrogen-hydrogen bond on protonated K121. The datum of crystal and calculated bond lengths were summarized in Table S1. The calculated results of def2-TZVP basis set (the average of the deviation is 0.060) are the closest to the crystal values, but the spent time is about three to four times than others. The calculated results of SDD basis set (the average of the deviation is 0.070) are better than those of LANL2DZ basis set, and its calculated time is much shorter than that of def2-TZVP. Therefore, we chose SDD basis sets to optimize the structure and add the def2-TZVP basis sets to calculate the valence electrons of metal in the single-point energy calculation with SMD.

Then, we tested the functional methods based on the SDD basis sets. The three functionals of ωB97X-D、M06-L and M06 were chosen. The compared results of different functionals were shown in Table S2. The datum of Table S2 demonstrated that M06-L method is the best for active site models, because its average of the deviation (0.051) is smaller than the others. By observing the bond length,

we found that most of the bond lengths change slightly (the deviation is below 0.1 Å) except Rh-N bond. This is because that Rh-N (the N atom of histidine) is a coordination bond which could be influenced by the protein environment.

According to the above test results, we confirmed that the calculated level for the active site models is M06-L/6-31+G(d,p) +def2-TZVP(SDD)//M06-L/6-31G(d,p)+SDD.

[1] Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, 125 (19):194101

[2] Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, 120(1), 215-241.

[3] Chai, J. D.; Head-Gordon, M. Long-range corrected hybrid density functionals with damped atom–atom dispersion corrections. *Phys. Chem. Chem. Phys.* **2008**, 10(44), 6615-6620.

[4] Li, H., Ma, X., Zhang, B., Lei, M.DFT Study on the Mechanism of Tandem Oxidative Acetoxylation/Ortho C–H Activation/Carbocyclization Catalyzed by Pd(OAc)2. *Organometallics* **2016**, 35 (19) 3301-3310.

[5] Li, H., Ma, X., Lei, M. Substituent effects and chemoselectivity of the intramolecular Buchner reaction of diazoacetamide derivatives catalyzed by the di-Rh(ii)-complex. *Dalton. Trans*. **2016**, 45 (20) 8506-8512.

[6] Lei, M., Pan, Y., Ma, X. The Nature of Hydrogen Production from Aqueous-Phase Methanol Dehydrogenation with Ruthenium Pincer Complexes Under Mild Conditions. *Eur. J. Inorg. Chem.* **2015**, 2015 (5) 794-803.

[7] Bergner, A., Dolg, M., Küchle, W., Stoll, H., Preuß, H. Ab initio energy-adjusted pseudopotentials for elements of groups 13–17. *Mol. Phys*. **1993**, 80 (6):1431-1441.

[8] Dolg, M., Wedig, U., Stoll, H., Preuss, H. Energy-adjusted abinitio pseudopotentials for the first row transition elements. *J. Chem. Phys.* **1987**, 86 (2):866-872.

[9] Eichkorn, K., Weigend, F., Treutler, O., Ahlrichs, R. Auxiliary basis sets for main row atoms and transition metals and their use to approximate Coulomb potentials. *Theor. Chem. Acc.* **1997**, 97 (1):119-124.

Table S1. The comparison of selected bond length with the crystal structures based on various basis sets in S112H.

Bond	Bond Length				Deviation		
	Crystal	M06/ LanL2DZ	M06/ def2-TZVP	M06/ SDD	M06/ LanL2DZ	M06/ def2-TZVP	M06/ SDD
Rh-N	2.334	2.166	2.151	2.154	0.168	0.183	0.180
Rh-C1	2.099	2.171	2.144	2.160	0.085	0.058	0.074
Rh-C2	2.112	2.158	2.136	2.150	0.083	0.061	0.075
Rh-C3	2.084	2.197	2.163	2.183	0.098	0.064	0.084
Rh-C4	2.086	2.197	2.167	2.184	0.085	0.055	0.072
Rh-C5	2.075	2.181	2.158	2.170	0.097	0.074	0.086
N-H1	1.008	1.027	1.022	1.027	0.019	0.014	0.019
N-H2	1.008	1.027	1.022	1.027	0.019	0.014	0.019
N-H3	1.008	1.026	1.020	1.026	0.018	0.012	0.018
The average deviation					0.075	0.060	0.070

Table S2. The comparison of selected bond length with the crystal structures based on various methods in S112H.

Bond	Bond Length				Deviation		
	Crystal	M06-L/ SDD	ωb97xd/ SDD	M06/ SDD	M06L/ SDD	ωb97xd/ SDD	M06/ SDD
Rh-N	2.334	2.179	2.138	2.154	0.155	0.196	0.180
Rh-	2.099	2.128	2.152	2.160	0.029	0.053	0.061
Rh-C2	2.112	2.123	2.133	2.150	0.011	0.021	0.038
Rh-C3	2.084	2.156	2.185	2.183	0.072	0.101	0.099
Rh-C4	2.086	2.160	2.169	2.184	0.074	0.083	0.098
Rh-C5	2.075	2.145	2.164	2.170	0.070	0.089	0.095
N-H1	1.008	1.024	1.036	1.027	0.016	0.028	0.019
N-H2	1.008	1.025	1.024	1.027	0.017	0.016	0.019
N-H3	1.008	1.024	1.023	1.026	0.016	0.015	0.018
The average deviation					0.051	0.067	0.070

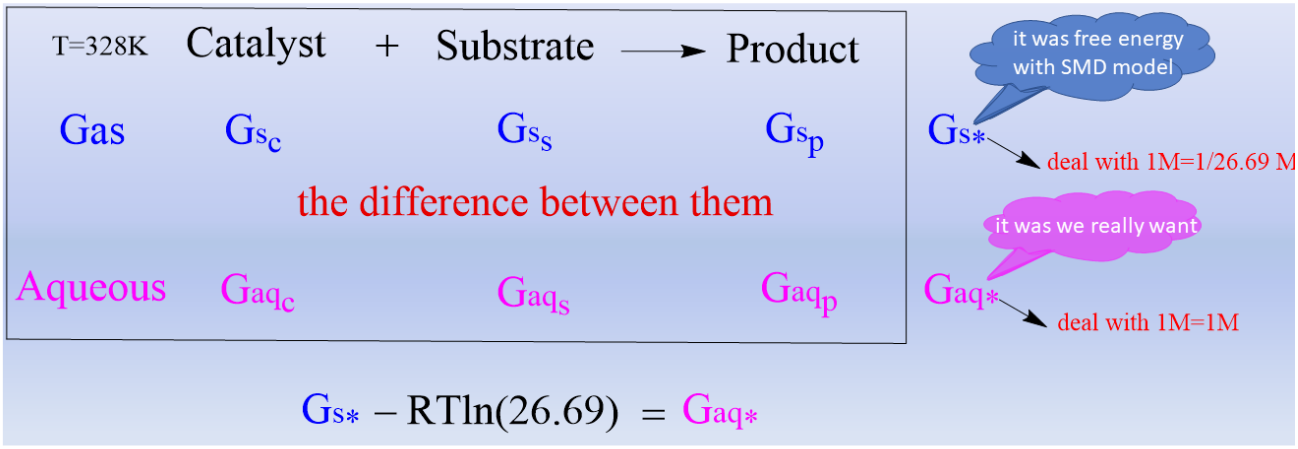

Figure S1. Thermodynamic diagram of phase transition. Standard molar volume *V*m = 26.69 L/mol at 328 K and ideal gas constant R=0.0019872 kcal/(mol·K).

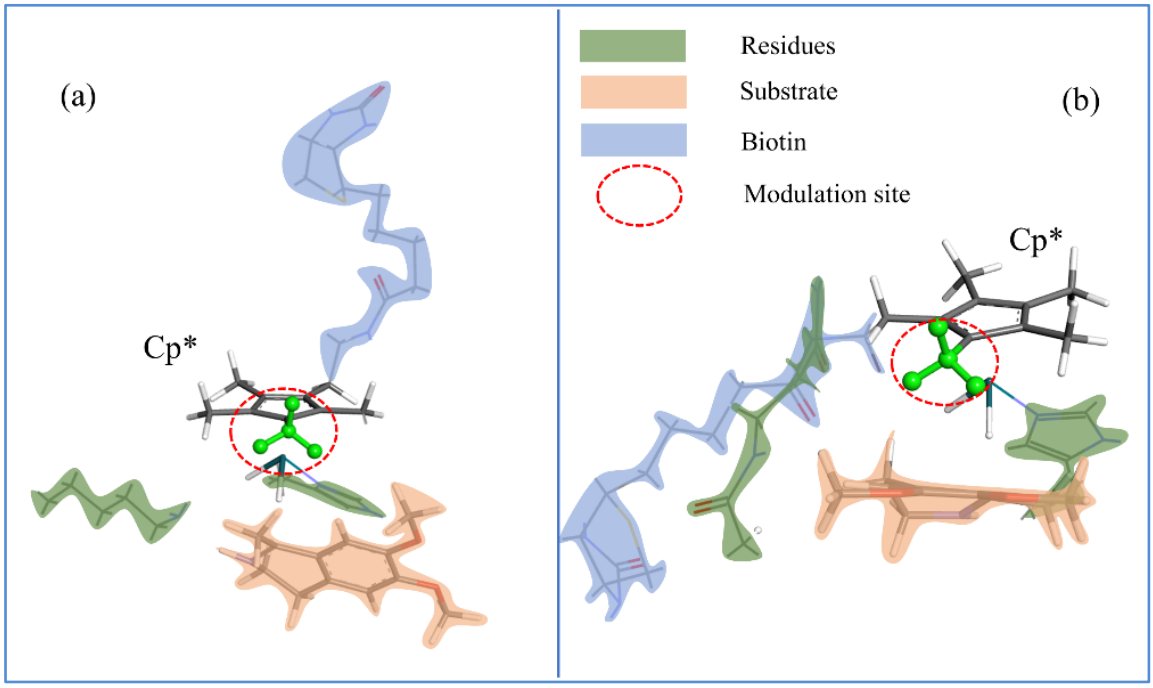

Figure S2. The position of the substituent group in S112H Sav (a) and K121H Sav (b), respectively.

Cartesian coordinates (in Å) of stability points of the favorable path in S112H system

$\mathbf{R_{eq}^{S}}$

	Coordinates (Angstroms)		
	X	Y	Z
H	-2.35091300	2.23422400	0.12843900
H	-3.26164900	1.09520300	1.74977600
N	3.15232200	-1.95329500	0.31957000
C	2.40857700	-0.94225100	1.04888400
C	1.05302900	-0.61370300	0.43641200
C	0.35347800	0.38166200	1.30799900
C	0.36598500	1.79233500	1.16268200
C	1.08827900	2.58076500	0.12615200
H	2.04069100	2.96338400	0.51350500
H	0.50475500	3.44243400	-0.20991600
H	1.31941000	1.97674500	-0.75614600
C	-0.41321300	2.34546900	2.25628300
C	-0.55751000	3.79534900	2.56679400
H	0.27263800	4.15320200	3.18845900
H	-1.48376600	3.99983200	3.11161200
H	-0.56595800	4.40000500	1.65590300
C	-0.81395000	1.25106000	3.11117000
C	-1.50398500	1.38607300	4.42336300
H	-0.77107800	1.48419900	5.23287400
H	-2.12540700	0.51559600	4.64725700
H	-2.14513500	2.27016700	4.45500700
C	-0.36728200	0.03212600	2.51876600
C	-0.49350000	-1.33569800	3.09444100
H	0.35576400	-1.58433400	3.74325700
H	-0.53136800	-2.10198300	2.31327200
H	-1.39952300	-1.43450200	3.69980400
H	1.17358000	-0.21371300	-0.57969300
H	0.44975800	-1.52719000	0.34283900
H	2.29039200	-1.30319900	2.07517900
H	3.01243700	-0.02700900	1.13512900
C	4.28978200	-2.42950200	0.87558100
C	5.24527400	-3.35215500	0.03765000
C	6.78508000	-3.08829700	0.47187700
C	7.14293400	-1.66622500	0.17769000

C	8.63495200	-1.51420300	0.10045500
C	8.93438400	-0.10045600	-0.41241500
S	9.19797500	-0.11395900	-2.22705000
C	9.92256100	1.52847100	-2.06414100
C	10.86843200	1.43524900	-0.73881900
C	10.18840000	0.44574800	0.20829000
H	9.93319200	0.91189200	1.16636900
N	11.24409600	-0.59821800	0.39761900
H	11.16881800	-1.41728500	0.95164700
C	12.34474700	-0.23649500	-0.33439900
O	13.37223100	-0.92219600	-0.37228800
N	12.21799600	0.85382000	-0.98184700
H	12.94778800	1.24594800	-1.55779900
H	10.94075600	2.43362700	-0.28014800
H	9.13821400	2.29155000	-1.97688700
H	10.56923500	1.77336700	-2.93064800
H	8.08173900	0.54390800	-0.18404000
H	9.06161800	-2.26029200	-0.60520700
H	9.08437600	-1.65808700	1.08696100
H	6.76618700	-1.02124700	0.96273200
H	6.69494600	-1.37428200	-0.79452400
H	7.45628100	-3.76609200	-0.11465700
H	6.90866400	-3.28870300	1.53138500
H	5.13702500	-3.13539700	-1.05381100
H	4.99051700	-4.40961400	0.19592700
O	4.60040700	-2.02462900	2.08264600
C	-1.70198600	0.56465200	-3.83376600
H	-1.24863900	1.42207100	-4.33471600
C	-1.62608000	0.70304900	-2.32699900
H	-2.11164500	1.62938900	-1.99229000
H	-0.58233700	0.81525900	-1.99835900
C	-2.24805800	-0.43176600	-1.59554900
C	-2.73198700	-1.62561500	-2.07265000
H	-2.78203000	-2.03386000	-3.07022100
N	-3.19807500	-2.31598800	-0.97814300
H	-3.71274100	-3.18489300	-0.99481000
C	-3.01566000	-1.54080100	0.11152500
H	-3.30844300	-1.82357500	1.11211400
N	-2.44111200	-0.39854400	-0.22644700
C	-4.15405500	8.66575900	-2.27744600
H	-3.79808600	9.67638700	-2.06492000
C	-3.93282800	7.73337900	-1.09860600
H	-4.44546100	8.12800900	-0.21098100
H	-2.86696700	7.70358300	-0.83668500

C	-4.42508500	6.31841200	-1.36891100
H	-3.89570900	5.90431000	-2.23880100
H	-5.48527800	6.35544600	-1.65858000
C	-4.26602500	5.37561000	-0.18281200
H	-4.76659600	5.80778600	0.69608600
H	-3.20594800	5.26992800	0.08607500
C	-4.85447600	4.01279300	-0.47928000
H	-4.31513000	3.51643500	-1.29362600
H	-5.90416100	4.09390600	-0.78143400
N	-4.79797900	3.08028100	0.67726500
H	-5.37351800	2.20004900	0.46249000
H	-5.13690800	3.51767900	1.53181900
H	2.96433500	-2.10417600	-0.66028700
Rh	-1.77158100	1.10643400	1.14547200
H	-5.21607900	8.73775300	-2.53296000
H	-3.62705500	8.31253500	-3.16974400
H	-2.74142600	0.49381700	-4.17378500
H	-1.18062300	-0.33124300	-4.18625100
C	-6.24810800	-0.29737200	0.49453600
N	-6.03658900	0.77859300	-0.19278600
C	-6.38837900	-0.16183000	1.97784700
H	-7.26916100	-0.69134900	2.35239700
H	-5.51360000	-0.58435800	2.48674000
H	-6.46270400	0.88741000	2.26626000
C	-6.55339700	-0.48208000	-2.29077600
H	-6.20409600	-0.62150200	-3.31959600
H	-7.61704300	-0.21226200	-2.36147200
C	-5.78549300	0.64529800	-1.62634100
H	-6.02424600	1.60130700	-2.10536900
H	-4.70015100	0.49335600	-1.75300100
C	-6.41223100	-1.74440600	-1.49621200
C	-6.30259500	-1.63350200	-0.10502400
C	-6.20900800	-2.80101500	0.67963900
H	-6.12875000	-2.71728900	1.75840300
C	-6.21597900	-4.05896000	0.09477300
C	-6.33478300	-4.16562100	-1.31861800
C	-6.43029400	-3.00665200	-2.08918700
H	-6.53156400	-3.08091100	-3.16762300
O	-6.12455100	-5.23429900	0.75476200
O	-6.34374900	-5.42066700	-1.80131800
C	-6.02845300	-5.17235400	2.16545000
H	-6.90651600	-4.68597700	2.60787000
H	-5.97390900	-6.20370900	2.50917300
H	-5.12456600	-4.63552700	2.48355300

C	-6.51636500	-5.58232400	-3.20071000
H	-5.69319200	-5.12247400	-3.76104500
H	-6.51950800	-6.65605100	-3.37856600
H	-7.46596500	-5.15128100	-3.53739200
H	-3.82509700	2.72343100	0.84163000

$\mathbf{I_{eq}^{S}}$

	Coordinates (Angstroms)		
	X	Y	Z
H	2.82753900	1.77381100	0.12013000
H	3.63838100	0.36792400	-1.12746000
N	-3.11250800	-1.85312400	0.12619000
C	-2.25939500	-1.00212500	-0.68153000
C	-0.93250200	-0.67048800	-0.01146800
C	-0.05787100	0.06844800	-0.97372500
C	0.09137700	1.47615400	-1.07628800
C	-0.61930800	2.51817200	-0.28438000
H	-1.48081500	2.91704600	-0.83473700
H	0.03458300	3.36314900	-0.04908300
H	-0.99886500	2.12246200	0.66220400
C	1.03006100	1.72896200	-2.15256400
C	1.36218600	3.06916100	-2.71240000
H	0.58850900	3.40652400	-3.41353800
H	2.30761600	3.05350200	-3.26345300
H	1.44189000	3.82787600	-1.92892500
C	1.36682400	0.45644300	-2.75454800
C	2.19918400	0.27377500	-3.97583200
H	1.58603300	0.34371500	-4.88225000
H	2.68630400	-0.70620100	-3.98860700
H	2.97909700	1.03783100	-4.05035400
C	0.70983300	-0.57503400	-2.02402800
C	0.71910500	-2.03154200	-2.33927400
H	-0.02191100	-2.29157000	-3.10603500
H	0.48541500	-2.63827200	-1.45824100
H	1.69661500	-2.35584100	-2.71315400
H	-1.09330900	-0.07228700	0.89587500
H	-0.43831600	-1.59789500	0.31176000
H	-2.09470300	-1.51812300	-1.63253400
H	-2.79127800	-0.07600900	-0.94446500

C	-4.22360900	-2.37863200	-0.43864100
C	-5.27139900	-3.13767100	0.45152700
C	-6.76462700	-2.90286800	-0.13522700
C	-7.08928200	-1.44373600	-0.08594700
C	-8.57621300	-1.24282500	-0.14810800
C	-8.85882800	0.23983600	0.12249400
S	-9.25376100	0.50952400	1.89276500
C	-9.90247300	2.12638800	1.43009500
C	-10.75248000	1.85729700	0.06447300
C	-10.04310000	0.71777700	-0.66822500
H	-9.70171200	1.02586900	-1.66264500
N	-11.12069400	-0.31491600	-0.78022300
H	-11.03618400	-1.21043800	-1.19781500
C	-12.25722600	0.18260600	-0.19807900
O	-13.30975400	-0.46227600	-0.13758700
N	-12.13698700	1.35506400	0.28661300
H	-12.89143200	1.84919300	0.73908500
H	-10.75380900	2.77579100	-0.54276300
H	-9.08578600	2.84655700	1.29053000
H	-10.60069300	2.51709600	2.19744900
H	-7.96827800	0.81945400	-0.13310300
H	-9.08066800	-1.86143900	0.62616200
H	-8.95792600	-1.52337200	-1.13373700
H	-6.63261100	-0.93579600	-0.92718100
H	-6.70240800	-1.01904300	0.86331000
H	-7.50159000	-3.46575000	0.49245900
H	-6.81841100	-3.25887800	-1.15911900
H	-5.23459400	-2.76026000	1.50327600
H	-5.04567100	-4.21320700	0.47361600
O	-4.43044400	-2.15410500	-1.71309000
C	1.51858800	1.13988400	4.21877600
H	1.29379200	2.17505600	4.48150300
C	1.92893900	1.02266700	2.76396200
H	2.79921600	1.66094200	2.55286400
H	1.14813400	1.41980000	2.10140800
C	2.22789900	-0.36966600	2.33322500
C	2.29027700	-1.52327000	3.07464700
H	2.15628400	-1.70632000	4.12932800
N	2.54370800	-2.54074400	2.18120900
H	2.64175400	-3.51939100	2.39835500
C	2.63833200	-1.99809100	0.94687900
H	2.84437600	-2.56431700	0.04966900
N	2.45001000	-0.68988600	1.00431700
C	4.37938400	8.84298100	1.66126100

H	3.90750200	9.81431700	1.49461200
C	4.03075900	7.84924000	0.56696900
H	4.34225800	8.24620500	-0.40860300
H	2.94112500	7.72806000	0.50186200
C	4.67827600	6.48836200	0.77839400
H	4.34865600	6.07068400	1.74101800
H	5.76643200	6.61979100	0.87406200
C	4.39645000	5.48858200	-0.33390000
H	4.69274700	5.92415200	-1.29983300
H	3.31679900	5.29350500	-0.40768700
C	5.13790200	4.17682400	-0.13263800
H	4.77046800	3.67985000	0.77618200
H	6.20328300	4.38584700	0.03897300
N	5.03909200	3.20165200	-1.22723500
H	5.90030100	1.76491300	-0.71181700
H	5.22580300	3.66333600	-2.11306300
H	-3.00350700	-1.85971000	1.12932100
Rh	2.12454700	0.57951800	-0.70031400
H	5.46041200	9.00777300	1.71734000
H	4.05437100	8.48370700	2.64336700
H	2.31061000	0.79744000	4.89321900
H	0.62554900	0.54348800	4.43140700
C	6.00686100	-0.24910000	-0.91359800
N	6.08323700	0.85122000	-0.20943200
C	6.08690300	-0.13229900	-2.39421500
H	6.92564300	-0.71263200	-2.78939800
H	5.16818400	-0.52376400	-2.84124800
H	6.19546800	0.90764800	-2.70382700
C	6.34846700	-0.36040600	1.90337900
H	5.95631900	-0.42131900	2.92344500
H	7.43977200	-0.26458700	1.99501300
C	5.77409200	0.85928700	1.21706900
H	6.16681400	1.78548600	1.64256500
H	4.67422500	0.88486000	1.29166700
C	6.01559300	-1.60493100	1.13542100
C	5.86427100	-1.52781000	-0.25957500
C	5.58181900	-2.69492200	-1.00312700
H	5.45458400	-2.62871100	-2.07792300
C	5.43723300	-3.91805800	-0.37333200
C	5.60822700	-3.99287400	1.03824200
C	5.90610300	-2.84107100	1.76395500
H	6.03439700	-2.89631400	2.84036200
O	5.13332800	-5.08469100	-0.97686200
O	5.43708100	-5.21282800	1.57161100

C	4.97380600	-5.05651000	-2.38510300
H	5.89085300	-4.72158400	-2.88438300
H	4.75162500	-6.07940500	-2.68286000
H	4.14342500	-4.40156900	-2.67946600
C	5.69225800	-5.36843800	2.96095100
H	5.00551400	-4.76322600	3.56635500
H	5.53248100	-6.42309900	3.17659700
H	6.72308700	-5.09350400	3.20800800
H	4.08692300	2.83195800	-1.27363900

P_{eq}^{S}

	Coordinates (Angstroms)		
	X	Y	Z
H	2.62288600	1.66883800	0.08085300
H	4.12976100	0.25005500	-0.78106300
N	-3.06964600	-1.62080300	0.24661400
C	-2.13998500	-0.94513300	-0.63164400
C	-0.80704500	-0.64341800	0.05177000
C	0.20659800	-0.27485500	-0.97897900
C	0.44544800	1.04568400	-1.51395700
C	-0.26653300	2.29231000	-1.12537500
H	-1.12898000	2.46031100	-1.78111600
H	0.38070900	3.16946000	-1.20111700
H	-0.64061600	2.24201600	-0.09947200
C	1.45252700	0.91754400	-2.53372300
C	1.94781300	2.00053000	-3.42724600
H	1.36280100	2.04909100	-4.35338900
H	2.99302800	1.84495300	-3.71159000
H	1.87562300	2.98010900	-2.94674500
C	1.74112300	-0.50084000	-2.68319400
C	2.63543900	-1.08913700	-3.71161900
H	2.04137700	-1.41811000	-4.57276600
H	3.16448300	-1.97089000	-3.33530100
H	3.36946600	-0.37219700	-4.08491400
C	0.98666500	-1.23498600	-1.73902800
C	0.98137700	-2.71380500	-1.56744800
H	0.31043500	-3.20323900	-2.28334300
H	0.64754600	-3.00420800	-0.56701800
H	1.98149900	-3.13792200	-1.71575200
H	-0.91942200	0.15940100	0.79195400

H	-0.46332100	-1.52967200	0.60065000
H	-1.99356700	-1.58630100	-1.50798500
H	-2.58818900	-0.02084200	-1.02212900
C	-4.15993100	-2.22177900	-0.28252500
C	-5.18762300	-2.94854600	0.65666200
C	-6.68431100	-2.80563400	0.04948500
C	-7.05632600	-1.35815100	-0.00790500
C	-8.54860500	-1.21099300	-0.08939400
C	-8.88062300	0.27728200	0.07239800
S	-9.29416300	0.66088400	1.81721900
C	-9.99225100	2.21807900	1.23673700
C	-10.82530400	1.82353200	-0.10870000
C	-10.07523000	0.65795200	-0.75475000
H	-9.73833800	0.90452100	-1.76768900
N	-11.11815900	-0.41482600	-0.79542300
H	-11.00231300	-1.33489000	-1.14691700
C	-12.27350600	0.08594100	-0.25456200
O	-13.30492400	-0.58698200	-0.15114100
N	-12.19406200	1.29360800	0.14452600
H	-12.96668000	1.79414100	0.55757900
H	-10.85291800	2.69530300	-0.78072900
H	-9.19853300	2.95263600	1.04822000
H	-10.70711900	2.64006500	1.97150800
H	-8.00787100	0.86577700	-0.22144200
H	-9.03716400	-1.78832400	0.72586700
H	-8.91541000	-1.57423500	-1.05344200
H	-6.61155900	-0.89754000	-0.88211700
H	-6.68882300	-0.85367100	0.90946400
H	-7.40622100	-3.34558400	0.71374200
H	-6.72070400	-3.23613200	-0.94617500
H	-5.16905900	-2.49524700	1.67850300
H	-4.92731800	-4.01171300	0.75718000
O	-4.36662000	-2.09671500	-1.57056300
C	1.43865000	1.80934500	4.12754900
H	1.14592900	2.85861000	4.19215300
C	1.76182900	1.41976200	2.69661500
H	2.56619600	2.05420300	2.29808400
H	0.90788300	1.61707500	2.03265900
C	2.16298100	-0.00487200	2.54996500
C	2.33084000	-0.95659100	3.52187400
H	2.21249400	-0.91321000	4.59278400
N	2.70159300	-2.11245400	2.87123900
H	2.93053500	-2.99495100	3.30034600
C	2.75559900	-1.85411000	1.55049500

H	3.06148500	-2.57567000	0.80391500
N	2.43804600	-0.58742700	1.32147800
C	4.06306400	9.39747300	1.02962700
H	3.54245700	10.32461000	0.77715000
C	3.68825000	8.26476500	0.09080500
H	3.92431500	8.54698700	-0.94415900
H	2.60167900	8.10350500	0.11164600
C	4.39762800	6.96046100	0.42373900
H	4.13598600	6.64968800	1.44593400
H	5.48359100	7.13441400	0.44091900
C	4.09384700	5.83071500	-0.54856200
H	4.34229300	6.15485300	-1.57039700
H	3.01364800	5.61682000	-0.55797800
C	4.86129200	4.55498900	-0.23695500
H	4.56606800	4.16898600	0.74878400
H	5.93275700	4.78280400	-0.16021800
N	4.70428000	3.46290200	-1.20238700
H	5.74478300	1.94183400	-0.41519800
H	4.89357700	3.81496800	-2.13708900
H	-2.91184500	-1.62669300	1.24292500
Rh	2.24720100	0.28584400	-0.62877000
H	5.13782700	9.60326900	0.99311600
H	3.81481800	9.15330800	2.06789100
H	2.30337600	1.66999700	4.78381700
H	0.61589800	1.21103500	4.53152000
C	5.31090300	0.02222900	-0.77072200
N	5.93155300	1.02235200	0.00255600
C	5.72888100	0.14763000	-2.22407300
H	6.79108700	-0.08970800	-2.32167500
H	5.16619900	-0.52068600	-2.87700900
H	5.57235300	1.17501600	-2.56471500
C	6.14497300	-0.30637600	2.01781900
H	5.73624700	-0.44578800	3.02634300
H	7.23362700	-0.22381200	2.13542000
C	5.60456000	0.97707000	1.41223400
H	6.03864700	1.85307700	1.90246600
H	4.50580200	1.03238300	1.55035500
C	5.82478400	-1.50166900	1.16343900
C	5.43824000	-1.35032700	-0.16829200
C	5.12234600	-2.48907500	-0.93119000
H	4.82784000	-2.36942800	-1.96889700
C	5.20516200	-3.76657900	-0.39583900
C	5.61565700	-3.92278600	0.95416800
C	5.91721700	-2.79362000	1.70404200

H	6.23595000	-2.90233600	2.73734200
O	4.93649100	-4.91585300	-1.06017100
O	5.67564400	-5.19793000	1.39836000
C	4.64668300	-4.80978800	-2.43826600
H	5.46304700	-4.32310900	-2.98684000
H	4.52112800	-5.82873700	-2.80129600
H	3.71706500	-4.24891500	-2.61819000
C	6.17100200	-5.40034400	2.70806400
H	5.51669600	-4.94465000	3.46446600
H	6.19525200	-6.47835100	2.85854900
H	7.18135100	-4.99052000	2.82435600
H	3.73442800	3.15313900	-1.20676000

Cartesian coordinates (in Å) of stability points of the favorable path in K121H system

$\mathbf{I}_{ax}^{\mathbf{R}}$

	Coordinates (Angstroms)		
	X	Y	Z
O	8.74222200	-3.83914200	-1.54274000
C	9.04939200	-2.65999900	-1.43627400
N	9.49120400	-2.03120900	-0.28682100
H	9.50831500	-2.62823100	0.52912100
C	9.06038800	-0.65564600	-0.19354700
H	9.87502000	0.05079800	-0.02006200
N	8.91529600	-1.62768800	-2.40391500
H	9.71019100	-1.62774600	-3.04379600
C	8.69733400	-0.38704700	-1.67964700
H	9.28414000	0.43830500	-2.07222800
C	7.23005900	-0.00309900	-1.69587400
H	7.01879800	0.61926500	-2.55209200
H	6.58826300	-0.89437900	-1.74404300
S	6.93723300	0.92080000	-0.14903900
C	7.83399300	-0.38402600	0.73625000
H	8.01021500	0.04287600	1.76175800
C	6.96646300	-1.62525900	0.94757800
H	6.60222400	-1.98197700	-0.02507200
H	7.67875700	-2.40567100	1.24956300
C	5.80881000	-1.48594000	1.94523000
H	5.59798800	-2.49139000	2.33148800
H	6.14112900	-0.89592200	2.81113000
C	4.48551400	-0.90030800	1.41651900
H	4.60667500	0.16507900	1.17591600
H	4.26882800	-1.34403000	0.43314800
C	3.37880700	-1.15739100	2.45011400
H	3.45135100	-2.21351200	2.75219900
H	3.60092100	-0.60253400	3.37399000
C	1.91771500	-0.88816900	2.09473500
O	1.52527800	-0.48023600	1.00044300
N	1.00379100	-1.12944700	3.09199600
H	1.35457900	-1.57621000	3.92758300
C	-0.38779100	-1.39206400	2.73460300
H	-0.65775400	-2.38591600	3.10726600

H	-0.44668600	-1.43645100	1.64399100
C	-1.38035900	-0.34210700	3.22183800
H	-1.02075600	0.64248300	2.90006600
H	-1.38603900	-0.31861700	4.32206200
C	-2.78840900	-0.53367500	2.73944700
C	-3.65062300	-1.64443100	3.01204000
C	-3.38509100	-2.83990300	3.86225300
H	-2.31828800	-3.02564700	4.00204000
H	-3.82330400	-2.72296800	4.86255400
H	-3.81652900	-3.74974300	3.43340100
C	-4.94086400	-1.31903100	2.45838800
C	-6.12868200	-2.21370500	2.54628100
H	-5.88111800	-3.24576300	2.27580700
H	-6.52120000	-2.24124700	3.56956700
H	-6.94618100	-1.87804500	1.90194100
C	-4.91039800	-0.01091800	1.89756700
C	-6.05681300	0.75859700	1.33829200
H	-6.85012000	0.10032000	0.97080100
H	-6.51088300	1.41412000	2.09214100
H	-5.74688600	1.39362500	0.50277500
C	-3.55390000	0.47012000	2.02726900
C	-3.09537900	1.84191600	1.66573700
H	-3.66406100	2.23892600	0.81973200
H	-3.21523000	2.54169100	2.50261900
H	-2.04029700	1.85818800	1.37645500
C	3.54538000	2.66333200	-0.37456800
O	4.10062500	3.74598100	-0.29688800
N	2.61701300	2.23212400	0.52708300
H	2.27293100	1.27821600	0.49854700
C	1.97317900	3.19281500	1.41179800
H	1.65062100	4.06588200	0.83241800
C	0.76564300	2.53942900	2.07696400
H	1.07623900	1.80388100	2.82961900
H	0.20086100	1.97298500	1.32456600
C	-0.15497400	3.58968700	2.65802300
O	-0.43444400	4.61478200	2.04755700
N	-0.56202600	3.36535700	3.94706900
H	-0.26607800	2.56132200	4.47262400
H	-1.12670600	4.06349900	4.40318500
C	-2.69809400	-5.78775100	-3.49671900
H	-2.62185800	-6.61379500	-4.20522400
C	-4.12627200	-5.62663800	-3.00377400
H	-4.46206200	-6.56404900	-2.54001100
H	-4.79668300	-5.47185600	-3.85940700

C	-4.31013800	-4.50617700	-2.03829700
N	-5.55772400	-3.99968000	-1.74040100
C	-5.42013400	-3.01168700	-0.82051900
H	-6.24350500	-2.43597500	-0.42410000
N	-4.14748000	-2.84811700	-0.50841900
H	-6.43036200	-4.32602700	-2.12578800
C	-3.44738500	-3.77118700	-1.25896200
H	-2.37560100	-3.86251100	-1.15558100
Rh	-3.42290400	-1.26239000	0.76305600
H	-3.35075700	-0.41269700	-0.57595900
H	-1.97933500	-1.65904800	0.19715700
C	-0.36089400	0.86603200	-1.01237700
C	-1.32002700	1.81837900	-1.64993800
C	-1.33253000	3.16800900	-1.32297400
H	-0.59690700	3.55839100	-0.62344200
C	-2.30054100	4.02446200	-1.85765800
O	-2.37730100	5.33071600	-1.62523300
C	-1.39566400	5.91795200	-0.76247500
H	-1.43231400	5.48119400	0.23903900
H	-1.64215500	6.97673300	-0.72598100
H	-0.39069700	5.78816300	-1.17828800
C	-3.30746400	3.50324800	-2.72758500
O	-4.18960400	4.41541900	-3.18259400
C	-5.20961400	3.94520300	-4.04263100
H	-4.79177800	3.50963000	-4.95922500
H	-5.81321500	4.81433600	-4.29803800
H	-5.83987900	3.19720100	-3.54422600
C	-3.31011900	2.15816600	-3.03148200
H	-4.06881700	1.75934700	-3.69566400
C	-2.31167100	1.30083900	-2.50964300
C	-2.34164200	-0.10771900	-2.75683000
C	-3.51880900	-0.78067500	-3.36820300
H	-3.44987600	-1.86822800	-3.27856200
H	-3.59461400	-0.52414200	-4.43067200
H	-4.43691400	-0.45484700	-2.87477100
N	-1.28606500	-0.84988700	-2.48076400
C	-0.05117200	-0.31065100	-1.90887800
H	0.60766500	-0.02105800	-2.73940600
H	0.44191300	-1.10241400	-1.34157400
H	-1.38243100	-1.85271000	-2.55712700
H	-0.79907400	0.48579200	-0.07436600
H	0.57492100	1.36649600	-0.74919100
C	3.75944600	1.78437000	-1.60702000
H	3.12391800	2.17710600	-2.40745900

H	4.79623200	1.86030900	-1.93455100
H	3.49996100	0.72912700	-1.45174100
H	2.67554700	3.57012900	2.16545500
H	-2.34659900	-4.88153600	-4.00118500
H	-2.01198400	-5.99824500	-2.67123500

$\mathbf{P}_{ax}^{\mathbf{R}}$

	Coordinates (Angstroms)		
	X	Y	Z

O	8.73326000	-3.96593000	-1.21759100
C	9.01906700	-2.77665400	-1.21484600
N	9.45477600	-2.04342900	-0.12656600
H	9.48692200	-2.56762000	0.73754100
C	8.99903200	-0.67293000	-0.14907700
H	9.80128500	0.06038800	-0.04221500
N	8.86115800	-1.83402100	-2.26674200
H	9.65278200	-1.87481400	-2.90937200
C	8.62381000	-0.53979000	-1.65038700
H	9.19331200	0.25916100	-2.11623300
C	7.14961700	-0.18516800	-1.69007200
H	6.92269100	0.35730200	-2.59522800
H	6.52420200	-1.08870900	-1.65731500
S	6.84730200	0.86297800	-0.22650600
C	7.77237700	-0.34445600	0.76183800
H	7.94567600	0.17221200	1.74570200
C	6.92901500	-1.57833300	1.08466300
H	6.56669300	-2.02392900	0.14864200
H	7.65710000	-2.31690100	1.44799400
C	5.77387000	-1.37457000	2.07410700
H	5.58358600	-2.34669000	2.54670400
H	6.09943900	-0.70633900	2.88392900
C	4.43739300	-0.86055000	1.50558000
H	4.53763400	0.18219200	1.17352600
H	4.22415500	-1.39107500	0.56540400
C	3.34069200	-1.04771400	2.56455700
H	3.43425500	-2.07237300	2.95583500
H	3.55701500	-0.41143300	3.43589100
C	1.87312700	-0.83636000	2.19680000
O	1.46792600	-0.53118500	1.07407400
N	0.96877700	-1.00732100	3.21707000

H	1.33345100	-1.37754100	4.08306900
C	-0.41699200	-1.34377000	2.90099200
H	-0.71776100	-2.15703100	3.56806300
H	-0.45230600	-1.72038100	1.87155600
C	-1.37564300	-0.16272300	3.01101800
H	-0.94040000	0.66928200	2.45223900
H	-1.43104800	0.17260000	4.05785400
C	-2.77166500	-0.37660500	2.51300500
C	-3.66916200	-1.48062400	2.77237600
C	-3.41175200	-2.68200500	3.61603300
H	-2.53872400	-3.24735100	3.28313700
H	-3.24114800	-2.39594300	4.66147800
H	-4.26378900	-3.36549300	3.60404200
C	-4.97503400	-1.11894000	2.23096200
C	-6.18511500	-1.97649200	2.33933300
H	-5.96819100	-3.01950300	2.08853100
H	-6.57178500	-1.96855400	3.36462800
H	-6.99286500	-1.62818100	1.69079900
C	-4.88518100	0.14923600	1.61716700
C	-5.96849000	0.91701800	0.94491500
H	-6.79033800	0.27064700	0.62436700
H	-6.39408700	1.67509000	1.61276000
H	-5.59659300	1.44586000	0.06091300
C	-3.50964100	0.59926500	1.75754000
C	-3.00451300	1.91639300	1.29692200
H	-3.58603200	2.31239900	0.46055700
H	-3.04968400	2.64995700	2.11121100
H	-1.96610800	1.86624000	0.96268000
C	3.42271200	2.51823800	-0.57903800
O	3.95819600	3.61337600	-0.59828700
N	2.50684800	2.14952800	0.36226000
H	2.14856800	1.20141000	0.38523500
C	1.84977400	3.17095900	1.16537500
H	1.50339900	3.98399200	0.51611400
C	0.65773200	2.55573600	1.89196800
H	0.98075800	1.88051200	2.69409700
H	0.11533700	1.93340900	1.16450500
C	-0.27928600	3.63526000	2.38656500
O	-0.58068200	4.59881100	1.69205800
N	-0.67582300	3.51537800	3.69271100
H	-0.24483700	2.84882100	4.31005300
H	-1.15904900	4.29745500	4.10599400
C	-2.67844000	-6.28133900	-2.92294400
H	-2.59425300	-7.15330100	-3.57275000

C	-4.11821000	-5.80396500	-2.85043100
H	-4.76070300	-6.61824100	-2.48956300
H	-4.48471300	-5.57031500	-3.85912400
C	-4.30960200	-4.61596800	-1.97355300
N	-5.55334800	-4.06113300	-1.74804400
C	-5.42242300	-3.01632300	-0.89928100
H	-6.24398500	-2.39584600	-0.57292900
N	-4.15256500	-2.86109000	-0.56196900
H	-6.42115400	-4.38668600	-2.14622700
C	-3.45030400	-3.84935500	-1.22521000
H	-2.38292500	-3.95023500	-1.09315500
Rh	-3.39476400	-1.26474400	0.65062800
H	-3.03120800	-0.45348100	-1.00012400
H	-1.96846700	-1.92444000	0.33983800
C	-0.35966200	0.51206600	-1.19042400
C	-1.23955000	1.64714800	-1.59833600
C	-0.85254500	2.98404000	-1.48694300
H	0.15516300	3.21852900	-1.15252500
C	-1.74359700	4.01062200	-1.79583100
O	-1.46513100	5.32194000	-1.75659800
C	-0.14331500	5.69928300	-1.38237000
H	0.05780200	5.41398000	-0.34512100
H	-0.10882100	6.78277300	-1.48266400
H	0.60162800	5.24873500	-2.05003500
C	-3.06231200	3.68045500	-2.21310400
O	-3.85944500	4.73999300	-2.48673800
C	-5.17969300	4.45827700	-2.89551800
H	-5.20169200	3.88739300	-3.83310800
H	-5.66205000	5.42249500	-3.04987800
H	-5.72944600	3.89638600	-2.12680700
C	-3.43857300	2.34836100	-2.33122300
H	-4.43488400	2.10533200	-2.68577200
C	-2.52394000	1.32468200	-2.03951800
C	-2.85690000	-0.12744600	-2.14033600
C	-4.15061600	-0.46587000	-2.85290800
H	-4.26692400	-1.54957400	-2.94443500
H	-4.14565300	-0.04017600	-3.85993000
H	-5.01915100	-0.07946800	-2.31028500
N	-1.78225700	-0.88534000	-2.67127000
C	-0.42042300	-0.64370700	-2.18143400
H	0.22834100	-0.43176000	-3.04204000
H	-0.02799600	-1.54916700	-1.69903400
H	-2.01118400	-1.87018100	-2.71885400
H	-0.67144800	0.14113200	-0.19858900

H	0.67673700	0.83655700	-1.07003300
C	3.64699500	1.54047300	-1.73274400
H	2.92331000	1.77957500	-2.52017700
H	4.64828200	1.68458400	-2.13740600
H	3.50559800	0.48801100	-1.45665600
H	2.55291600	3.62520900	1.87451600
H	-2.01941600	-5.50594400	-3.32444400
H	-2.30139700	-6.56427100	-1.93616500

Cartesian coordinates (in Å) of the catalysts and substrate in two systems

C- S112H

	Coordinates (Angstroms)		
	X	Y	Z
H	4.56650900	0.28755900	0.29048400
H	5.18184500	-1.42547800	-0.90073500
N	-1.86951800	-2.36899000	0.46575500
C	-0.84575900	-1.79740400	-0.38716700
C	0.50496300	-1.63701600	0.30336000
C	1.48885900	-1.10740900	-0.69164400
C	1.81771000	0.25218000	-0.91546000
C	1.27043800	1.44284800	-0.20836300
H	0.45902200	1.90518200	-0.78411400
H	2.03406700	2.21066700	-0.05131100
H	0.86214800	1.18275100	0.77211700
C	2.74831100	0.29105500	-2.02890100
C	3.21367700	1.53823400	-2.70160200
H	2.41160300	1.98800500	-3.29898800
H	4.03700700	1.34121800	-3.39722800
H	3.53482500	2.29853700	-1.98105700
C	2.90505800	-1.05719300	-2.52667000
C	3.65125500	-1.45538300	-3.75261500
H	2.98935100	-1.44523000	-4.62617400
H	4.06572600	-2.46234500	-3.66640100
H	4.48030700	-0.77498500	-3.96977700
C	2.15649100	-1.93116800	-1.68349000
C	1.97389200	-3.39822400	-1.86363100
H	1.12126900	-3.62310600	-2.51609300
H	1.78614900	-3.90119000	-0.90995900
H	2.85577800	-3.86185500	-2.31516800
H	0.42239500	-0.95766900	1.16232700
H	0.84208700	-2.60437000	0.69950100
H	-0.75647500	-2.44194900	-1.26703100
H	-1.18390400	-0.82558500	-0.77640000
C	-3.05911900	-2.69619700	-0.08896500
C	-4.26635800	-3.10385100	0.82909900
C	-5.65828000	-2.61225000	0.15827300
C	-5.64992500	-1.12106400	0.04345000
C	-7.05307000	-0.60615500	-0.10228900
C	-7.00262200	0.92286900	0.00221000

S	-7.36038200	1.46528800	1.71695400
C	-7.62308300	3.12448400	1.06335000
C	-8.48605600	2.90078500	-0.30232700
C	-8.03536600	1.55985300	-0.88315000
H	-7.61531500	1.67436200	-1.88852800
N	-9.31399000	0.78350200	-0.93419200
H	-9.42371500	-0.14894500	-1.25355000
C	-10.32146800	1.57953800	-0.45519400
O	-11.49232200	1.19251200	-0.37360800
N	-9.95163400	2.74276300	-0.08889400
H	-10.58507100	3.43726900	0.27785500
H	-8.27100300	3.72480600	-1.00025700
H	-6.66379700	3.62767500	0.88540400
H	-8.23068400	3.74090900	1.75605300
H	-6.00055500	1.26085000	-0.27345800
H	-7.69724100	-1.00995400	0.70928000
H	-7.46930300	-0.90226200	-1.06921600
H	-5.07577300	-0.82138100	-0.82532400
H	-5.19581000	-0.69035500	0.95963500
H	-6.51387500	-2.92697700	0.80853800
H	-5.77104200	-3.05781300	-0.82496100
H	-4.16588400	-2.63076400	1.83709500
H	-4.28683700	-4.19363200	0.97120800
O	-3.18680300	-2.57282100	-1.38737200
C	3.23547900	-0.03746900	4.42235200
H	2.97420900	0.99854500	4.64510900
C	3.39663800	-0.25363500	2.92994900
H	4.16367100	0.41643000	2.52077100
H	2.47823600	0.02546800	2.39318500
C	3.75397700	-1.65102800	2.57061400
C	3.92869600	-2.74029800	3.38499600
H	3.85412200	-2.85471700	4.45458700
N	4.25280900	-3.79136000	2.55802000
H	4.45244500	-4.73529800	2.84754100
C	4.27104900	-3.33594800	1.28777200
H	4.50502900	-3.94087200	0.42520500
N	3.97275300	-2.04641100	1.26370600
C	7.79079100	6.51995400	1.21083100
H	7.32762600	7.50032500	1.34066400
C	6.85531800	5.54862900	0.51017200
H	6.56414700	5.95329600	-0.46846200
H	5.92221000	5.44768500	1.08017600
C	7.47630400	4.17195600	0.31469300
H	7.74166000	3.74467500	1.29158800

H	8.42482300	4.27673200	-0.23130100
C	6.57357500	3.19964700	-0.43647700
H	6.29288300	3.63855000	-1.40551400
H	5.63688800	3.03869800	0.11494600
C	7.26548800	1.87276900	-0.66654300
H	7.46882200	1.35127600	0.27296500
H	8.21590100	2.00561800	-1.19159900
N	6.42031100	0.94598200	-1.48377700
H	6.92579100	0.10371900	-1.75909500
H	6.08287600	1.39804800	-2.33398100
H	-1.78310400	-2.29352900	1.46836400
Rh	3.73355300	-0.86810700	-0.50142600
H	8.71364200	6.66455300	0.64025100
H	8.07376500	6.15547100	2.20350300
H	4.16067500	-0.26626000	4.96037900
H	2.44605300	-0.67127400	4.83893600
H	5.56677200	0.57454100	-0.94537800

S- S112H

	Coordinates (Angstroms)		
	X	Y	Z
C	2.42795100	0.72629000	-0.06431900
N	3.42645700	-0.05429000	0.16272400
C	2.73041500	2.16891800	-0.33977900
H	2.26952700	2.50872700	-1.27373200
H	2.34112800	2.81493400	0.45621200
H	3.80980600	2.30860400	-0.39693300
C	1.91235800	-2.00922300	-0.24107200
H	1.66759400	-3.01124800	0.12961700
H	2.16121800	-2.12916900	-1.30694000
C	3.11785500	-1.44052000	0.49069000
H	4.00911100	-2.04475600	0.29072000
H	2.95138800	-1.49567400	1.57878600
C	0.74460800	-1.07891500	-0.10589700
C	1.01971800	0.29147700	-0.04455500
C	-0.04600100	1.20660700	0.01989000
H	0.16747300	2.26915500	0.06414300
C	-1.36202400	0.77203900	0.03637300
C	-1.63475200	-0.61588900	-0.02262100

C	-0.57896100	-1.51953100	-0.09929800
H	-0.77906400	-2.58567900	-0.15308200
O	-2.45570400	1.57797600	0.10436200
O	-2.94771600	-0.95404400	0.00063600
C	-2.21374500	2.96632500	0.15428800
H	-1.67989400	3.31902600	-0.73843000
H	-3.19290600	3.44306600	0.19896300
H	-1.63333300	3.24746100	1.04346800
C	-3.25113900	-2.33195300	-0.05880600
H	-2.82491000	-2.87811000	0.79275900
H	-4.33775700	-2.40357100	-0.02607000
H	-2.88492900	-2.78793800	-0.98788600

C-K121H

	Coordinates (Angstroms)		
	X	Y	Z
O	-7.70061700	4.31136400	0.97047200
C	-8.16683200	3.27755400	0.51227100
N	-8.57377700	2.17284500	1.23741200
H	-8.41590300	2.25220800	2.23303600
C	-8.34496900	0.92614200	0.54469500
H	-9.23278000	0.29467600	0.46837100
N	-8.29039900	2.90018000	-0.85238800
H	-9.13933300	3.29338500	-1.25982200
C	-8.18438700	1.45209800	-0.90790100
H	-8.92546300	1.00043700	-1.56095100
C	-6.80049900	1.02915100	-1.36237300
H	-6.77548500	0.93542800	-2.43739400
H	-6.04194400	1.76408000	-1.05729400
S	-6.48717200	-0.58739500	-0.57456700
C	-7.08163400	0.11933500	0.98672600
H	-7.21045100	-0.76824800	1.66537600
C	-6.02175200	0.99860300	1.65115300
H	-5.71294000	1.78536100	0.95000000
H	-6.57424400	1.55338700	2.42223500
C	-4.79918400	0.27335400	2.22927100
H	-4.40167200	0.90819900	3.03147300
H	-5.12255100	-0.65755200	2.71629200
C	-3.64081300	-0.04129900	1.26346400

H	-3.94374800	-0.80989000	0.53881300
H	-3.46527000	0.83551600	0.62218500
C	-2.40561000	-0.44562300	2.08200000
H	-2.28802400	0.29690000	2.88630800
H	-2.60926600	-1.38499300	2.61744500
C	-1.04636300	-0.59233900	1.40052800
O	-0.83645900	-0.39293400	0.20291400
N	-0.00694300	-0.97757000	2.21245800
H	-0.19923300	-1.01028800	3.20343500
C	1.36486800	-0.67145500	1.81960500
H	1.85589200	-0.11555400	2.62677000
H	1.32157000	0.00580900	0.96501500
C	2.21784500	-1.87837900	1.43479900
H	1.66798300	-2.46427100	0.68842800
H	2.35416000	-2.53449400	2.30735800
C	3.55289400	-1.49011800	0.86688500
C	4.78740300	-1.31374000	1.60372100
C	4.93042500	-1.42388000	3.08294400
H	4.02269700	-1.10127400	3.60088200
H	5.13086100	-2.46045000	3.38595900
H	5.75362800	-0.80964700	3.45795800
C	5.82904500	-1.09775600	0.66807400
C	7.27894300	-0.94015100	0.97415300
H	7.44233800	-0.41884100	1.92267900
H	7.79192500	-1.90923500	1.04483600
H	7.79845100	-0.37554300	0.19180600
C	5.25562300	-1.18058500	-0.66714000
C	6.03261100	-1.03686900	-1.92923300
H	6.71501100	-0.17844100	-1.89223300
H	6.65021500	-1.92171900	-2.12997700
H	5.37633300	-0.89208100	-2.79148100
C	3.87389200	-1.45775400	-0.54805800
C	2.89443200	-1.70691200	-1.64383900
H	3.23091800	-1.28287100	-2.59347700
H	2.73496900	-2.78230000	-1.80616000
H	1.92114300	-1.25869100	-1.41815200
C	-3.43496600	-2.19159600	-2.21879400
O	-4.13391100	-3.11053200	-2.61056700
N	-2.36329100	-2.36597200	-1.39286800
H	-1.80881500	-1.56381200	-1.11358800
C	-1.77965900	-3.69156900	-1.24256600
H	-1.64217100	-4.15720700	-2.22468800
C	-0.42553500	-3.57358300	-0.54981000
H	-0.53887100	-3.31476000	0.51077400

H	0.13240300	-2.74588300	-1.00810000
C	0.38490400	-4.83564100	-0.74745700
O	0.44276400	-5.40496200	-1.83100500
N	0.95407400	-5.35135300	0.38736500
H	1.03825400	-4.79243200	1.22032600
H	1.59600400	-6.11915200	0.27254400
C	3.63230600	6.16450100	-1.60378600
H	3.50044800	7.17953000	-1.98378900
C	5.10323400	5.77977100	-1.57423200
H	5.66122000	6.49560600	-0.95413300
H	5.53084400	5.87239100	-2.58262900
C	5.31830000	4.39942600	-1.06288300
N	6.56481900	3.81722100	-0.94373600
C	6.40559800	2.55872800	-0.45170200
H	7.22284800	1.88446800	-0.24239400
N	5.12597500	2.30347400	-0.25405100
H	7.44402600	4.24982400	-1.17503300
C	4.44296600	3.44001200	-0.62898400
H	3.36687100	3.47532500	-0.55795900
Rh	4.22128400	0.52165900	0.47092100
H	3.80223300	1.39810600	1.72303300
C	-3.64453900	-0.78381600	-2.77695700
H	-3.02381900	-0.67447400	-3.67144600
H	-4.68835000	-0.67184100	-3.07020700
H	-3.36525400	0.01378500	-2.07862600
H	-2.45181600	-4.34756500	-0.67604600
H	3.06062900	5.48889400	-2.24616000
H	3.19249900	6.12046400	-0.60345000
H	2.87931400	1.23446100	0.02219200

S-K121H

	Coordinates (Angstroms)		
	X	Y	Z

H	4.27231200	0.30027300	0.07292700
C	2.32722400	0.78963300	-0.06654700
N	3.32865700	-0.06158400	0.08563500
C	2.66506100	2.22243700	-0.27214300
H	2.14865300	2.62352400	-1.14714100
H	2.34043900	2.81254600	0.59072800

H	3.73711100	2.37926000	-0.39847300
C	1.89808400	-2.00841100	-0.23823400
H	1.66704400	-2.99873200	0.16190500
H	2.10010000	-2.14914400	-1.30927500
C	3.13150800	-1.46597400	0.45147700
H	4.02927400	-2.01884900	0.17234200
H	3.02978200	-1.51986300	1.54362700
C	0.73510300	-1.07360000	-0.07541400
C	0.98191200	0.31843200	-0.02173400
C	-0.10438900	1.22968100	0.02022100
H	0.08904500	2.29517200	0.06577000
C	-1.40557300	0.77480200	0.03175100
C	-1.64777800	-0.63500500	-0.01710100
C	-0.57312100	-1.52928900	-0.08023800
H	-0.76519100	-2.59562100	-0.13674700
O	-2.50953000	1.53388900	0.08500300
O	-2.92761300	-0.98490500	0.00008300
C	-2.32834800	2.94268600	0.12612400
H	-1.80119800	3.29943600	-0.76648600
H	-3.32815900	3.37041600	0.15302100
H	-1.77677800	3.24441900	1.02426500
C	-3.25727200	-2.37465500	-0.04691800
H	-2.84064300	-2.90291500	0.81609000
H	-4.34311300	-2.41662200	-0.01516200
H	-2.89660700	-2.82849000	-0.97499300
