Supporting Information for:

On the Role of Alkylcobalamins in the Vitamin B_{12}-Catalyzed Reductive Dehalogenation of Perchloroethylene and Trichloroethylene

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Table S1. Cartesian Coordinates of Relevant Structures

Tetrachloroethylcob(III)alamin

Co	-0.32086900	0.03710700	0.02724500
N	-0.59999500	-1.60120100	0.96418200
N	0.46629000	0.53943500	1.68223600
N	-0.06285000	1.83839500	-0.67897200
N	-1.40342200	-0.57570400	-1.47748200
C	0.10391300	-1.77005300	2.25519800
H	1.11282200	-2.15712000	2.04864600
C	0.63881500	2.84795100	-0.04629200
C	-1.38051600	-2.60694900	0.69308400
C	-0.55701900	2.26717700	-1.85607300
C	-0.73358700	-2.83885300	2.98110500
C	0.78505900	4.03548900	-0.97336600
C	-1.35796000	-3.63392200	1.80859300
C	-0.19101000	3.71198800	-2.11736900
C	1.13381700	2.79859000	1.23098600
C	-2.11098000	-2.71993600	-0.52751100
C	-1.32928100	1.50950000	-2.73303400
C	1.28261800	0.05907000	3.83920600
C	1.43104300	1.57172700	3.53217600
C	-2.75494700	-1.94606000	-2.87198600
C	-2.58337700	-0.56603800	-3.53130700
C	0.20111800	-0.35833200	2.83196400
H	-0.79339600	-0.09629900	3.22550100
C	1.01262800	1.65612700	2.07472800
C	-2.05850100	-1.78991700	-1.53533600
C	-1.71224300	0.18517400	-2.54754100
H	2.22332900	-0.46304800	3.62874300
H	1.00540000	-0.14137700	4.87688300
H	2.44352800	1.95632200	3.68850100
H	0.75490000	2.17980900	4.14911600
H	-2.26415800	-2.73912000	-3.44739600
H	-3.80184400	-2.24048600	-2.75036300
H	-2.09700000	-0.61763100	-4.51108900
H	-3.53528700	-0.04262200	-3.67680700
H	1.67010100	3.66164400	1.60980700
H	-2.69309200	-3.62040900	-0.69071200
H	-1.65706800	1.99456400	-3.64642100
H	-0.13962200	-3.46285600	3.65279900
H	-1.52271600	-2.35817000	3.57185500
H	1.82011200	4.08083900	-1.33321100
H	0.57530700	4.98225800	-0.46809800
H	-0.72200800	-4.47704800	1.50522600
H	-2.34953800	-4.04176600	2.02779900
H	0.24570700	3.83578500	-3.11285400
H	-1.09300100	4.33578100	-2.08261900
C	1.46096100	-0.69081000	-0.88387300
N	-2.16188900	0.83337100	0.89967200
C	-3.33745200	0.22361900	0.95972000
N	-4.25363700	1.01282700	1.57066700
C	-3.63474900	2.19391700	1.92209900
C	-2.33937100	2.06750900	1.49990700
H	-3.55726300	-0.76268900	0.58119600
H	-5.22268300	0.77576900	1.73404300

H	-4.15725500	2.99344500	2.42384400
H	-1.53237900	2.77690700	1.58502900
C	2.77905600	-0.73299000	-0.05315500
Cl	3.48620300	0.89114100	0.25817300
Cl	4.10032600	-1.74853800	-0.76100900
Cl	1.13742100	-2.43784000	-1.32700400
H	2.56466600	-1.16779800	0.91908000
Cl	1.80582700	0.15639500	-2.44532500

1,1,2-Trichloroethylcob(III)alamin

Co	0.15866100	0.00839700	0.06737200
N	0.47886400	1.72693100	-0.67222500
N	-0.69728300	1.03796200	1.41973600
N	-0.18350500	-1.62676800	1.07392500
N	1.29141300	-0.84112300	-1.26601800
C	-0.27039700	2.85860400	-0.08498200
H	-1.25725600	2.89098400	-0.57003200
C	-1.02345000	-1.72991600	2.16317800
C	1.26228500	2.10437200	-1.63807500
C	0.35978900	-2.82536500	0.77201700
C	0.56290500	4.08506200	-0.49734100
C	-1.18880600	-3.18333100	2.55705800
C	1.22742800	3.61022500	-1.81375500
C	-0.09467200	-3.89504400	1.74103800
C	-1.62087600	-0.67621700	2.81422900
C	2.00096600	1.18400600	-2.44420300
C	1.22764600	-3.07066300	-0.28561700
C	-1.60020400	3.06428400	2.23264600
C	-1.88666700	1.90704600	3.22502000
C	2.67889200	-1.17066700	-3.16623500
C	2.56240500	-2.49300500	-2.38655400
C	-0.44380700	2.49731400	1.39208400
H	0.51709100	2.67360500	1.89928300
C	-1.39919200	0.68825300	2.46017900
C	1.95671300	-0.17592400	-2.28036700
C	1.63365400	-2.14226800	-1.24391600
H	-2.47734100	3.24418400	1.59978800
H	-1.34665400	4.00182100	2.73291900
H	-2.94028900	1.82066800	3.50858900
H	-1.31280100	2.01567300	4.15566100
H	2.17199200	-1.22644800	-4.13654400
H	3.71209900	-0.86871500	-3.36090900
H	2.14764800	-3.31097900	-2.98433300
H	3.52723500	-2.84050400	-1.99824000
H	-2.26225600	-0.89064500	3.66190700
H	2.59022300	1.58366400	-3.26240300
H	1.58911200	-4.08701500	-0.40190700
H	-0.04025800	4.98675300	-0.62577600
H	1.32911100	4.29227500	0.25959800
H	-2.18900500	-3.52649000	2.26594000
H	-1.09893100	-3.32811200	3.63714000
H	0.60996000	3.85330100	-2.68948600
H	2.21915300	4.03837000	-1.98977900
H	-0.45348700	-4.78287700	1.21226700
H	0.74741300	-4.21284000	2.36858200
C	-1.53633700	-0.27249600	-1.10752100

N	1.97631200	0.22055000	1.28031900
C	3.18067600	0.59862500	0.88009500
N	4.04914500	0.60523000	1.92092700
C	3.36484100	0.21093500	3.05163300
C	2.08153100	-0.02333400	2.63737500
H	3.45363600	0.87192400	-0.12771000
H	5.02753800	0.85509600	1.87339600
H	3.84053500	0.13350000	4.01692000
H	1.23511900	-0.35131100	3.21991400
C	-2.81058300	0.16477500	-0.39185400
Cl	-4.36164700	-0.06556000	-1.30134800
Cl	-1.43054500	0.63930800	-2.68225200
H	-2.75676000	1.22779100	-0.16663900
Cl	-1.71953200	-2.02320100	-1.56122900
H	-2.92042700	-0.40078300	0.53146800

1,1,2-Trichloroethylcob(II)alamin

Co	0.15943000	0.00213600	0.07390400
N	0.51934300	1.76033000	-0.55831200
N	-0.79019500	0.97419400	1.41931800
N	-0.25510200	-1.68119700	0.99166400
N	1.39184200	-0.77205900	-1.23491100
C	-0.27426200	2.84924300	0.02712700
H	-1.23674800	2.91320500	-0.50774300
C	-1.13467200	-1.82128600	2.00889400
C	1.36036300	2.18650600	-1.47708100
C	0.33209800	-2.88062600	0.66216600
C	0.57166200	4.09996500	-0.27323100
C	-1.32165000	-3.29278900	2.33973500
C	1.29496100	3.70194200	-1.58349500
C	-0.14981100	-3.97098400	1.59937200
C	-1.79205000	-0.78626300	2.69160800
C	2.15856800	1.32828600	-2.25044000
C	1.25469100	-3.06058800	-0.36258400
C	-1.75299400	2.95605700	2.25270100
C	-2.09868800	1.76629900	3.18527900
C	2.93447800	-0.99761400	-3.00604800
C	2.76458600	-2.37534500	-2.32958100
C	-0.53760500	2.42234200	1.47346300
H	0.38657500	2.60041700	2.05168300
C	-1.56179600	0.56781500	2.41308400
C	2.11050800	-0.06497500	-2.13319900
C	1.73148100	-2.10723300	-1.25098000
H	-2.58388500	3.14903300	1.56273600
H	-1.54562700	3.88170100	2.79815600
H	-3.16844900	1.67782500	3.40318900
H	-1.58139800	1.85564900	4.15113900
H	2.53398600	-0.99142300	-4.02751500
H	3.97898000	-0.67282800	-3.07389200
H	2.42615100	-3.14612000	-3.03150100
H	3.70633300	-2.73741800	-1.89466700
H	-2.48059000	-1.05347900	3.48606200
H	2.80209500	1.75649800	-3.01155200
H	1.63455100	-4.07134500	-0.49358600
H	-0.02517000	5.01155800	-0.37161800
H	1.30327100	4.25603800	0.53015400

H	-2.29054800	-3.63287600	1.94923300
H	-1.32737400	-3.47890600	3.41871600
H	0.69661700	3.97867100	-2.46281300
H	2.28057300	4.16459400	-1.70330800
H	-0.44960700	-4.87743900	1.06315700
H	0.64670000	-4.26259700	2.30020200
C	-1.45822700	-0.22765800	-1.20747700
N	1.86875400	0.15561300	1.38468900
C	3.07352500	0.59082100	1.06278400
N	3.89517700	0.55584200	2.14383700
C	3.16880800	0.07042800	3.21521500
C	1.91393200	-0.17155600	2.72477500
H	3.37346300	0.93452600	0.08334600
H	4.86653800	0.83028500	2.15543200
H	3.60247100	-0.05634700	4.19494200
H	1.04331300	-0.55519600	3.23393200
C	-2.76643000	0.13942800	-0.52633700
Cl	-4.30046100	-0.06621500	-1.50714100
Cl	-1.31135900	0.79547400	-2.72460000
H	-2.75248200	1.18914300	-0.24524700
Cl	-1.59852600	-1.94842000	-1.79597400
H	-2.90605400	-0.47745900	0.35859400

1,2,2-Trichloroethylcob(III)alamin

Co	-0.27424400	0.05051000	0.06387200
N	-0.63192400	-1.68577600	-0.60179500
N	0.73234800	-0.92175100	1.34312900
N	0.21918200	1.74063400	0.91813200
N	-1.51455900	0.85413500	-1.20760900
C	0.19711400	-2.78859100	-0.06566900
H	1.13394400	-2.80456300	-0.63694000
C	1.13895200	1.87715500	1.94127600
C	-1.50621100	-2.10287900	-1.46596600
C	-0.24040100	2.94641700	0.52055000
C	-0.64895600	-4.03961600	-0.36109400
C	1.36822200	3.34481600	2.25110500
C	-1.45647700	-3.61167700	-1.61193900
C	0.34665300	4.06682300	1.35293600
C	1.77778800	0.84338800	2.58052700
C	-2.35579300	-1.21682300	-2.20261400
C	-1.14301300	3.15943900	-0.51651900
C	1.72395000	-2.92106900	2.13525000
C	2.10891600	-1.72410000	3.04367600
C	-3.11807000	1.10305100	-2.94995000
C	-2.75273600	2.48981600	-2.38868600
C	0.49639900	-2.38413200	1.37962700
H	-0.41745000	-2.54728500	1.97176400
C	1.53473400	-0.53736200	2.29105100
C	-2.30268300	0.14692400	-2.10021600
C	-1.73989900	2.17436100	-1.30853200
H	2.53606500	-3.13452800	1.43389400
H	1.50890800	-3.83009700	2.70193500
H	3.18723600	-1.62454100	3.20231300
H	1.64259900	-1.79356600	4.03617300
H	-2.83979900	0.99579700	-4.00366200
H	-4.18851000	0.88473600	-2.87923100

H	-2.31502800	3.15247300	-3.14320000
H	-3.61264900	3.01998000	-1.96396100
H	2.49151100	1.08460200	3.36079300
H	-3.03072200	-1.65106400	-2.93242600
H	-1.41827500	4.18815400	-0.72461400
H	-0.04362600	-4.93309100	-0.53014300
H	-1.32978400	-4.24178800	0.47492800
H	2.39908900	3.62378200	2.00529300
H	1.22813600	3.55300200	3.31614600
H	-0.92852500	-3.86450300	-2.54165100
H	-2.45183000	-4.06281300	-1.67343700
H	0.79791000	4.83525500	0.71738400
H	-0.44482600	4.55789300	1.93136700
C	1.20340500	0.42467900	-1.26356500
N	-1.95812200	-0.10698600	1.46571300
C	-3.19256200	-0.51364700	1.21249300
N	-3.95307300	-0.46011100	2.33380700
C	-3.16310200	0.00546500	3.36410000
C	-1.93016000	0.21907100	2.80918600
H	-3.56288900	-0.84561200	0.25454500
H	-4.92835200	-0.71743900	2.40034300
H	-3.54058900	0.13921000	4.36593600
H	-1.03244200	0.58408200	3.28304600
C	2.65221900	0.38909500	-0.78952100
Cl	3.69296700	1.51037200	-1.77761400
Cl	3.41920900	-1.24249900	-0.75538700
Cl	1.04044900	-0.39829400	-2.86683300
H	2.72520500	0.76837700	0.22466300
H	0.99797200	1.47227600	-1.48328800

1,2,2-Trichloroethylcob(II)alamin

Co	-0.27119900	0.05975000	0.06693400
N	-0.76020800	-1.63091600	-0.64457800
N	0.71527400	-1.02492400	1.27836700
N	0.35354200	1.68612800	0.98330400
N	-1.50874400	0.97362300	-1.14500100
C	0.01566100	-2.79176400	-0.17760200
H	0.93614300	-2.86349300	-0.77422600
C	1.28190800	1.71903600	1.96675800
C	-1.70242800	-1.96172500	-1.49818700
C	-0.04799500	2.95397100	0.62217700
C	-0.91758100	-3.97965300	-0.47725000
C	1.64248600	3.15722300	2.30803600
C	-1.73034300	-3.46977700	-1.69273000
C	0.60050300	3.98545200	1.52598600
C	1.88638400	0.61048900	2.57533700
C	-2.52988000	-1.02146100	-2.14084500
C	-0.94113700	3.24225900	-0.40637800
C	1.60355200	-3.10057200	1.96004000
C	2.06918500	-1.97852700	2.92351500
C	-3.22858300	1.38410500	-2.70747500
C	-2.55558000	2.72684000	-2.35245800
C	0.38573400	-2.45922500	1.27090300
H	-0.51723700	-2.61035400	1.88926500
C	1.56135100	-0.71634700	2.23985300
C	-2.37265600	0.35723700	-1.98046600

C	-1.61323900	2.34496100	-1.22754900
H	2.38427900	-3.30479800	1.22036100
H	1.36305000	-4.03440600	2.47733100
H	3.15325200	-1.95870900	3.07744000
H	1.60477900	-2.08210900	3.91468500
H	-3.26465200	1.18872000	-3.78394300
H	-4.26357700	1.33781900	-2.34052900
H	-1.99155700	3.12174800	-3.20920500
H	-3.27007500	3.50324100	-2.05734900
H	2.63138500	0.79144200	3.34279900
H	-3.27372800	-1.37508300	-2.84692900
H	-1.13738900	4.29675500	-0.58687400
H	-0.37872000	-4.90978300	-0.68056400
H	-1.58638400	-4.15349300	0.37592900
H	2.66596100	3.36933600	1.97133800
H	1.62084000	3.33959700	3.38786400
H	-1.23105800	-3.72431000	-2.63795700
H	-2.74738600	-3.87343400	-1.74538200
H	1.04824200	4.81071000	0.96138300
H	-0.14297100	4.43219100	2.20202600
C	1.18640800	0.40410200	-1.27503700
N	-1.90708100	-0.04772800	1.50102500
C	-3.15545000	-0.39931400	1.25226700
N	-3.90121100	-0.34406900	2.38701700
C	-3.07655700	0.06646000	3.41765300
C	-1.84395300	0.24420700	2.84861400
H	-3.54034500	-0.69504200	0.28683000
H	-4.88474400	-0.55978400	2.45824500
H	-3.43583700	0.19170900	4.42726000
H	-0.91907600	0.55892400	3.30717100
C	2.62965200	0.27436700	-0.81962500
Cl	3.74109900	1.41847700	-1.73975900
Cl	3.34295200	-1.38396400	-0.90795500
Cl	0.96948300	-0.34618700	-2.92047200
H	2.73093300	0.58131000	0.21666800
H	1.03250300	1.46763700	-1.45586400

1,2-Dichloroethylcob(III)alamin

Co	0.06984100	-0.04676700	0.04648300
N	1.16521600	1.38056100	-0.53797800
N	-0.83891100	1.35965800	0.94416800
N	-1.18652000	-1.35869500	0.76922800
N	1.23851200	-1.36083900	-0.78261800
C	0.63248300	2.74504300	-0.34193800
H	-0.06249900	2.95128200	-1.16943700
C	-2.32206100	-1.05913200	1.49585800
C	2.32233300	1.38226900	-1.12694700
C	-1.09429400	-2.68782900	0.54847100
C	1.88463500	3.63408900	-0.45079500
C	-3.12261000	-2.31884900	1.76837900
C	2.81661900	2.79659700	-1.36258400
C	-2.23296800	-3.44114700	1.20289700
C	-2.69900200	0.19653200	1.90718300
C	2.98180200	0.18186100	-1.54051400
C	-0.08580800	-3.31208100	-0.17852400
C	-1.29577200	3.65237100	1.28500500

C	-2.25180900	2.77777700	2.13666100
C	3.06072900	-2.33480700	-1.96507100
C	2.09177300	-3.44387200	-1.51480500
C	-0.15429100	2.67259800	0.96808600
H	0.56989000	2.65015100	1.79714600
C	-1.93704400	1.37609300	1.64331400
C	2.43220600	-1.06682700	-1.41906400
C	1.00528300	-2.68373300	-0.78456400
H	-1.79472200	3.96417500	0.35993200
H	-0.95866500	4.55007100	1.80859000
H	-3.30924800	3.03191700	2.01425200
H	-2.02530800	2.85317500	3.20927100
H	3.14199700	-2.27154200	-3.05525400
H	4.07511700	-2.47475400	-1.57749700
H	1.66777900	-4.00409700	-2.35532800
H	2.55971000	-4.17831200	-0.84971800
H	-3.62425900	0.29824100	2.46386500
H	3.93376100	0.27556500	-2.05208000
H	-0.14437500	-4.39138100	-0.27381300
H	1.66963700	4.62493400	-0.85733400
H	2.34140900	3.76382900	0.53778300
H	-4.09049600	-2.26504100	1.25749100
H	-3.33256800	-2.43309000	2.83629200
H	2.68217600	3.04979800	-2.42306400
H	3.88073900	2.91549100	-1.13552100
H	-2.75046500	-4.07720600	0.47766100
H	-1.84518000	-4.10344600	1.98581100
C	-1.04469400	-0.05435800	-1.63012500
N	1.28046900	-0.26144600	1.89092600
C	2.59923900	-0.31190100	1.99621100
N	2.97157100	-0.45925600	3.29220500
C	1.82800700	-0.50479600	4.06191300
C	0.78994000	-0.38040500	3.17812200
H	3.30000600	-0.24609300	1.17779100
H	3.92133000	-0.52452900	3.63193700
H	1.85825000	-0.61954800	5.13429900
H	-0.26953700	-0.37044900	3.38120400
C	-2.35525600	0.69738800	-1.56594100
Cl	-3.51896500	0.19699300	-2.88337800
Cl	-0.15447200	0.44856800	-3.13938300
H	-2.88044000	0.48408200	-0.63782400
H	-1.23723500	-1.11653600	-1.78027200
H	-2.22306500	1.77432700	-1.67318200

1,2-Dichloroethylcob(II)alamin

Co	0.06746400	-0.05402200	0.04337200
N	1.24819000	1.27801600	-0.61546800
N	-0.77520600	1.46205700	0.83344100
N	-1.26449000	-1.24698900	0.85657800
N	1.18664800	-1.47172200	-0.70024300
C	0.78369300	2.66843500	-0.51597400
H	0.10567400	2.87577800	-1.36071700
C	-2.35156300	-0.84444600	1.55342800
C	2.42261500	1.17529800	-1.19625400
C	-1.23686900	-2.61540300	0.70654400
C	2.08199500	3.48492600	-0.65683400

C	-3.24613200	-2.03308300	1.87070700
C	2.97260700	2.55600300	-1.51927100
C	-2.38075500	-3.24851700	1.47594400
C	-2.67288000	0.47438300	1.90728700
C	3.02914100	-0.05888300	-1.49402900
C	-0.27119600	-3.31769100	-0.01035100
C	-1.10191300	3.78248900	1.03415300
C	-2.08763300	3.02740200	1.96284700
C	3.00787600	-2.62317700	-1.65852800
C	1.84840600	-3.62014200	-1.45231600
C	-0.01665400	2.72044300	0.78815600
H	0.70651900	2.72671100	1.62348400
C	-1.87051900	1.57355700	1.56224200
C	2.38824100	-1.28387500	-1.28735800
C	0.84180000	-2.80482500	-0.66466200
H	-1.59586900	4.03668500	0.08817000
H	-0.71628400	4.70619100	1.47635400
H	-3.12993300	3.34315500	1.84676700
H	-1.82368500	3.17171200	3.02042200
H	3.40244900	-2.61942100	-2.67942400
H	3.85271900	-2.84186500	-0.98988700
H	1.42091200	-3.92678100	-2.41757300
H	2.15116500	-4.53531100	-0.93200600
H	-3.59221000	0.64534900	2.45742000
H	3.99808700	-0.06234400	-1.98201100
H	-0.40130300	-4.39650500	-0.05764300
H	1.92585300	4.46962400	-1.10720000
H	2.53671900	3.63167600	0.33141200
H	-4.16030000	-1.97364400	1.26476700
H	-3.56160900	-2.04433900	2.91955300
H	2.83569000	2.75867600	-2.59049700
H	4.04317200	2.64982300	-1.30667200
H	-2.92766300	-3.98813500	0.88101900
H	-2.00343200	-3.77420300	2.36532300
C	-1.04137100	-0.11601600	-1.62435600
N	1.25215200	-0.20553300	1.88835900
C	2.56802000	-0.26604200	1.97872800
N	2.95422000	-0.35258800	3.27939600
C	1.81435500	-0.34597400	4.06140400
C	0.76986200	-0.25316400	3.18070800
H	3.25278700	-0.24677900	1.14287900
H	3.90559900	-0.41794900	3.61033000
H	1.85455300	-0.40756900	5.13786000
H	-0.29013200	-0.21469700	3.38025900
C	-2.32261900	0.67292500	-1.56842900
Cl	-3.55345300	0.17522700	-2.85762600
Cl	-0.15992600	0.31607800	-3.17772700
H	-2.84248500	0.50836800	-0.62790800
H	-1.25683200	-1.17799800	-1.73861600
H	-2.16589600	1.73979200	-1.72308000

Methylcob(III)alamin
See: *JACS*, **2005**, *127*, 384-396.

Methylcob(II)alamin
See: *JACS*, **2005**, *127*, 384-396.

Base-off Tetrachloroethylcob(III)alamin

Co	-0.22506800	0.00838000	-0.57161600
N	-0.65127600	1.86071400	-0.63713700
N	1.43035200	0.66804400	-1.23950800
N	0.34902000	-1.80188600	-1.02221700
N	-2.10994400	-0.46613800	-0.55976200
C	0.48118300	2.81557000	-0.71910100
H	0.89391100	2.94929600	0.29197400
C	1.64118100	-2.18790700	-1.35080600
C	-1.80316400	2.47586600	-0.67526200
C	-0.45316300	-2.89251700	-0.99335400
C	-0.16036800	4.12171100	-1.22336200
C	1.75874500	-3.69509800	-1.39250900
C	-1.63767400	3.97560000	-0.79266100
C	0.30105500	-4.16690100	-1.29374500
C	2.67828600	-1.33824700	-1.62164500
C	-3.04644600	1.79593300	-0.58273300
C	-1.82092000	-2.87157300	-0.75976300
C	2.99215200	2.41596200	-1.58179100
C	3.58413400	1.06942500	-2.06342700
C	-4.48941800	-0.28686300	-0.40160100
C	-4.09740500	-1.77127600	-0.46518600
C	1.49056000	2.10899800	-1.60970300
H	1.12271400	2.18947500	-2.64510500
C	2.53659500	0.06983900	-1.61030700
C	-3.16382900	0.43633300	-0.50915600
C	-2.59236100	-1.72909500	-0.59053300
H	3.32124000	2.63093700	-0.55826600
H	3.27055900	3.25959900	-2.21757000
H	4.56972300	0.84218900	-1.64573500
H	3.68150400	1.03644300	-3.15750100
H	-4.98400300	-0.02463600	0.53972000
H	-5.16394800	0.00902500	-1.21130200
H	-4.38268900	-2.32584200	0.43585000
H	-4.54297200	-2.29716700	-1.31637200
H	3.64214500	-1.76241000	-1.88037600
H	-3.95364800	2.39021100	-0.57525200
H	-2.33992900	-3.82434500	-0.76396400
H	0.31815000	5.01257000	-0.81092100
H	-0.09095000	4.17579400	-2.31587400
H	2.35539700	-4.03762700	-0.53872800
H	2.26709800	-4.03547500	-2.29890900
H	-1.82557200	4.43176000	0.18911300
H	-2.34821100	4.42128900	-1.49514000
H	0.13543300	-4.91100700	-0.50817400
H	-0.06175600	-4.60576100	-2.23083900
C	-0.01714600	-0.08146400	1.45551300
C	1.35144000	0.41520000	2.00645800
Cl	2.71437200	-0.66423300	1.56172000
Cl	1.38796500	0.64292000	3.79559900
Cl	-1.27832100	0.99561500	2.19237700
H	1.56815800	1.38897200	1.57526800
Cl	-0.33597000	-1.74146000	2.06384100

Base-off Tetrachloroethylcob(II)alamin

Co	-0.30120700	0.09655200	-0.69973900
N	-0.28867700	1.98988400	-0.56104500
N	1.40349500	0.41216900	-1.48009100
N	-0.18030800	-1.77994700	-1.17733500
N	-2.24972500	0.05298100	-0.48552600
C	1.02102100	2.65633000	-0.71747000
H	1.55828800	2.59584300	0.23985000
C	0.98750200	-2.42450600	-1.54236200
C	-1.26336900	2.85003000	-0.45274800
C	-1.19321400	-2.66292200	-1.09314300
C	0.66759600	4.11695600	-1.06267500
C	0.78465200	-3.92669800	-1.53201400
C	-0.75729500	4.28029500	-0.48362000
C	-0.74127600	-4.07415000	-1.40932000
C	2.16800000	-1.81458000	-1.87414700
C	-2.62524200	2.46326900	-0.30859000
C	-2.51595400	-2.34203000	-0.79873400
C	3.30080800	1.78169600	-1.82539600
C	3.56771400	0.35227100	-2.35995900
C	-4.50071400	0.75199600	-0.11693100
C	-4.47377100	-0.77193700	-0.32778000
C	1.76475300	1.81598600	-1.75904800
H	1.35367100	2.08092900	-2.74779800
C	2.33833700	-0.40188000	-1.88316000
C	-3.05125700	1.16102000	-0.30687500
C	-3.00175300	-1.06477800	-0.54326000
H	3.72071700	1.88612200	-0.81839100
H	3.72427400	2.56561900	-2.45972200
H	4.49360600	-0.09091800	-1.97908800
H	3.62598900	0.33270700	-3.45781000
H	-4.83363400	1.02256400	0.89128400
H	-5.15818100	1.26962400	-0.82340400
H	-4.85142300	-1.32749200	0.53761400
H	-5.06457200	-1.09107700	-1.19448500
H	3.01053600	-2.43929700	-2.15173300
H	-3.36656100	3.24596200	-0.18467600
H	-3.23279100	-3.15725300	-0.79029900
H	1.38239700	4.83602200	-0.65357900
H	0.64555600	4.24710100	-2.15178700
H	1.29592500	-4.35066000	-0.65944000
H	1.20237000	-4.40623000	-2.42237900
H	-0.73668600	4.68012200	0.53971900
H	-1.39786700	4.94229600	-1.07552700
H	-1.04767900	-4.76962500	-0.62160400
H	-1.20173900	-4.42082600	-2.34338500
C	0.14570700	-0.25886300	1.54390900
C	1.47561600	0.15674600	2.13645200
Cl	2.86738900	-0.72766600	1.37964500
Cl	1.70626800	0.02864100	3.97667100
Cl	-1.07988700	0.80541800	2.45147000
H	1.64099000	1.21245000	1.93616200
Cl	-0.20031700	-1.99239300	2.04590000

Base-off 1,1,2-Trichloroethylcob(III)alamin

Co	-0.03504900	0.10562200	-0.50386900
N	1.27389200	1.47323100	-0.50401700
N	1.46749800	-0.94222300	-1.01300300
N	-1.19144100	-1.39316600	-0.94688500
N	-1.45991600	1.41207100	-0.57610100
C	2.69484500	1.04953000	-0.48946100
H	2.96068900	0.80579000	0.54998900
C	-0.78246700	-2.71051800	-1.07947400
C	1.16178000	2.77380100	-0.51410200
C	-2.53982000	-1.31965800	-1.06412100
C	3.45768200	2.29765900	-0.96702900
C	-1.97700300	-3.63689600	-1.14429500
C	2.51423600	3.45251900	-0.55665700
C	-3.15723600	-2.67178700	-1.33697100
C	0.52028200	-3.13137000	-1.16301500
C	-0.09334100	3.43877300	-0.45464600
C	-3.28271900	-0.15284300	-0.96817000
C	3.81036300	-1.28663600	-1.16379700
C	3.05043700	-2.57973400	-1.54872500
C	-2.63697200	3.48336300	-0.41026100
C	-3.63496600	2.35907900	-0.72935000
C	2.72422200	-0.21490100	-1.33784800
H	2.66255000	0.08679700	-2.39506400
C	1.61316900	-2.22731200	-1.21480700
C	-1.29437400	2.78772500	-0.46739200
C	-2.76754000	1.12146200	-0.75139300
H	4.13506700	-1.33447200	-0.11755800
H	4.69088100	-1.10753400	-1.78492500
H	3.39039700	-3.47057800	-1.01144800
H	3.13722100	-2.80001200	-2.62161200
H	-2.79368700	3.89513500	0.59352400
H	-2.68743400	4.31977300	-1.11302300
H	-4.43098600	2.26011500	0.01579400
H	-4.12370800	2.49374000	-1.70154300
H	0.71598000	-4.19201300	-1.27524500
H	-0.09631600	4.52238600	-0.41192500
H	-4.35767900	-0.23745600	-1.08853100
H	4.45262200	2.38108600	-0.52433600
H	3.57130300	2.27444800	-2.05716400
H	-2.06138200	-4.19116400	-0.20150600
H	-1.87680100	-4.37441300	-1.94505100
H	2.75145400	3.83672900	0.44516500
H	2.53474900	4.30518600	-1.24185200
H	-3.99808600	-2.86630300	-0.66470100
H	-3.55078800	-2.70163400	-2.36058600
C	-0.09108600	-0.16163200	1.49530400
C	0.90395500	-1.25013500	1.88883400
Cl	0.94571800	-1.66018800	3.64904100
Cl	0.30528000	1.36678300	2.37050200
H	1.91173100	-0.93317800	1.62816800
Cl	-1.74759700	-0.64920800	2.01978200
H	0.65982900	-2.17211300	1.36370600

Base-off 1,1,2-Trichloroethylcob(II)alamin

Co	-0.07956000	0.15574300	-0.60718000
N	1.04281200	1.66905800	-0.50211600
N	1.52742900	-0.66418100	-1.21124500
N	-1.07289700	-1.45850500	-1.03527200
N	-1.67656700	1.28046600	-0.51780700
C	2.49678600	1.41087600	-0.51091900
H	2.78417800	1.10797500	0.50616800
C	-0.50101700	-2.69427500	-1.26454700
C	0.77815400	2.93978300	-0.40704100
C	-2.41927700	-1.54929000	-1.08353500
C	3.11410100	2.77505400	-0.87151600
C	-1.56899100	-3.77151800	-1.29901300
C	2.04412200	3.77516500	-0.37159100
C	-2.87616600	-2.96406100	-1.37960700
C	0.83860300	-2.93816900	-1.44351400
C	-0.55231500	3.44364600	-0.31406400
C	-3.29853400	-0.48581200	-0.92233300
C	3.88989100	-0.71940800	-1.34895700
C	3.29373600	-2.07171100	-1.81582800
C	-3.08561700	3.18370600	-0.22832000
C	-3.95397600	1.95593100	-0.55444400
C	2.68041100	0.22521900	-1.46180900
H	2.59588100	0.60548300	-2.49337300
C	1.82278600	-1.90802400	-1.46970300
C	-1.66853100	2.65296000	-0.34917800
C	-2.93784800	0.83583200	-0.66514500
H	4.21169600	-0.79264500	-0.30307600
H	4.74697800	-0.39737300	-1.94703100
H	3.74172000	-2.94165300	-1.32416100
H	3.41583200	-2.21595500	-2.89901400
H	-3.25855000	3.54439400	0.79224000
H	-3.26072100	4.02783500	-0.90292000
H	-4.69324100	1.73404300	0.22254400
H	-4.50458600	2.06914100	-1.49644800
H	1.15622600	-3.96107400	-1.61735100
H	-0.68523400	4.51489300	-0.20283900
H	-4.35925500	-0.70251000	-1.00330200
H	4.09554600	2.93392500	-0.41662200
H	3.22685700	2.85933700	-1.95981700
H	-1.52275400	-4.36095600	-0.37499700
H	-1.42799800	-4.46435700	-2.13395300
H	2.23893300	4.09042800	0.66283500
H	1.97122300	4.68272500	-0.98009400
H	-3.63598100	-3.29390700	-0.66433700
H	-3.32916000	-3.01452300	-2.37814300
C	0.02867300	-0.29513800	1.58591000
C	1.02066100	-1.37456500	1.87342400
Cl	1.26669200	-1.96296600	3.63591600
Cl	0.48819900	1.19862200	2.57803900
H	2.01675600	-1.05029100	1.57256100
Cl	-1.62213500	-0.83826300	2.20231700
H	0.74758900	-2.28073100	1.33382600

Base-off 1,2,2-Trichloroethylcob(III)alamin

Co	-0.28261200	0.07238200	-0.55909200
N	-0.14766700	1.94852600	-0.43034300
N	1.49129500	0.25232200	-1.18116000
N	-0.25019400	-1.81810700	-1.01650300
N	-2.21190100	0.15112000	-0.40492000
C	1.21645200	2.53203600	-0.48422500
H	1.65455900	2.44258400	0.51757000
C	0.88620600	-2.55101300	-1.32364800
C	-1.06089100	2.87311600	-0.31796700
C	-1.32516000	-2.64245500	-0.94528100
C	0.97111100	4.00363000	-0.85892300
C	0.56502000	-4.02809700	-1.42675400
C	-0.45540500	4.26114000	-0.31898200
C	-0.96252800	-4.07710000	-1.25686400
C	2.13885700	-2.02589100	-1.51029900
C	-2.44687300	2.57651500	-0.18574600
C	-2.61662300	-2.23676600	-0.64208200
C	3.50314500	1.49321900	-1.40789400
C	3.71074600	0.03499200	-1.88712800
C	-4.42690500	0.98385000	-0.06001800
C	-4.47641100	-0.54577200	-0.20953700
C	1.97439100	1.63323800	-1.45372500
H	1.65156600	1.88992800	-2.47503200
C	2.40370500	-0.62844500	-1.49864600
C	-2.95594900	1.31044300	-0.21267100
C	-3.02850800	-0.92235700	-0.42587100
H	3.86165300	1.60563400	-0.37979500
H	4.01604100	2.22463900	-2.03651900
H	4.57233000	-0.46099600	-1.42946800
H	3.84589700	-0.02497700	-2.97596500
H	-4.79096600	1.32112400	0.91599500
H	-5.02185600	1.50075700	-0.81982200
H	-4.87064900	-1.04920400	0.68029300
H	-5.08947500	-0.87445200	-1.05588400
H	2.95312500	-2.70418000	-1.74112400
H	-3.13564700	3.40455400	-0.05803500
H	-3.38366700	-3.00387500	-0.61775600
H	1.71630700	4.67873900	-0.43253100
H	0.98676400	4.12403100	-1.94865000
H	1.08685500	-4.58442100	-0.63995500
H	0.90277900	-4.43760100	-2.38352000
H	-0.43891700	4.64417900	0.71083600
H	-1.03454800	4.97052900	-0.91769200
H	-1.28773900	-4.74505900	-0.45268400
H	-1.47532800	-4.40544400	-2.16831800
C	-0.09425300	-0.38872500	1.35733700
C	1.26803200	-0.92531900	1.78835300
Cl	1.08542600	-1.99721200	3.24034500
Cl	2.51676600	0.32686000	2.11556600
Cl	-0.71231400	0.85834100	2.48355700
H	1.67947200	-1.56546300	1.01266700
H	-0.79563200	-1.21959700	1.43382800

Base-off 1,2,2-Trichloroethylcob(II)alamin

Co	-0.36739300	0.03389300	-0.61989700
N	-0.49933400	1.90076800	-0.44145100
N	1.30860200	0.47883400	-1.38618200
N	-0.09516200	-1.83996900	-1.06249700
N	-2.28963400	-0.17100200	-0.30347600
C	0.76985700	2.65151300	-0.53504300
H	1.28295200	2.55142300	0.42991700
C	1.11326500	-2.38850400	-1.45400400
C	-1.51404600	2.68622400	-0.22996300
C	-1.03133100	-2.80348000	-0.93519500
C	0.32328800	4.10357400	-0.79198200
C	1.01759500	-3.90404600	-1.50326600
C	-1.09310400	4.14235700	-0.16908100
C	-0.48266900	-4.17335900	-1.28673300
C	2.25227000	-1.68396400	-1.74816900
C	-2.84275100	2.19591800	-0.04944600
C	-2.35364900	-2.58854300	-0.55815400
C	3.11547000	1.99214400	-1.64646300
C	3.50726400	0.58820500	-2.17402500
C	-4.58276200	0.34086600	0.12805200
C	-4.41126400	-1.18638600	0.03035500
C	1.57894900	1.91450300	-1.60716600
H	1.15961800	2.18525900	-2.59042300
C	2.31975700	-0.25715400	-1.74731300
C	-3.17250900	0.86936100	-0.07411100
C	-2.93826800	-1.34838100	-0.29404700
H	3.50537000	2.12899600	-0.63281800
H	3.48782600	2.80554400	-2.27565900
H	4.44870000	0.21459400	-1.75791000
H	3.60965800	0.57582200	-3.26884400
H	-4.98041700	0.65955100	1.09712300
H	-5.25891800	0.73225800	-0.64052600
H	-4.64900800	-1.69548000	0.97195900
H	-5.03979900	-1.64094000	-0.74360600
H	3.14048300	-2.23992400	-2.03079300
H	-3.63254000	2.91830000	0.13028500
H	-2.99891000	-3.45999000	-0.50153900
H	1.00216000	4.84178800	-0.35677200
H	0.26277900	4.29327500	-1.87126300
H	1.62727600	-4.34337400	-0.70471700
H	1.39552900	-4.30176800	-2.45027800
H	-1.06358500	4.46496200	0.88083200
H	-1.78716800	4.80726700	-0.69414300
H	-0.68127500	-4.89782600	-0.49003800
H	-0.96946300	-4.55503600	-2.19295700
C	0.11962800	-0.37209200	1.49169500
C	1.48848600	-0.80316700	1.82117400
Cl	1.69693000	-1.77446800	3.46470600
Cl	2.74025300	0.51218600	1.85624000
Cl	-0.51553400	0.87282400	2.68119100
H	1.84310900	-1.53180800	1.09678800
H	-0.52494500	-1.24118900	1.64882100

Base-off 1,2-Dichloroethylcob(III)alamin

Co	-0.08810900	-0.05403900	-0.45309000
N	-1.54517000	1.13637000	-0.35309900
N	0.84174000	1.54583600	-0.84909400
N	1.51407600	-1.08560700	-0.82797100
N	-1.26776000	-1.58038700	-0.53142500
C	-1.22526800	2.57640700	-0.20963000
H	-0.98617000	2.76233000	0.84791500
C	2.78715800	-0.56345700	-0.99009500
C	-2.83245600	0.92766800	-0.38491800
C	1.56613100	-2.44119700	-0.83627300
C	-2.52976000	3.28683600	-0.61423900
C	3.81764400	-1.66992200	-1.08571500
C	-3.61187800	2.22348100	-0.30970700
C	2.97416000	-2.95472500	-1.03696300
C	3.09437500	0.77168000	-1.06098100
C	-3.39790900	-0.37676400	-0.44668300
C	0.46766200	-3.27712100	-0.69596900
C	1.02303900	3.90901800	-0.79813600
C	2.35763700	3.27730600	-1.26521800
C	-3.25040200	-2.91495500	-0.55039800
C	-2.01811000	-3.83490200	-0.54144400
C	0.02562400	2.77102300	-1.05901800
H	-0.28357300	2.78056400	-2.11589500
C	2.11162000	1.79691000	-1.04177600
C	-2.65623900	-1.52268500	-0.49596700
C	-0.85980900	-2.86513000	-0.58985600
H	1.06749800	4.13737400	0.27336100
H	0.77424100	4.82837200	-1.33310100
H	3.23457400	3.63728900	-0.71842200
H	2.54516800	3.46440000	-2.33166200
H	-3.91491000	-3.08590800	0.30201600
H	-3.85300000	-3.03853200	-1.45680100
H	-1.95503100	-4.44430300	0.36780100
H	-1.98710100	-4.52710300	-1.38918400
H	4.13401600	1.05461300	-1.18510500
H	-4.47891500	-0.46487600	-0.44782500
H	0.65220000	-4.34609200	-0.71891400
H	-2.68784300	4.22259000	-0.07366600
H	-2.51720400	3.51262600	-1.68693800
H	4.52473100	-1.60367000	-0.25152600
H	4.40246200	-1.57911000	-2.00635300
H	-4.02146500	2.33534000	0.70368200
H	-4.45824700	2.24467400	-1.00280500
H	3.26039500	-3.62685200	-0.22110600
H	3.03834500	-3.53660800	-1.96336100
C	0.20778600	-0.27943700	1.49118000
C	1.25860900	0.65804600	2.04429200
Cl	1.87130600	0.09950800	3.66532200
Cl	-1.30154300	-0.18207100	2.46924700
H	2.13351500	0.68083600	1.39735300
H	0.53456400	-1.31653300	1.56624200
H	0.87683200	1.66925100	2.18629700

Base-off 1,2-Dichloroethylcob(II)alamin

Co	0.12862700	0.08979400	-0.51473600
N	1.38918300	-1.29797700	-0.41959700
N	-1.00880200	-1.32558200	-1.07025300
N	-1.28136400	1.38391900	-0.84305500
N	1.54723800	1.43635600	-0.44049300
C	0.83911700	-2.66572900	-0.34630300
H	0.50517800	-2.83131300	0.68794700
C	-2.60598800	1.06454400	-1.07673300
C	2.68950300	-1.29378000	-0.37267900
C	-1.12270100	2.72275900	-0.78208200
C	2.03769300	-3.56901300	-0.69504400
C	-3.46364400	2.31839600	-1.08062200
C	3.25288500	-2.69995900	-0.29011500
C	-2.43139400	3.45768800	-1.00134100
C	-3.10482900	-0.19956800	-1.26705200
C	3.45466800	-0.08927000	-0.36524100
C	0.08910800	3.37627000	-0.57740800
C	-1.54970400	-3.63008000	-1.08667200
C	-2.76139400	-2.79163400	-1.56747600
C	3.70811300	2.44854800	-0.35900300
C	2.62920500	3.54599700	-0.30712100
C	-0.38087300	-2.64698300	-1.27281900
H	-0.01397500	-2.69148500	-2.31165700
C	-2.29334300	-1.37282400	-1.28841600
C	2.90073300	1.16142400	-0.38078100
C	1.33711100	2.76419400	-0.44942500
H	-1.66399600	-3.87741400	-0.02442000
H	-1.42335600	-4.56308400	-1.64312300
H	-3.69494500	-3.03260100	-1.04808700
H	-2.94651200	-2.92827000	-2.64286900
H	4.38276000	2.47325700	0.50264500
H	4.33159400	2.52747200	-1.25737300
H	2.63470600	4.08859800	0.64607100
H	2.73496500	4.29468100	-1.09986600
H	-4.17249100	-0.30949200	-1.42821300
H	4.53604600	-0.17239000	-0.32542100
H	0.06695000	4.46166100	-0.55568300
H	2.01018500	-4.53286800	-0.17962300
H	2.05879300	-3.76330900	-1.77485000
H	-4.13296400	2.31490400	-0.21227900
H	-4.09589600	2.37105100	-1.97269400
H	3.56792200	-2.90192200	0.74288300
H	4.12920800	-2.84448300	-0.93101900
H	-2.63032400	4.16299000	-0.18750600
H	-2.38801700	4.04433000	-1.92743000
C	-0.24931300	0.17393500	1.64226900
C	-1.46447900	-0.54212800	2.05007100
Cl	-2.18303200	-0.14491900	3.80543700
Cl	1.19047200	-0.36276500	2.67406200
H	-2.30774000	-0.27830700	1.41257600
H	-0.32644100	1.24536700	1.83718900
H	-1.34769400	-1.62490700	2.09692200

Base-off Methylcob(III)alamin
See: *JACS*, **2005**, *127*, 384-396.

Base-off Methylcob(II)alamin
See: *JACS*, **2005**, *127*, 384-396.

Tetrachloroethyl radical

C	-0.72112100	-0.19274700	-0.22123800
C	0.62537200	0.36407300	-0.48826900
H	0.59027700	1.00674400	-1.36490500
Cl	-2.07885400	0.74638700	-0.71545000
Cl	-0.96658900	-1.38070300	0.98684600
Cl	1.21336700	1.44011000	0.87925200
Cl	1.83114800	-0.92548300	-0.81994500

1,1,2-Trichloroethyl radical

C	-0.51278800	0.00013300	0.41745400
C	0.85375400	-0.00128200	0.95804800
H	1.03739900	-0.89885000	1.54813000
Cl	-1.20608300	-1.47054600	-0.15515300
Cl	2.16742000	-0.00058700	-0.35787700
Cl	-1.20379400	1.47178400	-0.15470100
H	1.03857900	0.89466100	1.55026700

1,2,2-Trichloroethyl radical

C	-0.79674400	-0.52528600	0.47532500
C	0.35207300	-0.08665300	-0.32477800
H	0.15116400	-0.09430500	-1.39383100
Cl	-2.38505600	-0.22328300	-0.09896700
Cl	0.81648400	1.66120000	0.05765400
Cl	1.75776900	-1.17034700	-0.01937800
H	-0.69949400	-0.78275600	1.52230000

1,2-Dichloroethyl radical

C	0.64731000	0.73539100	0.41306000
C	-0.57721800	0.87705500	-0.37097800
Cl	-1.85620300	-0.42065700	0.07153000
Cl	1.87635100	-0.36374200	-0.07665900
H	-1.07080800	1.82704800	-0.16150700
H	0.72374700	1.07825400	1.43786500
H	-0.41601600	0.75480400	-1.44165000

Methyl radical
See: *JACS*, **2005**, *127*, 384-396.

Table S2. Raw data for Co-C BDE calculations.

	Ee	*ZPE*	*E(0K)*	*Hvib*	*H(298K)*
Methylcobalamin	-2604.541180	0.489019	-2604.061648	0.515625	-2604.035485
(U)BP86	-2604.761457				-2604.255762
1,2-Dichloroethylcobalamin	-3563.030982	0.500607	-3562.540087	0.530516	-3562.510685
(U)BP86	-3563.313792				-3562.793495
1,2,2-Trichloroethylcobalamin	-4022.612052	0.491035	-4022.130543	0.522046	-4022.100061
(U)BP86	-4022.928045				-4022.416053
1,1,2Trichloroethylcobalamin	-4022.605593	0.490461	-4022.124647	0.521428	-4022.094207
(U)BP86	-4022.922477				-4022.411091
Tetrachloroethylcobalamin	-4482.172807	0.480146	-4481.701976	0.512305	-4481.670368
(U)BP86	-4482.522928				-4482.020489
Cob(II)alamin	-2564.661533	0.450862	-2564.219417	0.475696	-2564.194992
(U)BP86	-2564.867107				-2564.400566
Methyl	-39.837517	0.029822	-39.808274	0.033868	-39.804233
(U)BP86	-39.830288				-39.797006
1,2-Dichloroethyl	-998.347533	0.044459	-998.303937	0.050377	-998.298060
(U)BP86	-998.403089				-998.353616
1,2,2-Trichloroethyl	-1457.930211	0.034859	-1457.896028	0.041842	-1457.889107
(U)BP86	-1458.018995				-1457.977891
1,1,2-Trichloroethyl	-1457.937619	0.035820	-1457.902494	0.042668	-1457.895705
(U)BP86	-1458.026706				-1457.984792
Tetrachloroethyl	-1917.516894	0.026130	-1917.491271	0.034109	-1917.483374
(U)BP86	-1917.639435				-1917.605914

Table S2. Raw data redox calculations.

	Ee	*Gcorr*	*G*	*Gsolv*	*Ee (plus electron)*
Methylcob(III)alamin	-2604.541180	0.434642	-2604.106538	-33.58	-2604.66611
baseoff	-2378.308198	0.36772	-2377.940478	-37.75	-2378.446608
Methylcob(II)alamin	-2604.671653	0.429247	-2604.242406	-4.10	
baseoff	-2378.452048	0.363205	-2378.088843	-4.35	
1,2-Dichloroethylcob(III)alamin	-3563.030982	0.441677	-3562.589305	-36.23	-3563.168206
baseoff	-3336.796937	0.373272	-3336.423665	-40.23	-3336.947628
1,2-Dichloroethylcob(II)alamin	-3563.174228	0.437365	-3562.736863	-4.66	
baseoff	-3336.959462	0.366796	-3336.592666	-10.14	
1,2,2-Trichloroethylcob(III)alamin	-4022.612052	0.430624	-4022.181428	-32.65	-4022.750565
baseoff	-3796.376964	0.362035	-3796.014929	-35.56	-3796.534438
1,2,2-Trichloroethylcob(II)alamin	-4022.756642	0.426477	-4022.330165	-0.71	
baseoff	-3796.547563	0.35645	-3796.191113	-5.79	
1,1,2-Trichloroethylcob(III)alamin	-4022.605593	0.431073	-4022.17452	-39.54	-4022.744278
			guess=alter		-4022.739788
baseoff	-3796.372125	0.363063	-3796.009062	-40.49	-3796.540363
1,1,2-Trichloroethylcob(II)alamin	-4022.750031	0.425564	-4022.324467	-5.53	
baseoff	-3796.551488	0.356903	-3796.194585	-9.21	
Tetrachloroethylcob(III)alamin	-4482.172807				-4482.317507
baseoff	-4255.940978	0.350633	-4255.590345	-39.47	
Tetrachloroethylcob(II)alamin					
baseoff	-4256.130802	0.344789	-4255.786013	-7.46	