Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Outer-Sphere Electron Transfer Does Not Underpin B_{12}-Dependent Olefinic Reductive Dehalogenation in Anaerobes

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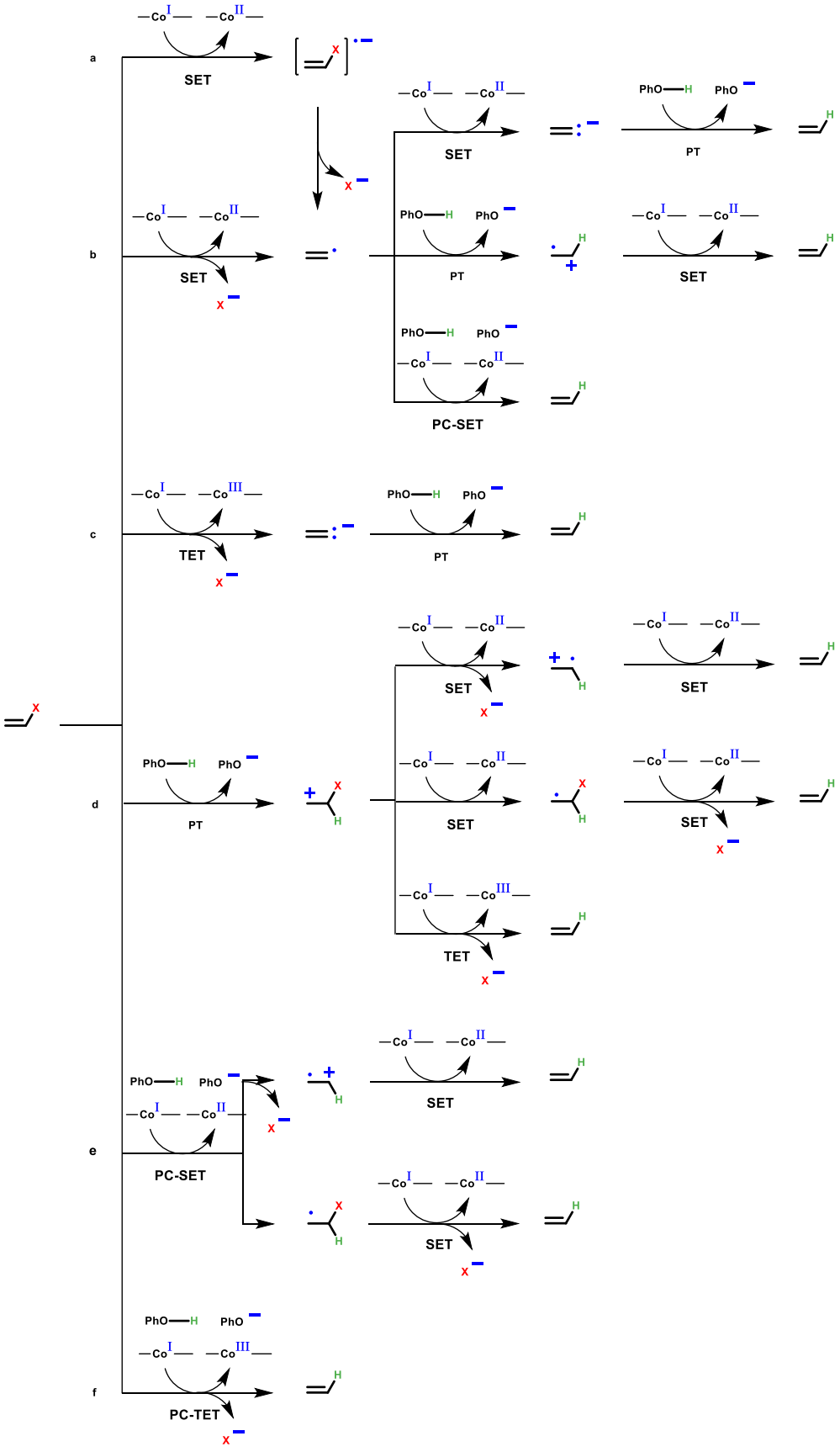
I. Schematic Representation of Outer-Sphere Electron Transfer Routes

The full reaction routes potentially underlying B_{12}-dependent olefinic reductive dehalogenation within the framework of outer-sphere electron transfer is illustrated in Scheme S1.

Scheme S1. Alternative outer-sphere electron transfer routes for B_{12}-dependent reductive dehalogenation of olefins[a]


a
SET
b
SET
PT
SET
PC-SET
c
TET
PT
d
SET
PT
SET
SET
TET
e
PC-SET
SET
SET
f
PC-TET

II. Experimental Data Set

The experimental data set consists of dehalogenation pathways of 6 chlorinated ethenes 4 brominated ethenes and 1 fluorinated ethene mediated by *Sulfurospirillum multivorans*, *Dehalococcoides mccartyi* strain 195, *Desulfitobacterium* sp. PCE-S, and *Sporomusa ovata* strain H1 (Table S1). Larger experimental data set was not constructed. Because halogenated olefins were reductively metabolized by bacterial species mainly from phyla of Protobacteria, Chloroflexi, and Firmicutes[1], covering *S. multivorans*, *D. mccartyi* strain 195, *D.* sp. PCE-S, and *S. ovata* strain H1, respectively.

Table S1. Experimental dehalogenation pathways

phylum	strain	parent substrate	one step product	reference
Protobacteria	*Sulfurospirillum multivorans*	TCE	*cis*-DCE	2, 3
		PCE	TCE	2, 3
		cis-DBE	VB	4
		trans-DBE	VB	4
		TBE[a]	***cis*-DBE**, 1,1-DBE, *trans*-DBE	4
Chloroflexi	*Dehalococcoides mccartyi* 195	VC	ethene	5, 6
		1,1-DCE	VC	6
		cis-DCE	VC	6
		trans-DCE	VC	6
		TCE	1,1-DCE, ***cis*-DCE**, *trans*-DCE	6
		PCE	TCE	5, 6
Firmicutes	*Desulfitobacterium* sp. PCE-S	TCE	*cis*-DCE	7
		PCE	TCE	7
		VB	ethene	4
		cis-DBE	VB	4
		trans-DBE	VB	4
Firmicutes	*Sporomusa ovata* strain H1	TFE	*cis*-DFE	8

[a]Substrate tested with reductive dehalogenase. Products in bold are major products.

III. Energetic Difference of Radical Anions at Distinct Symmetries

The highly symmetric radical anions would subject to pseudo-Jahn-Teller distortions, which would affect the magnitudes of free energy barriers and thus would alter the conclusion. Regarding this issue, we studied the ground state free energy difference of radical anions of perhalogenated ethenes (PFE, PCE, and PBE) at C_1 and D_{2h} symmetries, considering density functionals (BP86, PBE, PBE0, TPSS, and TPSSh) at distinct levels of Jacob's ladder. The C_1 symmetry was assigned by computational algorithm; while the D_{2h} is the highest possible symmetry of radical anions of perhalogenated ethenes. The respective free energy differences were given in Table S2.

Table S2. Free energy differences (eV) of radical anions at distinct symmetries

compound	symmetry	BP86	PBE	PBE0	TPSS	TPSSh
PFE	C_1	0.00	0.00	0.00	0.00	0.00
	D_{2h}	2.15	1.81	1.77	1.87	1.85
PCE	C_1	0.00	0.00	0.00	0.00	0.00
	D_{2h}	1.34	1.29	1.09	1.37	1.28
PBE	C_1	0.00	0.00	0.00	0.00	0.00
	D_{2h}	0.64	0.64	0.94	0.68	0.80

Energies of radical anions at C_1 symmetry were taken as references. The calculations were done at the theoretical levels of above functionals with basis set Def2SVP.

IV. Free Energy Barriers of Outer-Sphere Electron Transfer.

The free energy barrier of outer-sphere ET ($\Delta G^{\neq}_{\mathrm{OS-ET}}$) was calculated according to Marcus theory,[9, 10] which defines the $\Delta G^{\neq}_{\mathrm{OS-ET}}$ in terms of intrinsic barrier (λ) and corrected driving force ($\Delta G^{\mathrm{corr.}}$) of the reaction.

$$\Delta G^{\neq}_{\mathrm{OS-ET}} = \frac{(\lambda + \Delta G^{\mathrm{corr.}})^2}{4\lambda}$$

The term λ is raised by geometry distortions of reactants (λ_{i}) and their surrounding solvent (λ_{s}).

$$\lambda = \lambda_{\mathrm{i}} + \lambda_{\mathrm{s}}$$

Regarding non-dissociative reaction, its λ_{i} was calculated via Nelsen's four-point scheme.[11]

$$\lambda_{\mathrm{i}} = \frac{\lambda_{\mathrm{i,D}} + \lambda_{\mathrm{i,A}}}{2}$$

$$\lambda_{\mathrm{i,D}} = E(\mathrm{D}^+|\mathrm{D}) - E(\mathrm{D}|\mathrm{D}) + E(\mathrm{D}|\mathrm{D}^+) - E(\mathrm{D}^+|\mathrm{D}^+)$$

$$\lambda_{\mathrm{i,A}} = E(\mathrm{A}^-|\mathrm{A}) - E(\mathrm{A}|\mathrm{A}) + E(\mathrm{A}|\mathrm{A}^-) - E(\mathrm{A}^-|\mathrm{A}^-)$$

Here the $\lambda_{\mathrm{i,D}}$ and $\lambda_{\mathrm{i,A}}$ are the reorganization energies of electron donor and acceptor. $E(\mathrm{D}^+|\mathrm{D})$ and its analogues depict the vertical energy of D^+ at geometry of D. The λ_{i} was treated by arithmetic mean instead of other average schemes proposed recently.[12] Because distinct average approaches goes to the consistent conclusion for outer-sphere ET reactions and arithmetic mean for calculating λ_{i} is widely applied.[13]

By contrast, the λ_{i} of dissociative reaction was calculated via Savéant method,[14] which splits the λ_{i} into two contributors, $\lambda_{\mathrm{i,D}}$ and the carbon-halogen bond dissociation energy of substrate ($\mathrm{BDE}_{\mathrm{C-X}}$ here).

$$\lambda_{\mathrm{i}} = \lambda_{\mathrm{i,D}} + \mathrm{BDE}_{\mathrm{C-X}}$$

The external contribution of the intrinsic barrier resulted from solvent, λ_{s}, is characterized by

$$\lambda_{\mathrm{s}} = \frac{(\Delta e)^2}{4\pi\varepsilon_0}\left(\frac{1}{2r_{\mathrm{D}}} + \frac{1}{2r_{\mathrm{A}}} - \frac{1}{2r_{\mathrm{DA}}}\right)\left(\frac{1}{\varepsilon_{\mathrm{op}}} - \frac{1}{\varepsilon_{\mathrm{s}}}\right)$$

where r_{D} and r_{A} are the non-penetrating hard sphere radii of electron donor and acceptor. r_{DA} is the sum of r_{D} and r_{A}, representing the center-to-center distance between the electron donor and acceptor. The half of the longest point-to-point distances of the electron donor and acceptor respectively give r_{D} and r_{A}. $\varepsilon_{\mathrm{op}}$ and ε_{s} are the optical and static dielectric constants of proteins ($\varepsilon_{\mathrm{op}}$ = 2.41 and ε_{s} = 4.0).[13]

The $\Delta G^{\mathrm{corr.}}$calibrates the free energy of the reaction (ΔG) with electrostatic interactions (w) of electron donor and acceptor before and after the reaction event.[10]

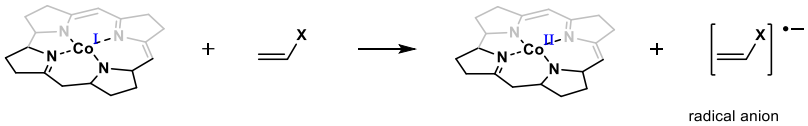
$$\Delta G^{\mathrm{corr.}} = w + \Delta G$$

$$w = (Z_{\mathrm{D}} - Z_{\mathrm{A}} - 1)\frac{e^2}{\varepsilon_{\mathrm{s}} * r_{\mathrm{DA}}}$$

Here Z_{D} and Z_{A} refer to the charges of individual electron donor and acceptor. The free energy barriers of the initial PT and PC-ET reactions were calculated by the analogue way as ET and thus were not articulated.[15-17] The reaction with free energy barrier smaller than 20 kcal/mol is feasible at physiological condition.[13]

The free energy barriers of non-dissociative SET, dissociative SET, TET, PT, non-dissociative PC-SET, dissociative PC-SET, and PC-TET covering full congeners of fluorinated, chlorinated, and brominated ethenes are given in Tables S3-S9.

Table S3. Free energy barriers (kcal/mol) of the outer-sphere non-dissociative single-electron transfer ($\Delta G^{\neq}_{\mathrm{oSET}}$), considering four averages of internal reorganization energy proposed recently[12]

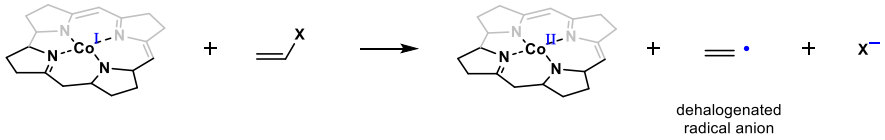


substrate	radical anion	$\Delta G^{\neq}_{\mathrm{oSET}}$				radical anion	$\Delta G^{\neq}_{\mathrm{oSET}}$				radical anion	$\Delta G^{\neq}_{\mathrm{oSET}}$			
		$\bar{\lambda}_{i,1}$	$\bar{\lambda}_{i,2}$	$\bar{\lambda}_{i,3}$	$\bar{\lambda}_{i,4}$		$\overline{\lambda_{i,1}}$	$\overline{\lambda_{i,2}}$	$\overline{\lambda_{i,3}}$	$\overline{\lambda_{i,4}}$		$\overline{\lambda_{i,1}}$	$\overline{\lambda_{i,2}}$	$\overline{\lambda_{i,3}}$	$\overline{\lambda_{i,4}}$
VX	VF	79.0	81.3	74.0	80.1	VC	45.8	45.4	47.9	45.6	VB	37.0	36.8	38.4	36.9
1,1-DXE	1,1-DFE	61.0	61.0	60.5	61.0	1,1-DCE	36.4	35.7	39.0	36.0	1,1-DBE	26.5	26.2	27.9	26.3
cis-DXE	*cis*-DFE	60.8	60.9	60.4	60.9	*cis*-DCE	35.9	35.4	38.3	35.6	*cis*-DBE	31.4	31.3	32.3	31.3
trans-DXE	*trans*-DFE	58.9	59.1	58.4	59.0	*trans*-DCE	41.5	40.9	43.8	41.2	*trans*-DBE	25.5	25.4	26.4	25.5
TXE	TFE	52.0	52.0	52.0	52.0	TCE	33.9	33.4	36.0	33.7	TBE	20.7	20.7	21.5	20.7
PXE	PFE	41.3	40.9	39.5	41.1	PCE	29.0	28.6	31.1	28.8	PBE	18.2	18.0	19.2	18.1

Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, PFE = perfluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, PCE = perchloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene, PBE = perbromoethene. The internal reorganization energies, λ_1 and λ_2, are energies of reactants at the geometries of products referred to energies of reactants and energies of products at the geometries of reactants referred to energies of products. $\bar{\lambda}_{i,1}$, $\bar{\lambda}_{i,2}$, and $\bar{\lambda}_{i,3}$ are arithmetic, harmonic, and geometric averages of the λ_1 and λ_2. $\bar{\lambda}_{i,4}$ is the arithmetic average of the $\bar{\lambda}_{i,1}$ and $\bar{\lambda}_{i,2}$.

The free energy barrier ($\Delta G^{\neq}_{\mathrm{oSET}}$) derived from $\bar{\lambda}_{i,1}$, $\bar{\lambda}_{i,2}$, $\bar{\lambda}_{i,3}$, and $\bar{\lambda}_{i,4}$ yield a consistent conclusion: the non-dissociative outer-sphere SET from cob(I)alamin to all above substrates except PBE is not feasible, considering 20 kcal/mol as a free energy barrier threshold of a viable reaction under physiological conditions.[13] It is in line with our recent study, where different average approaches adopted in the free energy barrier calculations of all potential outer-sphere electron transfer routes from cob(I)alamin to aromatics did not alter the feasibility of dehalogenation.[13] For clarity, free energy barriers calculations of other outer-sphere ET routes in the present study are constrained to arithmetic average, $\bar{\lambda}_{i,1}$.

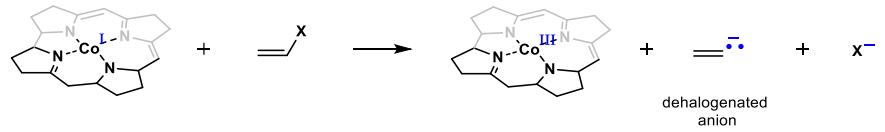
Table S4. Free energy barriers (kcal/mol) of the outer-sphere dissociative single-electron transfer ($\Delta G^{\neq}_{\mathrm{odSET}}$)



substrate	dehalogenated radical anion	$\Delta G^{\neq}_{\mathrm{odSET}}$	dehalogenated radical anion	$\Delta G^{\neq}_{\mathrm{odSET}}$	dehalogenated radical anion	$\Delta G^{\neq}_{\mathrm{odSET}}$
VX	E	58.9	E	43.1	E	35.2
1,1-DXE	VF	62.6	VC	37.3	VB	29.6
cis-DXE	VF	58.2	VC	40.7	VB	35.8
trans-DXE	VF	57.5	VC	43.4	VB	33.8
TXE	*cis*-DFE	64.1	*cis*-DCE	35.9	*cis*-DBE	30.1
	trans-DFE	65.5	*trans*-DCE	37.7	*trans*-DBE	33.0
	1,1-DFE	57.6	1,1-DCE	41.5	1,1-DBE	34.9
PXE	TFE	64.2	TCE	35.2	TBE	30.1

Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, E = ethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene.

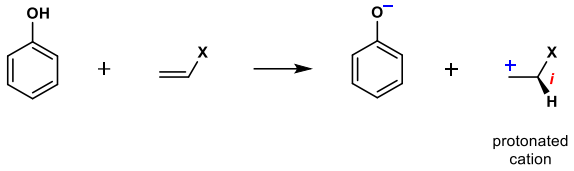
Table S5. Free energy barriers (kcal/mol) of the outer-sphere two-electron transfer ($\Delta G^{\neq}_{\mathrm{oTET}}$)



substrate	dehalogenated anion	$\Delta G^{\neq}_{\mathrm{oTET}}$	dehalogenated anion	$\Delta G^{\neq}_{\mathrm{oTET}}$	dehalogenated anion	$\Delta G^{\neq}_{\mathrm{oTET}}$
VX	E	140	E	121	E	114
1,1-DXE	VF	127	VC	96.5	VB	83.4
cis-DXE	VF	121	VC[a]		VB[a]	
trans-DXE	VF	118	VC[a]		VB[a]	
TXE	*cis*-DFE	115	*cis*-DCE	85.8	*cis*-DBE	71.1
	trans-DFE	116	*trans*-DCE	88.6	*trans*-DBE	74.8
	1,1-DFE	110	1,1-DCE	92.3	1,1-DBE	75.8
PXE	TFE	108	TCE	81.0	TBE	66.1

[a]The geometry optimization of dehalogenated anions derived from *cis*-DCE, *trans*-DCE, *cis*-DBE, and *trans*-DBE gives an acetylene and a halide (chloride and bromide). Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, E = ethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene.

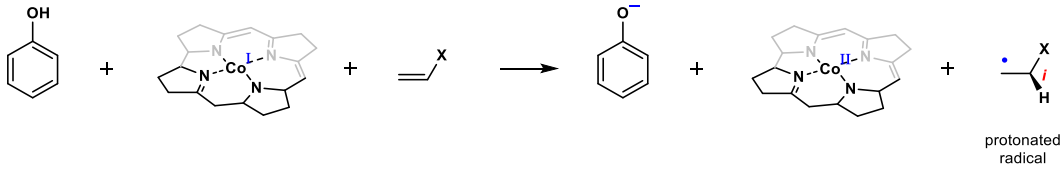
Table S6. Free energy barriers (kcal/mol) of proton transfer ($\Delta G^{\neq}_{\mathrm{PT}}$)



substrate	protonated cation	$\Delta G^{\neq}_{PT}$	protonated cation	$\Delta G^{\neq}_{PT}$	protonated cation	$\Delta G^{\neq}_{PT}$
VX	p_1-VF	88.7	p_1-VC	87.6	p_1-VB	88.1
	p_2-VF	88.7	p_2-VC	87.6	p_2-VB	88.1
1,1-DXE	p_1-1,1-DFE	82.8	p_1-1,1-DCE	81.8	p_1-1,1-DBE	88.3
	p_2-1,1-DFE	82.8	p_2-1,1-DCE	94.4	p_2-1,1-DBE	81.9
cis-DXE	p_1-*cis*-DFE	100	p_1-*cis*-DCE	98.8	p_1-*cis*-DBE	96.5
trans-DXE	p_1-*trans*-DFE	101	p_1-*trans*-DCE	97.5	p_1-*trans*-DBE	90.3
TXE	p_1-TFE	116	p_1-TCE	90.9	p_1-TBE	94.2
	p_2-TFE	92.1	p_2-TCE	100	p_2-TBE	89.6
PXE	p_1-PFE	98.6	p_1-PCE	99.4	p_1-PBE	91.3

Phenol represents tyrosine as proton donor in reductive dehalogenase. p_i gives the position of olefinic carbon protonated. Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, PFE = perfluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, PCE = perchloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene, PBE = perbromoethene.

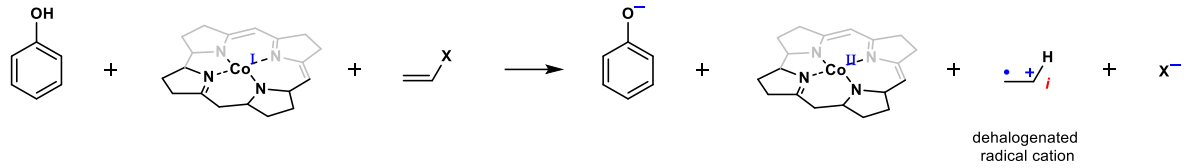
Table S7. Free energy barriers (kcal/mol) of non-dissociative proton-coupled single-electron transfer ($\Delta G^{\neq}_{oPC-SET}$).[a]



substrate	protonated radical	$\Delta G^{\neq}_{oPC-SET}$	protonated radical	$\Delta G^{\neq}_{oPC-SET}$	protonated radical	$\Delta G^{\neq}_{oPC-SET}$
VX	p_1-VF	46.4	p_1-VC	42.6	p_1-VB	40.9
	p_2-VF	43.3	p_2-VC	44.9	p_2-VB	41.2
1,1-DXE	p_1-1,1-DFE	43.7	p_1-1,1-DCE	40.4	p_1-1,1-DBE	41.5
	p_2-1,1-DFE	40.9	p_2-1,1-DCE	45.2	p_2-1,1-DBE	38.8
cis-DXE	p_1-*cis*-DFE	41.8	p_1-*cis*-DCE	40.8	p_1-*cis*-DBE	38.6
trans-DXE	p_1-*trans*-DFE	40.6	p_1-*trans*-DCE	42.1	p_1-*trans*-DBE	38.0
TXE	p_1-TFE	38.5	p_1-TCE	39.1	p_1-TBE	39.4
	p_2-TFE	39.3	p_2-TCE	42.0	p_2-TBE	36.2
PXE	p_1-PFE	34.5	p_1-PCE	39.3	p_1-PBE	36.1

Phenol represents tyrosine as proton donor in reductive dehalogenase; Co ligated with a deprotonated corrin ring represents full size cobalamin employed in calculations. p_i shows the position of aromatic carbon protonated. Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, PFE = perfluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, PCE = perchloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene, PBE = perbromoethene.

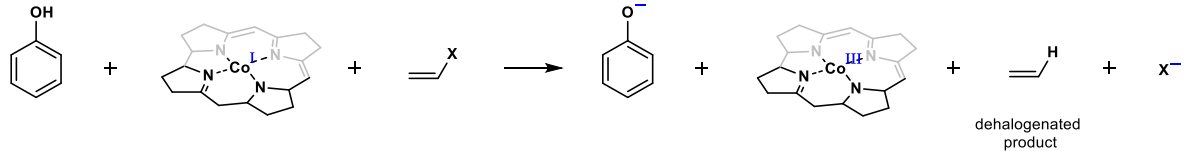
Table S8. Free energy barriers (kcal/mol) of dissociative proton-coupled single-electron transfer ($\Delta G^{\neq}_{\mathrm{odPC-SET}}$).[a]



substrate	dehalogenated radical cation	$\Delta G^{\neq}_{\mathrm{odPC-SET}}$	dehalogenated radical cation	$\Delta G^{\neq}_{\mathrm{odPC-SET}}$	dehalogenated radical cation	$\Delta G^{\neq}_{\mathrm{odPC-SET}}$
VX	p_1-E	128	p_1-E	112	p_1-E	104
1,1-DXE	p_1-VF	126	p_1-VC	115	p_1-VB	89.8
	p_2-VF	144	p_2-VC	100	p_2-VB	107
cis-DXE	p_1-VF	119	p_1-VC	101	p_1-VB	92.7
trans-DXE	p_1-VF	117	p_1-VC	102	p_1-VB	91.6
TXE	p_1-*cis*-DFE	117	p_1-*cis*-DCE	93.0	p_1-*cis*-DBE	83.2
	p_1-*trans*-DFE	118	p_1-*trans*-DCE	91.7	p_1-*trans*-DBE	83.1
	p_2-1,1-DXE	114	p_2-1,1-DCE	96.3	p_2-1,1-DBE	87.3
PXE	p_1-TFE	113	p_1-TCE	88.5	p_1-TBE	78.4

Phenol represents tyrosine as proton donor in reductive dehalogenase; Co ligated with a deprotonated corrin ring represents full size cobalamin employed in calculations. p_i shows the position of olefenic carbon protonated. Stable geometry of p_2-E can not be obtained during optimization. Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, E = ethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene.

Table S9. Free energy barriers (kcal/mol) of outer-sphere proton-coupled two-electron transfer ($\Delta G^{\neq}_{\mathrm{odPC-TET}}$)

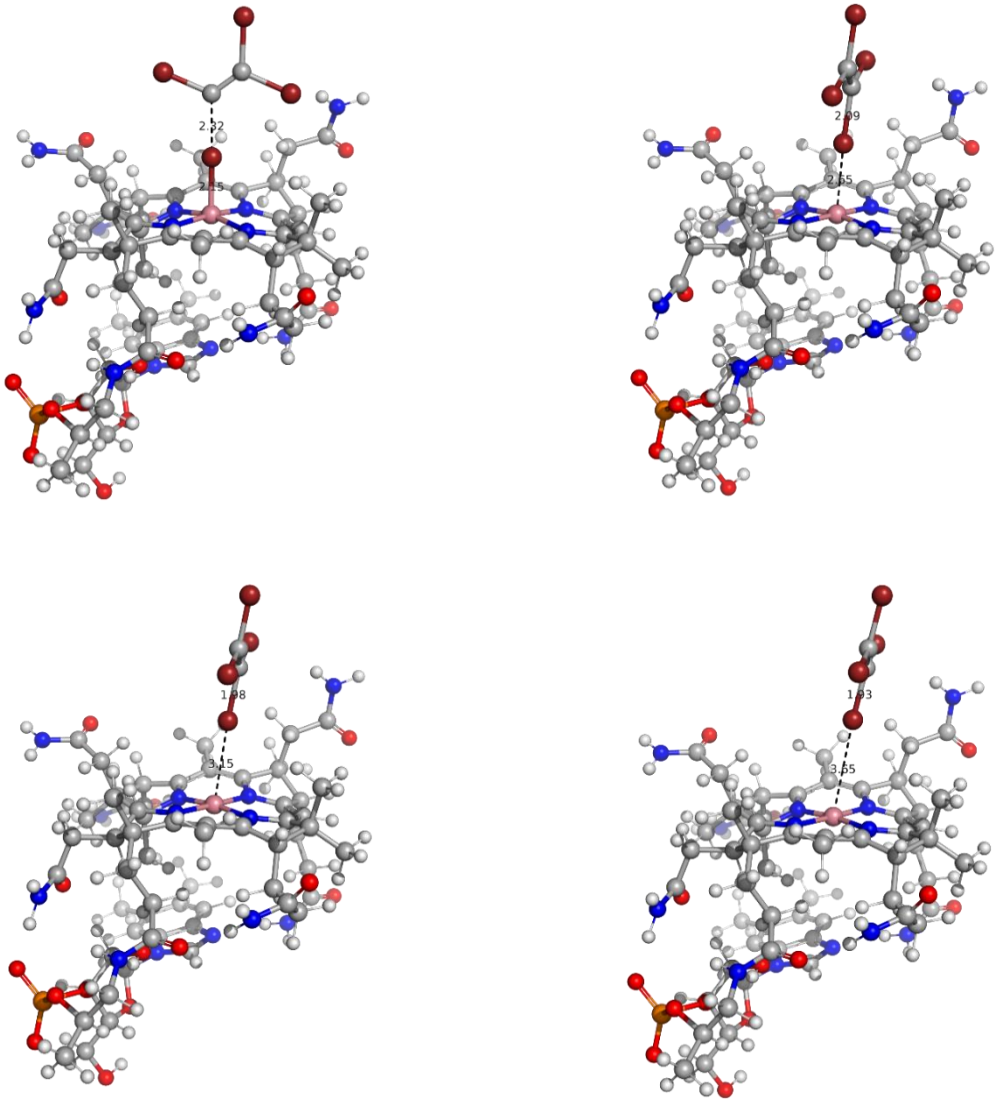


substrate	dehalogenated product	$\Delta G^{\neq}_{\mathrm{odPC-TET}}$	dehalogenated product	$\Delta G^{\neq}_{\mathrm{odPC-TET}}$	dehalogenated product	$\Delta G^{\neq}_{\mathrm{odPC-TET}}$
VX	E	89.2	E	75.6	E	63.9
1,1-DXE	VF	90.6	VC	71.0	VB	58.9
cis-DXE	VF	83.0	VC	70.8	VB	61.8
trans-DXE	VF	81.2	VC	73.7	VB	60.2
TXE	*cis*-DFE	86.2	*cis*-DCE	68.0	*cis*-DBE	57.0
	trans-DFE	87.6	*trans*-DCE	69.3	*trans*-DBE	57.9
	1,1-DXE	78.6	1,1-DCE	70.6	1,1-DBE	59.9
PXE	TFE	83.2	TCE	66.6	TBE	55.1

The proton donor tyrosine in reductive dehalogenase is represented by phenol; Co ligated with deprotonated corrin ring illustrates full size cobalamin adopted calculations. Compound abbreviations: VX = vinyl halide DXE = dihaloethene, TXE = trihaloethene, PXE = perhaloethene, E = ethene, VF = vinyl fluoride, DFE = difluoroethene, TFE = trifluoroethene, VC = vinyl chloride, DCE = dichloroethene, TCE = trichloroethene, VB = vinyl bromide, DBE = dibromoethene, TBE = tribromoethene.

V. Electronic Structures and Free Energies of Substrate-Cobalamin Complexes

The free energy barrier (18.2 kcal/mol, Table S3) implies the occurrence of outer-sphere SET from cob(I)alamin (B_{12s}) to perbromoethene (PBE) under ambient condition. To further confirm the feasibility of this reaction event, we studied the electronic structures (fragment charges and C-Br bond order) and free energies of PBE··· B_{12s} complexes at Co···Br and Co···C coordinations, considering coordination distances at 2.15, 2.65, 3.15, 3.65, and 4.15 Å. The optimized geometries, electronic structures (fragment charge, bond order, electron density difference) and free energies of these complexes are given in Figures 2, S1-S4 and Table S10-S12, respectively.



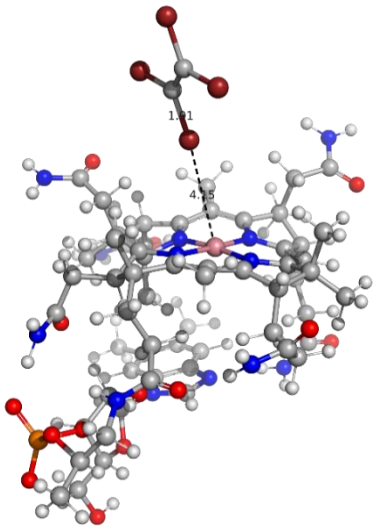
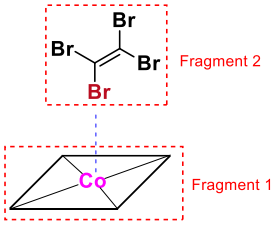


Fig. S1 Optimized geometries of PBE··· B_{12s} complexes at distinct Co···Br distances. The Co···Br and C···Br distances are given in Å. The optimizations and vibrational analyses were done at spin-unrestricted BP86 with a basis set Def2SVP.

Table S10. Fragment charges and bond orders of PBE-cobalamin complexes at distinct Co···Br distances



Co···Br distance (Å)	Hirshfeld charge		Mayer bond order	
	fragment 1	fragment 2	Co···Br	C···Br
2.15	-0.560	-0.440	1.050	0.370
2.65	-0.744	-0.256	0.677	0.690
3.15	-0.880	-0.120	0.342	0.935
3.65	-0.952	-0.049	0.181	1.049
4.15	-0.960	-0.040	0.086	1.099

The calculations were done at spin-unrestricted BP86/Def2TZVPP//BP86/Def2SVP. The Hirshfeld population and bond order analyses were carried out by Gaussian 09 Rev.E and Multiwfn 3.7, respectively.

Co···Br distance, 2.15 Å

Co···Br distance, 2.65 Å

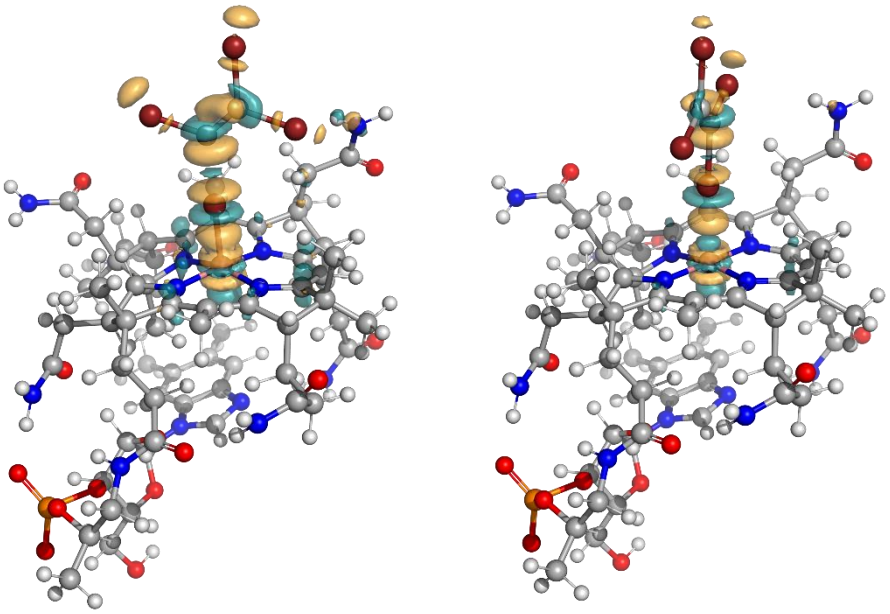
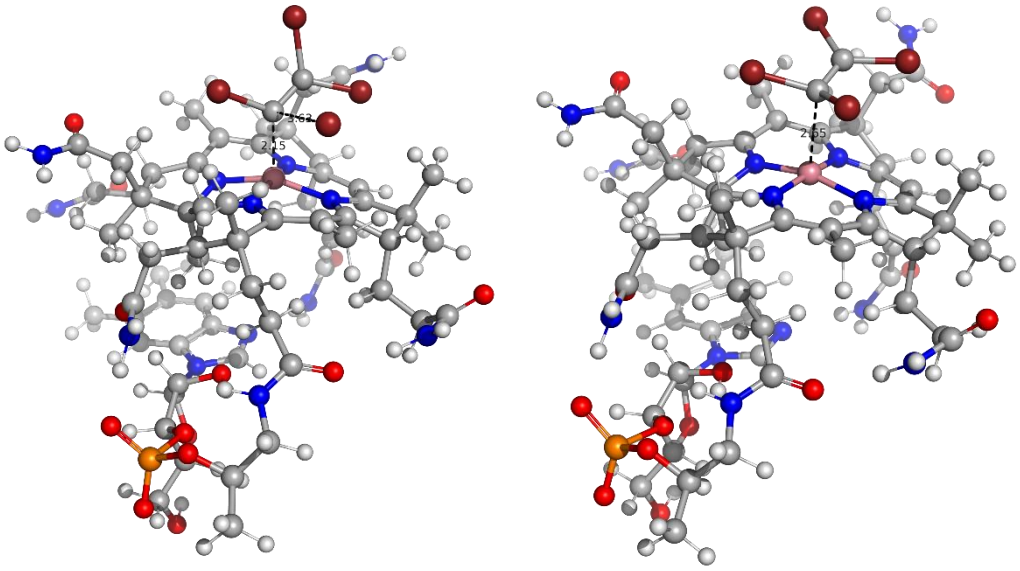


Fig. S2 The electron density difference maps of cob(I)alamin-PBE complexes, considering Co···Br distances at 2.15 and 2.65 Å. The surfaces of electron density difference calculated at spin-unrestricted BP86/Def2TZVPP//BP86/Def2SVP are depicted at the isovalues of 0.003 (orange) and -0.003 (teal), respectively. Atoms and bonds in the complexes are represented by balls and sticks. The color code of balls: pink, Co; gray, C; white, H; red, O; blue, N; yellow, P; dark red, Br.



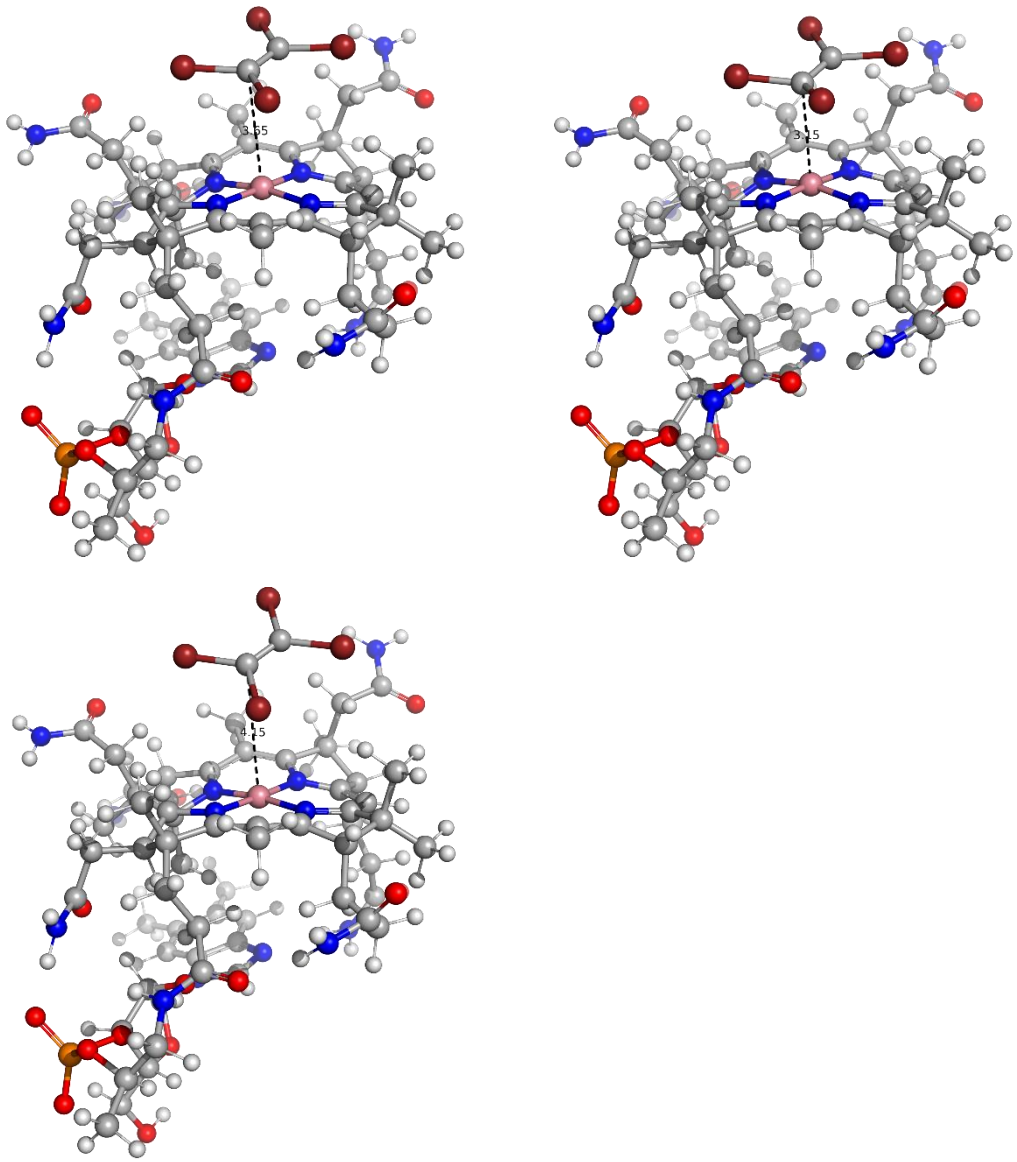
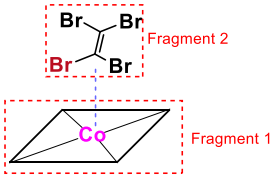


Fig. S3 Optimized geometries of PBE··· B_{12s} complexes at distinct Co···C distances. The Co···C distances are given in Å. The optimizations and vibrational analyses were done at spin-unrestricted BP86 with a basis set Def2SVP.

Table S11. Fragment charges and bond orders of PBE-cobalamin complexes at distinct Co···C distances

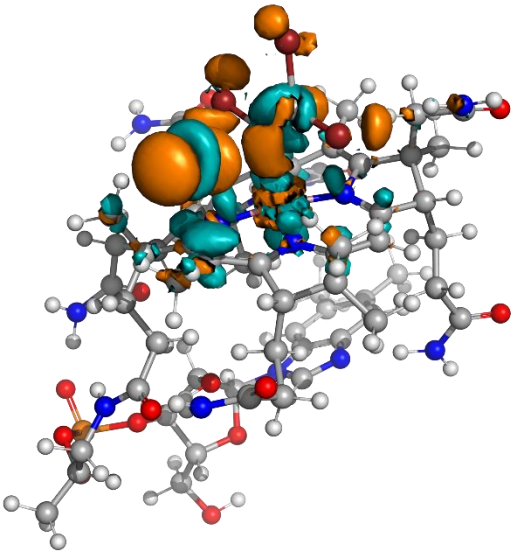


Co···C distance (Å)	Hirshfeld charge		Mayer bond order	
	fragment 1	fragment 2	Co···C	C···Br
2.15	-0.428	-0.572	0.711	0.067

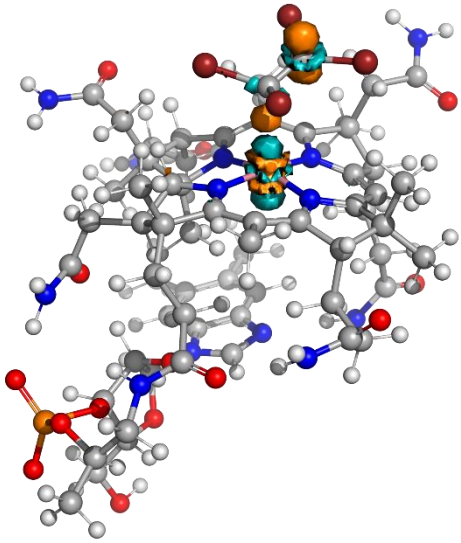
2.65	-0.918	-0.082	0.388	0.978
3.15	-1.068	0.068	0.174	1.035
3.65	-1.116	0.117	0.065	1.077
4.15	-1.070	0.071	< 0.050	1.100

The calculations were done at spin-unrestricted BP86/Def2TZVPP//BP86/Def2SVP. The Hirshfeld population and bond order analyses were carried out by Gaussian 09 Rev.E and Multiwfn 3.7, respectively.

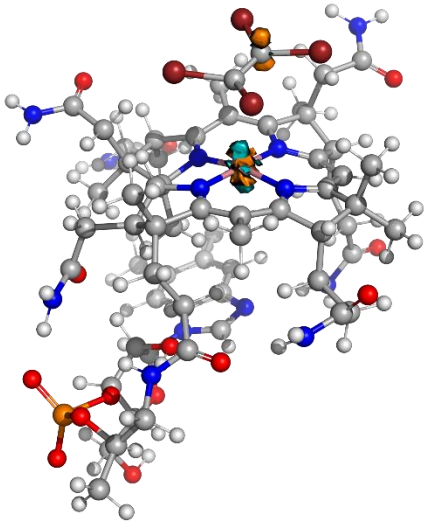
Co···C distance, 2.15 Å



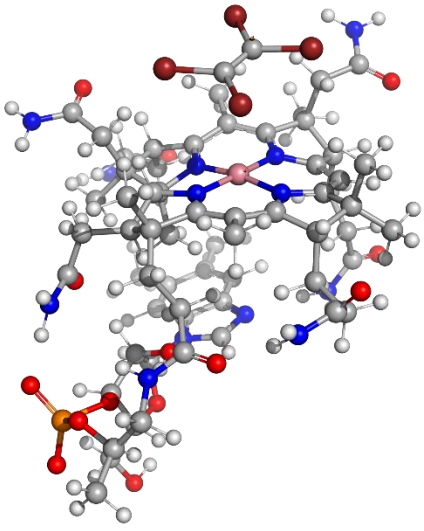
Co···C distance, 2.65 Å



Co···C distance, 3.15 Å



Co···C distance, 3.65 Å



Co···C distance, 4.15 Å

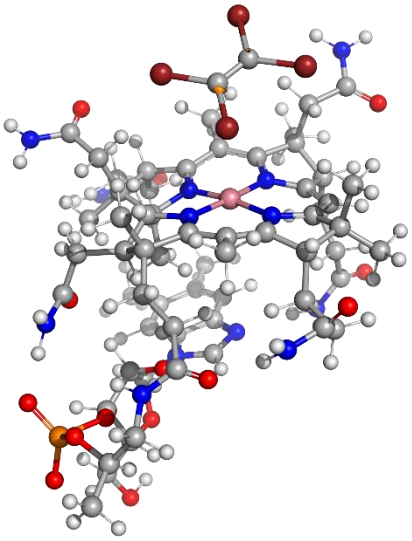


Fig. S4 The electron density difference maps of cob(I)alamin-PBE complexes, considering Co···C distances at 2.15, 2.65, 3.15, 3.65, and 4.15 Å. The surfaces of electron density difference calculated at spin-unrestricted BP86/Def2TZVPP//BP86/Def2SVP are depicted at the isovalues of 0.003 (orange) and -0.003 (teal), respectively. Atoms and bonds in the complexes are represented by balls and sticks. The color code of balls: pink, Co; gray, C; white, H; red, O; blue, N; yellow, P; dark red, Br.

Table S12. Gibbs free energies (G) of Co···PBE complexes at different Co···Br and Co···C distances[a]

	distance(A)	G (Hartree)	ΔG[b] (kcal/mol)	ΔG[c] (kcal/mol)
Co···Br complex	2.15	-16279.67073940	18.7	0.00
	2.65	-16279.70053140	0.00	0.00
	3.15	-16279.69955410	0.61	0.00
	3.65	-16279.69165600	5.57	0.00
	4.15	-16279.69154160	5.64	0.00
Co···C complex	2.15	-16279.66305540	23.5	4.82
	2.65	-16279.65436840	29.0	29.0
	3.15	-16279.66398640	22.9	22.3
	3.65	-16279.67661240	15.0	9.44
	4.15	-16279.68370980	10.6	4.91

[a]The G were calculated at spin unrestricted BP86/Def2TZVPP//BP86/Def2SVP, including the zero-point energy (ZPE), entropy, thermal energy (298 K) corrections. The ΔG[b] is the energy difference between a complex and the energy lowest complex. The ΔG[c] is the energy difference between Co-C complex and Co-Br complex at the same coordination distance.

VI. Cartesian Coordinates of Species

A. Cartesian Coordinates of Olefins

Ethene, 6 atoms

atom	X	Y	Z
C	0.00000000	0.67105100	0.00000000
H	0.93812200	1.25158000	0.00000000
H	-0.93811900	1.25158600	0.00000000
C	0.00000000	-0.67105100	0.00000000
H	0.93811900	-1.25158600	0.00000000
H	-0.93812200	-1.25158000	0.00000000

MFE, 6 atoms

atom	X	Y	Z
C	1.19793200	-0.16615900	0.00000000
H	2.10848900	0.44936300	0.00000000
H	1.29075600	-1.26272400	0.00000000
C	0.00000000	0.43061800	0.00000000
H	-0.16434300	1.52283300	0.00000000
F	-1.15805400	-0.25513600	0.00000000

11-DFE, 6 atoms

atom	X	Y	Z
C	0.00000400	1.39751900	0.00000000
H	-0.95259900	1.94109100	0.00000000
H	0.95261000	1.94108600	0.00000000
C	0.00000000	0.06027400	0.00000000
F	1.08835300	-0.70161100	0.00000000
F	-1.08835700	-0.70160400	0.00000000

***cis*-DFE**, 6 atoms

atom	X	Y	Z
C	0.00000000	-0.88232500	0.00000000
H	-0.33674900	-1.93164800	0.00000000
C	-0.87094600	0.14126300	0.00000000
F	-0.49552100	1.42918600	0.00000000
F	1.33141800	-0.71794700	0.00000000
H	-1.96064800	-0.02313500	0.00000000

***trans*-DFE**, 6 atoms

atom	X	Y	Z
C	-0.33157700	0.58419300	0.00000000
C	0.33157700	-0.58419300	0.00000000
F	-0.33157700	-1.75411400	0.00000000
H	1.43054400	-0.67204100	0.00000000
H	-1.43054400	0.67204100	0.00000000
F	0.33157700	1.75411400	0.00000000

TFE, 6 atoms

atom	X	Y	Z
C	-0.69344200	-0.71161200	0.00000000
C	0.00000000	0.44077300	0.00000000
F	-0.58980800	1.63086800	0.00000000
H	-1.79263700	-0.73413800	0.00000000
F	-0.06979200	-1.90183500	0.00000000
F	1.32107600	0.53309700	0.00000000

PFE, 6 atoms

atom	X	Y	Z
C	0.00000000	0.67272200	0.00000000
C	0.00000000	-0.67272200	0.00000000
F	-1.11084600	-1.39816600	0.00000000
F	1.11084600	1.39816600	0.00000000
F	1.11084600	-1.39816500	0.00000000
F	-1.11084600	1.39816500	0.00000000

MCE, 6 atoms

atom	X	Y	Z
C	0.00000000	0.75912700	0.00000000
H	-0.79283800	1.52431500	0.00000000
C	1.30955100	1.04884200	0.00000000
H	1.62866700	2.10293000	0.00000000
H	2.08331200	0.26596100	0.00000000
Cl	-0.63390900	-0.86711900	0.00000000

11-DCE, 6 atoms

atom	X	Y	Z
C	0.00000000	0.42264100	0.00000000
C	0.00000700	1.76719100	0.00000000
H	-0.94979900	2.32016500	0.00000000
H	0.94981600	2.32016000	0.00000000
Cl	1.46528700	-0.52292400	0.00000000
Cl	-1.46529100	-0.52291900	0.00000000

***cis*-DCE**, 6 atoms

atom	X	Y	Z
C	1.10557900	0.40785200	0.00000000
C	0.00000000	1.17839800	0.00000000
Cl	1.10392800	-1.32271500	0.00000000
H	2.10555900	0.86863100	0.00000000
H	0.08618000	2.27605700	0.00000000
Cl	-1.62305900	0.57788100	0.00000000

***trans*-DCE**, 6 atoms

atom	X	Y	Z

C	-0.36820100	0.56337900	0.00000000
C	0.36820100	-0.56337900	0.00000000
H	1.46891900	-0.56694200	0.00000000
Cl	0.36820100	2.13896700	0.00000000
Cl	-0.36820100	-2.13896700	0.00000000
H	-1.46891900	0.56694200	0.00000000

TCE, 6 atoms

atom	X	Y	Z
C	-1.05207000	-0.40308000	0.00000000
C	0.00000000	0.44935900	0.00000000
Cl	-0.89150900	-2.12348900	0.00000000
H	-2.08283400	-0.02057200	0.00000000
Cl	1.65290100	-0.06186700	0.00000000
Cl	-0.26755300	2.17023200	0.00000000

PCE, 6 atoms

atom	X	Y	Z
C	0.00000100	0.68268500	0.00000000
C	-0.00000100	-0.68268500	0.00000000
Cl	1.46833600	1.60063100	0.00000000
Cl	1.46833600	-1.60063500	0.00000000
Cl	-1.46833600	-1.60063100	0.00000000
Cl	-1.46833600	1.60063500	0.00000000

MBE, 6 atoms

atom	X	Y	Z
C	-0.44483900	-2.10417500	0.00000000
H	-1.52999600	-1.91853600	0.00000000
H	-0.09575600	-3.14996900	0.00000000
C	0.45792200	-1.11370300	0.00000000
H	1.54725400	-1.27425300	0.00000000
Br	0.00000000	0.73285800	0.00000000

11-DBE, 6 atoms

atom	X	Y	Z
C	0.00000500	2.05392100	0.00000000
H	-0.94831400	2.61204400	0.00000000
H	0.94832700	2.61204100	0.00000000
C	0.00000000	0.71033100	0.00000000
Br	-1.60515900	-0.31156500	0.00000000
Br	1.60515700	-0.31156700	0.00000000

***cis*-DBE**, 6 atoms

atom	X	Y	Z
C	1.18524800	0.78445400	0.00000000
H	2.12497500	1.35854000	0.00000000
C	0.00000000	1.42132300	0.00000000
Br	-1.69502200	0.59569900	0.00000000
Br	1.43226400	-1.08470000	0.00000000
H	-0.03992900	2.52180800	0.00000000

***trans*-DBE**, 6 atoms

atom	X	Y	Z
C	-0.38184100	0.55246100	0.00000000
C	0.38184100	-0.55246100	0.00000000
Br	-0.38184100	-2.28921600	0.00000000
H	1.48196900	-0.54338200	0.00000000
H	-1.48196900	0.54338200	0.00000000
Br	0.38184100	2.28921600	0.00000000

TBE, 6 atoms

atom	X	Y	Z
C	1.20860800	-0.13564300	0.00000000
C	0.00000000	0.46965300	0.00000000
Br	-0.08992300	2.37066900	0.00000000
H	2.13592000	0.45576300	0.00000000
Br	1.47522800	-2.00049500	0.00000000
Br	-1.65352200	-0.44045500	0.00000000

PBE, 6 atoms

atom	X	Y	Z
C	0.00000100	0.68185500	0.00000000
C	-0.00000100	-0.68185500	0.00000000
Br	1.59565400	-1.69950600	0.00000000
Br	-1.59565400	1.69950600	0.00000000
Br	-1.59565400	-1.69950500	0.00000000
Br	1.59565400	1.69950500	0.00000000

B. Cartesian Coordinates of Olefinic Radical Anions

MFE_ra, 6 atoms

atom	X	Y	Z
C	1.22679400	-0.23825900	0.13609400
H	2.12826300	0.41952900	0.13965200
H	1.43452900	-1.18908000	-0.42389200
C	0.02312300	0.47451200	-0.21866900
H	-0.07511600	1.49238200	0.25425600
F	-1.22079800	-0.23781700	0.05838200

11-DFE_ra, 6 atoms

atom	X	Y	Z
C	1.40880900	-0.00007200	-0.17205900
H	1.97171400	0.91678200	0.11614100
H	1.97160000	-0.91698500	0.11615600
C	0.05563800	0.00000100	0.34130300
F	-0.70728800	-1.13442700	-0.06932000

F	-0.70715600	1.13449700	-0.06932000

***cis*-DFE_ra**, 6 atoms

atom	X	Y	Z
C	-0.64042700	0.52069200	0.30742800
H	-1.15825900	1.50560000	0.19075700
C	0.64043500	0.52069600	-0.30743100
F	1.58073800	-0.51442100	0.09856600
F	-1.58074400	-0.51441500	-0.09856600
H	1.15827500	1.50559300	-0.19074300

***trans*-DFE_ra**, 6 atoms

atom	X	Y	Z
C	0.59636600	0.34396400	-0.41698500
C	-0.59637700	-0.34397500	-0.41698700
F	-1.81901700	0.12909900	0.31838200
H	-0.60760600	-1.45260100	-0.36349800
H	0.60763800	1.45258600	-0.36354200
F	1.81902100	-0.12909000	0.31838100

TFE_ra, 6 atoms

atom	X	Y	Z
C	-0.78386500	0.52062500	0.34277300
C	0.41096400	0.01136400	-0.31379600
F	1.50884400	0.85303800	-0.02748500
H	-0.87320100	1.62396900	0.18151800
F	-1.98544200	-0.10000100	-0.11897700
F	0.82222000	-1.28813700	0.10697500

PFE_ra, 6 atoms

atom	X	Y	Z
C	0.66219200	-0.00001100	-0.34756200
C	-0.66218900	-0.00001100	0.34755100
F	-1.41290000	1.11899600	-0.05428100
F	1.41294900	-1.11899400	0.05430900
F	-1.41296700	-1.11897500	-0.05430600
F	1.41291700	1.11898800	0.05428600

MCE_ra, 6 atoms

atom	X	Y	Z
C	0.98592900	0.50924700	0.20713200
H	0.90393500	1.54034100	-0.18991000
C	2.03444900	-0.29788600	-0.03847600
H	2.90756200	-0.01551600	-0.68128200
H	2.07038000	-1.34024800	0.34406500
Cl	-1.41200900	-0.08545500	-0.02851800

11-DCE_ra, 6 atoms

atom	X	Y	Z
C	0.28402800	0.32614800	-0.00000200
C	0.35704800	1.67058100	0.00000000
H	-0.60164400	2.21657300	0.00000000
H	1.30451100	2.24664000	0.00000300
Cl	1.86783100	-0.60018800	0.00000000
Cl	-2.13543900	-0.36708200	0.00000000

***cis*-DCE_ra**, 6 atoms

atom	X	Y	Z
C	0.33374600	1.08315500	0.28916000
C	-0.91032500	0.96284300	-0.16918400
Cl	2.16302500	-0.38683700	-0.04434400
H	0.88738500	2.02949700	0.16723200
H	-1.53274200	1.70091100	-0.71233800
Cl	-1.92156400	-0.55471600	0.03406400

***trans*-DCE_ra**, 6 atoms

atom	X	Y	Z
C	0.47440500	-0.43750100	0.00000200
C	-0.47441000	0.43748100	0.00000100
H	-0.52610500	1.52886900	-0.00000500
Cl	2.66004600	0.04532900	0.00000000
Cl	-2.66004300	-0.04532100	0.00000000
H	0.52608700	-1.52888900	-0.00000700

TCE_ra, 6 atoms

atom	X	Y	Z
C	0.74959800	-0.95062000	-0.16866500
C	-0.35405300	-0.31317300	0.27908300
Cl	2.37523100	-0.24913500	0.03935300
H	0.78905600	-1.92270000	-0.69269100
Cl	-0.67638300	1.99991200	-0.04357100
Cl	-1.88486700	-1.19163200	0.00599300

PCE_ra, 6 atoms

atom	X	Y	Z
C	0.70423000	-0.17960800	-0.16724600
C	-0.54465500	0.27146900	-0.36888900
Cl	1.10368100	-1.88668100	-0.28670300
Cl	-2.41477500	-0.92407700	0.33894200
Cl	-0.89822300	1.97759200	-0.26567300
Cl	2.15299700	0.80074500	0.40265800

MBE_ra, 6 atoms

atom	X	Y	Z
C	-2.71796600	0.32432700	-0.03397200
H	-2.66883200	1.38951100	0.27597300
H	-3.67159700	0.03818600	-0.54708900

C	-1.69359200	-0.51454100	0.16731200
H	-1.67452400	-1.57579800	-0.14854700
Br	0.98526600	0.03684000	-0.01086800

11-DBE_ra, 6 atoms

atom	X	Y	Z
C	-0.30797900	1.96267000	0.00000000
H	-1.23916200	2.56053500	0.00000000
H	0.66015300	2.49355200	0.00000200
C	-0.26607200	0.61784200	-0.00000200
Br	-2.04877100	-0.34303800	0.00000000
Br	2.16372300	-0.24373800	0.00000000

***cis*-DBE_ra**, 6 atoms

atom	X	Y	Z
C	0.00000000	1.69365600	0.00000000
H	0.47906100	2.67584800	0.00000000
C	-1.19029800	1.21001700	0.00000000
Br	-1.73493500	-1.06342000	0.00000000
Br	1.98868500	0.44403400	0.00000000
H	-2.21853800	1.58062000	0.00000000

***trans*-DBE_ra**, 6 atoms

atom	X	Y	Z
C	-0.00000400	0.64281500	0.00000000
C	0.00000000	-0.64280900	0.00000000
Br	-2.00907500	-1.96558100	0.00000000
H	0.73965200	-1.44562500	0.00000000
H	-0.73964100	1.44564300	0.00000000
Br	2.00907600	1.96557900	0.00000000

TBE_ra, 6 atoms

atom	X	Y	Z
C	-0.60974800	-0.99022300	0.00003900
C	0.28786700	-0.01607800	0.00000800
Br	2.78311500	-0.78191800	-0.00000400
H	-0.34201200	-2.05556300	0.00002800
Br	-2.64349900	-0.82878700	-0.00000500
Br	-0.07466500	1.84194400	0.00000000

PBE_ra, 6 atoms

atom	X	Y	Z
C	0.46868700	0.39892800	-0.00001300
C	-0.66571700	-0.29030600	-0.00000800
Br	-0.71569800	-2.19261800	-0.00001100
Br	0.55435100	2.28134000	-0.00001100
Br	-2.58652000	0.48443200	0.00001400
Br	2.78164300	-0.59177500	0.00001200

C. Cartesian Coordinates of Dehalogenated Olefinic Radicals

MFE_dr, 5 atoms

atom	X	Y	Z
C	0.04884200	-0.59201000	0.00000000
H	-0.89378600	-1.18334200	0.00000000
H	0.98483900	-1.18337600	0.00000000
C	0.04884200	0.72765500	0.00000000
H	-0.67715500	1.55284400	0.00000000

11-DFE_dr, 5 atoms

atom	X	Y	Z
C	1.21225700	-0.11785600	0.00000000
H	2.10454100	0.52425800	0.00000000
H	1.34120100	-1.21715800	0.00000000
C	0.00000000	0.42801400	0.00000000
F	-1.19103200	-0.12978300	0.00000000

***cis*-DFE_dr**, 5 atoms

atom	X	Y	Z
C	0.00000000	0.38284600	0.00000000
H	-0.31278400	1.44864700	0.00000000
C	1.26111100	-0.01359000	0.00000000
F	-1.05754200	-0.45408800	0.00000000
H	2.26399700	0.42260500	0.00000000

***trans*-DFE_dr**, 5 atoms

atom	X	Y	Z
C	0.00000000	0.44470700	0.00000000
C	1.27562600	0.09908400	0.00000000
H	1.95963400	-0.75464200	0.00000000
H	-0.35786400	1.49095500	0.00000000
F	-1.02839200	-0.44434000	0.00000000

TFE_dr1, 5 atoms

atom	X	Y	Z
C	-0.23337800	1.42158200	0.00000000
C	0.00000000	0.12054400	0.00000000
F	-0.93652800	-0.83365100	0.00000000
H	-1.05086500	2.14389500	0.00000000
F	1.20887500	-0.43264400	0.00000000

TFE_dr2, 5 atoms

atom	X	Y	Z
C	0.00000000	0.88329200	0.00000000
C	-0.87654600	-0.12419700	0.00000000

H	-0.32667600	1.93419600	0.00000000
F	1.34239400	0.70405600	0.00000000
F	-0.72173300	-1.42503000	0.00000000

TFE_dr3, 5 atoms

atom	X	Y	Z
C	0.00000000	0.65813600	0.00000000
C	0.00593200	-0.67748300	0.00000000
F	1.03329600	-1.49484600	0.00000000
H	0.92574100	1.26564100	0.00000000
F	-1.14011100	1.36711700	0.00000000

PFE_dr, 5 atoms

atom	X	Y	Z
C	0.42580000	0.05820500	0.00001300
C	-0.79433400	0.59766900	-0.00000600
F	-1.97427800	0.02516300	0.00000000
F	1.53316600	0.78836100	-0.00000200
F	0.68680100	-1.25077300	-0.00000300

MCE_dr, 5 atoms

atom	X	Y	Z
C	0.04884300	0.72765900	0.00000000
H	-0.67717000	1.55284000	0.00000000
C	0.04884300	-0.59201300	0.00000000
H	-0.89378600	-1.18333200	0.00000000
H	0.98483900	-1.18338200	0.00000000

11-DCE_dr, 5 atoms

atom	X	Y	Z
C	0.00000000	0.71060900	0.00000000
C	1.22390400	1.22783400	0.00000000
H	2.13499300	0.59730800	0.00000000
H	1.35820700	2.32260200	0.00000000
Cl	-0.63744900	-0.85591600	0.00000000

***cis*-DCE_dr**, 5 atoms

atom	X	Y	Z
C	-1.26634800	-1.19845600	0.00000000
C	0.00000000	-0.84182500	0.00000000
H	0.85103900	-1.54379100	0.00000000
Cl	0.53147300	0.85825900	0.00000000
H	-2.28798800	-0.80492700	0.00000000

***trans*-DCE_dr**, 5 atoms

atom	X	Y	Z
C	1.25895100	1.17401900	0.00000000
C	0.00000000	0.78539800	0.00000000
H	-0.86364400	1.47988700	0.00000000
Cl	-0.50297100	-0.90149000	0.00000000
H	1.86044900	2.08894700	0.00000000

TCE_dr1, 5 atoms

atom	X	Y	Z
C	-0.04875900	1.78879400	0.00000100
C	0.00324300	0.47202300	-0.00000700
H	-0.74743400	2.62948700	0.00000800
Cl	1.50630500	-0.41722300	0.00000100
Cl	-1.44627400	-0.53538800	0.00000100

TCE_dr2, 5 atoms

atom	X	Y	Z
C	1.11113200	0.36696600	0.00000000
C	0.00000000	1.09633400	0.00000000
Cl	1.13577200	-1.39633300	0.00000000
H	2.10987100	0.83070100	0.00000000
Cl	-1.65204600	0.83101000	0.00000000

TCE_dr3, 5 atoms

atom	X	Y	Z
C	-0.53453400	0.49929100	-0.00000200
C	0.53291100	-0.29563600	-0.00000200
Cl	-2.16508500	-0.12833800	0.00000100
H	-0.47677100	1.60368500	0.00000300
Cl	2.19370300	-0.03787500	0.00000100

PCE_dr, 5 atoms

atom	X	Y	Z
C	-0.74914200	0.75022000	0.00000000
C	0.41953400	0.11093300	0.00000200
Cl	1.92021700	0.99476800	0.00000000
Cl	0.56389400	-1.63841000	0.00000000
Cl	-2.36777900	0.33970500	0.00000000

MBE_dr, 5 atoms

atom	X	Y	Z
C	0.04884200	-0.59201000	0.00000000
H	0.98483900	-1.18337700	0.00000000
H	-0.89378600	-1.18334200	0.00000000
C	0.04884200	0.72765500	0.00000000
H	-0.67715600	1.55284400	0.00000000

11-DBE_dr, 5 atoms

atom	X	Y	Z
C	0.25312400	-2.21308900	0.00000000
H	-0.28749400	-3.17618800	0.00000000

H	1.36051400	-2.25018600	0.00000000
C	-0.43196100	-1.07566000	0.00000000
Br	0.00000000	0.71882500	0.00000000

***cis*-DBE_dr**, 5 atoms

atom	X	Y	Z
C	0.40112200	-1.19233100	0.00000000
H	1.49316800	-1.37163700	0.00000000
C	-0.53240100	-2.11229800	0.00000000
Br	0.00000000	0.69691700	0.00000000
H	-0.70549300	-3.19266600	0.00000000

***trans*-DBE_dr**, 5 atoms

atom	X	Y	Z
C	0.45650800	-1.22024600	0.00000000
C	-0.45887600	-2.15447400	0.00000000
H	-1.53405100	-2.35658800	0.00000000
H	1.54825600	-1.36814600	0.00000000
Br	0.00000000	0.68494400	0.00000000

TBE_dr1, 5 atoms

atom	X	Y	Z
C	-0.03508600	2.05475800	0.00000000
C	0.00000000	0.74616700	0.00000000
Br	-1.61032500	-0.32668100	0.00000000
H	-0.67407600	2.94107200	0.00000000
Br	1.63559900	-0.23750800	0.00000000

TBE_dr2, 5 atoms

atom	X	Y	Z
C	1.19481100	0.71576200	0.00000000
C	0.00000000	1.28422400	0.00000000
H	2.13023500	1.29703700	0.00000000
Br	1.49283400	-1.19205800	0.00000000
Br	-1.75852300	0.81214500	0.00000000

TBE_dr3, 5 atoms

atom	X	Y	Z
C	0.33450600	0.72322300	0.00000000
C	0.00000000	-0.55956600	0.00000000
Br	0.90127000	-2.15395000	0.00000000
H	1.36676600	1.11715600	0.00000000
Br	-0.99766400	2.09397600	0.00000000

PBE_dr, 5 atoms

atom	X	Y	Z
C	-0.74239900	-0.81398200	0.00000800
C	0.40547200	-0.15215400	0.00000400
Br	2.05157600	-1.10905200	-0.00000100
Br	-2.52999700	-0.48882800	-0.00000100
Br	0.53618000	1.76350300	0.00000000

D. Cartesian Coordinates of Dehalogenated Olefinic Anions

MFE_da, 5 atoms

atom	X	Y	Z
C	0.06872300	-0.57183400	0.00000000
H	-0.81601900	-1.28889000	0.00000000
H	1.02994600	-1.16036800	0.00000000
C	0.06872300	0.79585100	0.00000000
H	-1.03860000	1.10515400	0.00000000

11-DFE_da, 5 atoms

atom	X	Y	Z
C	1.14671600	-0.10395600	0.00000000
H	2.12949500	0.41120000	0.00000000
H	1.17272800	-1.22541300	0.00000000
C	0.00000000	0.64850000	0.00000000
F	-1.13139100	-0.27256100	0.00000000

***cis*-DFE_da**, 5 atoms

atom	X	Y	Z
C	0.00000000	0.40069600	0.00000000
H	-0.60657100	1.34979700	0.00000000
C	1.30835000	0.13027300	0.00000000
F	-1.00532400	-0.63165000	0.00000000
H	1.80438300	1.14923500	0.00000000

***trans*-DFE_da**, 5 atoms

atom	X	Y	Z
C	0.00000000	0.46064200	0.00000000
C	1.33061500	0.38917200	0.00000000
H	1.63014900	-0.70171500	0.00000000
H	-0.64147900	1.37256600	0.00000000
F	-0.99692900	-0.64108200	0.00000000

TFE_da1, 5 atoms

atom	X	Y	Z
C	-0.11261200	1.53203100	0.00000000
C	0.00000000	0.21008200	0.00000000
F	-0.97484500	-0.83704500	0.00000000
H	-1.21232900	1.76236300	0.00000000
F	1.18462300	-0.52018300	0.00000000

TFE_da2, 5 atoms

atom	X	Y	Z
C	0.00000000	0.86002700	0.00000000
C	-1.07654800	0.02868900	0.00000000
H	-0.12235000	1.96164200	0.00000000
F	1.39379000	0.54006100	0.00000000
F	-0.66249700	-1.35049800	0.00000000

TFE_da3, 5 atoms

atom	X	Y	Z
C	0.00000000	0.54921900	0.00000000
C	-0.21025400	-0.79380700	0.00000000
F	1.10835800	-1.40647000	0.00000000
H	0.96844800	1.10832200	0.00000000
F	-1.07579400	1.44638200	0.00000000

PFE_da, 5 atoms

atom	X	Y	Z
C	0.00000000	0.37787800	0.00000000
C	-1.03949500	-0.49240500	0.00000000
F	-0.51429500	-1.83517800	0.00000000
F	-0.17356900	1.74191400	0.00000000
F	1.38086000	0.16961500	0.00000000

MCE_da, 5 atoms

atom	X	Y	Z
C	0.06872300	0.79585100	0.00000000
H	-1.03860000	1.10515400	0.00000000
C	0.06872300	-0.57183400	0.00000000
H	-0.81601900	-1.28889000	0.00000000
H	1.02994600	-1.16036800	0.00000000

11-DCE_da, 5 atoms

atom	X	Y	Z
C	0.00000000	1.04119100	0.00000000
C	1.35859500	0.92941200	0.00000000
H	1.97980700	0.00341500	0.00000000
H	1.92756500	1.88713300	0.00000000
Cl	-0.70934900	-0.80671600	0.00000000

***cis*-DCE_da**, 5 atoms

atom	X	Y	Z
C	-2.29296600	-0.99349600	0.00000000
C	-1.07520500	-1.13213100	0.00000000
H	0.00000000	-1.25453600	0.00000000
Cl	1.38493500	0.86619400	0.00000000
H	-3.33486800	-0.71700100	0.00000000

***trans*-DCE_da**, 5 atoms

atom	X	Y	Z
C	2.91452800	-0.66294100	-0.11364600
C	1.84029500	0.29253300	0.13563700
H	0.56583500	3.96616800	-0.28610000
H	0.85531100	1.16414400	0.35273900
Cl	-1.76177000	-0.17105100	-0.01168100

TCE_da1, 5 atoms

atom	X	Y	Z
C	-0.22963400	1.96252300	0.00000000
C	0.00000000	0.67994500	0.00000000
H	-1.28863400	2.28842700	0.00000000
Cl	1.54990900	-0.18653100	0.00000000
Cl	-1.39306000	-0.88071900	0.00000000

TCE_da2, 5 atoms

atom	X	Y	Z
C	0.00000000	1.19755900	0.00000000
C	-1.22919900	0.67045500	0.00000000
Cl	1.74802500	0.36048700	0.00000000
H	0.20139100	2.28094500	0.00000000
Cl	-1.32603600	-1.15395900	0.00000000

TCE_da3, 5 atoms

atom	X	Y	Z
C	0.00000000	0.51392300	0.00000000
C	-0.28561200	-0.81044200	0.00000000
Cl	-1.38976400	1.70169000	0.00000000
H	0.95213500	1.07991300	0.00000000
Cl	1.43456100	-1.66056100	0.00000000

PCE_da, 5 atoms

atom	X	Y	Z
C	-1.30408400	0.10078300	0.00000000
C	0.00000000	0.42871800	0.00000000
Cl	0.50389200	2.14431100	0.00000000
Cl	1.54194800	-0.62969500	0.00000000
Cl	-1.58557500	-1.70149900	0.00000000

MBE_da, 5 atoms

atom	X	Y	Z
C	0.06872300	-0.57183400	0.00000000
H	1.02994500	-1.16037000	0.00000000
H	-0.81601800	-1.28889200	0.00000000
C	0.06872300	0.79585100	0.00000000
H	-1.03859900	1.10515900	0.00000000

11-DBE_da, 5 atoms

atom	X	Y	Z
C	0.41591900	-2.11025100	0.00000000
H	0.22171700	-3.20807300	0.00000000
H	1.48808900	-1.81630500	0.00000000
C	-0.70088700	-1.33588700	0.00000000
Br	0.00000000	0.73432000	0.00000000

***cis*-DBE_da**, 5 atoms

atom	X	Y	Z
C	-0.00006500	-2.26618700	0.00000000
H	0.00000000	-1.13436000	0.00000000
C	-0.00016900	-3.49396500	0.00000000
Br	0.00005000	1.15058700	0.00000000
H	-0.00034500	-4.57525400	0.00000000

***trans*-DBE_da**, 5 atoms

atom	X	Y	Z
C	0.00000000	0.00000000	2.26653800
C	0.00000000	0.00000000	3.49430600
H	0.00000000	0.00000000	4.57559500
H	0.00000000	0.00000000	1.13473700
Br	0.00000000	0.00000000	-1.15072600

TBE_da1, 5 atoms

atom	X	Y	Z
C	-0.34060200	2.30557600	0.00000000
C	0.00000000	1.07127800	0.00000000
Br	-1.57824200	-0.83529300	0.00000000
H	-1.34373300	2.75140300	0.00000000
Br	1.67502300	0.17779200	0.00000000

TBE_da2, 5 atoms

atom	X	Y	Z
C	0.00000000	1.45700000	0.00000000
C	-1.25298500	1.04739600	0.00000000
H	0.36004700	2.49505400	0.00000000
Br	1.90360100	0.34787600	0.00000000
Br	-1.69909100	-0.84848900	0.00000000

TBE_da3, 5 atoms

atom	X	Y	Z
C	0.00000000	0.49503900	0.00000000
C	-0.31009700	-0.81731200	0.00000000
Br	1.56888200	-1.75212800	0.00000000
H	0.92483400	1.09781400	0.00000000
Br	-1.54214700	1.77600900	0.00000000

PBE_da, 5 atoms

atom	X	Y	Z
C	1.33359100	0.43968400	0.00000000
C	0.00000000	0.48383600	0.00000000
Br	-0.90513200	2.20184500	0.00000000
Br	2.12658100	-1.35313600	0.00000000
Br	-1.45006400	-1.00702700	0.00000000

E. Cartesian Coordinates of Protonated Olefins

MFE_p1, 7 atoms

atom	X	Y	Z
C	1.16983900	-0.18291900	0.00000100
H	1.74839300	0.24884600	-0.86346600
H	1.16050400	-1.28871500	0.00001500
C	-0.12009300	0.43509300	-0.00000100
H	-0.29436700	1.53604600	0.00000400
F	-1.18460000	-0.25089900	0.00000000
H	1.74840200	0.24887000	0.86344900

MFE_p2, 7 atoms

atom	X	Y	Z
C	-1.16983800	-0.18291900	0.00000000
H	-1.74839300	0.24885900	-0.86345800
H	-1.16050600	-1.28871600	0.00000100
C	0.12009300	0.43509200	0.00000000
H	0.29436400	1.53604600	0.00000000
F	1.18460000	-0.25089900	0.00000000
H	-1.74839700	0.24886100	0.86345500

11-DFE_p1, 7 atoms

atom	X	Y	Z
C	-1.39510700	0.00000500	0.01495000
H	-1.79534800	0.93109100	0.46579400
H	-1.70808900	-0.00004400	-1.06598200
C	0.05379200	0.00000100	0.01359300
F	0.74147800	-1.06145300	-0.00205200
F	0.74148600	1.06144900	-0.00205200
H	-1.79534900	-0.93104600	0.46586400

11-DFE_p2, 7 atoms

atom	X	Y	Z
C	-1.39510700	-0.00000300	-0.01495000
H	-1.79534900	0.93105800	-0.46584500
H	-1.79534800	-0.93108000	-0.46581200
C	0.05379200	0.00000000	-0.01359300
F	0.74148400	-1.06145000	0.00205200
F	0.74148000	1.06145200	0.00205200
H	-1.70808800	0.00002000	1.06598200

H	-0.87587200	-0.00000200	1.47603900

***cis*-DFE_p**, 7 atoms

atom	X	Y	Z
C	-0.74152600	0.53839800	-0.00000300
H	-1.36720600	1.46111900	-0.00000100
C	0.70894900	0.56823500	0.00000100
F	1.31915400	-0.61715200	-0.00000100
F	-1.36799800	-0.55587400	0.00000000
H	1.00115100	1.22817300	-0.87665900
H	1.00112500	1.22814900	0.87668000

***trans*-DFE_p**, 7 atoms

atom	X	Y	Z
C	-0.57345800	0.45510800	0.00000400
C	0.59994500	-0.41044700	0.00000300
F	1.75685800	0.10072300	-0.00000500
H	0.55894700	-1.52624800	0.00002000
H	-0.47703100	1.16174700	-0.88151500
F	-1.73061500	-0.21907700	-0.00000600
H	-0.47703200	1.16172000	0.88155400

TFE_p1, 7 atoms

atom	X	Y	Z
C	-0.82262000	-0.63527400	-0.02414200
C	0.49986300	-0.00646800	0.22124800
F	1.54165600	-0.73089100	-0.15288600
H	-0.98315100	-1.73655900	0.06215600
F	-1.85116200	0.08903200	-0.07559500
F	0.59538700	1.27832200	-0.06309400
H	0.34675100	-0.14116300	1.37938000

TFE_p2, 7 atoms

atom	X	Y	Z
C	0.81055000	-0.68775400	0.00000500
C	-0.50840200	-0.00701400	0.00000600
F	-1.58826500	-0.66169200	-0.00000300
H	0.81763000	-1.37493300	-0.89343400
F	1.82435000	0.18574400	-0.00000400
F	-0.61921500	1.24467000	0.00000100
H	0.81765400	-1.37494800	0.89342500

PFE_p, 7 atoms

atom	X	Y	Z
C	-0.79786500	0.00000000	0.35046600
C	0.73534800	0.00000000	0.04087400
F	1.38605700	-1.06623500	-0.04613600
F	-1.31656100	1.11204100	-0.16631100
F	1.38606400	1.06623100	-0.04613800
F	-1.31656300	-1.11203700	-0.16631400

MCE_p1, 7 atoms

atom	X	Y	Z
C	0.41541500	0.51708800	0.00000300
H	0.45383100	1.62787800	-0.00000100
C	1.62867700	-0.26277300	0.00000200
H	2.25589900	0.09010900	-0.86424200
H	1.50106400	-1.36003400	0.00003100
Cl	-1.10184100	-0.11611800	0.00000000
H	2.25594900	0.09016100	0.86418800

MCE_p2, 7 atoms

atom	X	Y	Z
C	-0.41541500	0.51708800	0.00000100
H	-0.45383100	1.62787900	-0.00000100
C	-1.62867800	-0.26277300	0.00000000
H	-2.25591300	0.09013100	-0.86422300
H	-1.50106600	-1.36003400	0.00000400
Cl	1.10184100	-0.11611800	0.00000000
H	-2.25592700	0.09013700	0.86421200

11-DCE_p1, 7 atoms

atom	X	Y	Z
C	0.00000000	0.30107900	0.01895700
C	0.00000100	1.77142100	0.01197800
H	0.92286000	2.18501300	0.46582700
H	-0.00002000	2.09159500	-1.06455400
Cl	-1.43406600	-0.55578300	-0.00155100
Cl	1.43406600	-0.55578300	-0.00155100
H	-0.92284500	2.18501100	0.46585700

11-DCE_p2, 7 atoms

atom	X	Y	Z
C	-0.38414600	0.39583700	0.54925500
C	0.65984200	1.08387000	-0.22937400
H	1.19574600	1.90006700	0.29234900
H	0.45020300	1.27786000	-1.29738500
Cl	-1.76116900	-0.23766600	-0.12270500
Cl	1.58493600	-0.49135900	-0.02829900
H	-0.30416200	0.33725400	1.65282000

***cis*-DCE_p**, 7 atoms

atom	X	Y	Z
C	0.52712400	0.58984400	0.16141900
C	-0.56448800	-0.37769600	0.23186400
H	-0.36889800	-1.42301900	0.55650600
Cl	2.11595600	-0.13426100	-0.10525300
Cl	-2.13083800	-0.00383100	-0.10561900

H	0.33175200	1.44379200	-0.52756200
H	0.51432900	1.05391300	1.19617900

***trans*-DCE_p**, 7 atoms

atom	X	Y	Z
C	0.68805000	0.97865300	0.00000500
C	-0.76488800	0.91647600	-0.00000700
Cl	1.62234900	-0.49622100	-0.00000300
H	0.96909900	1.64218000	-0.86800700
H	-1.34535100	1.86377800	-0.00002600
Cl	-1.63010100	-0.47547600	0.00000200
H	0.96906800	1.64212300	0.86806400

TCE_p1, 7 atoms

atom	X	Y	Z
C	-0.64866000	-1.00454700	0.00000700
C	0.51213300	-0.06926800	0.00000300
Cl	-2.25308200	-0.29210200	-0.00000300
H	-0.52606000	-1.68125600	-0.88392900
Cl	0.30384600	1.57733400	0.00000100
Cl	2.05931200	-0.70844400	-0.00000200
H	-0.52606400	-1.68125000	0.88394400

TCE_p2, 7 atoms

atom	X	Y	Z
C	0.74123700	-0.15549800	0.69696400
C	-0.74124100	-0.15547000	0.69697000
Cl	1.64394000	0.96161400	-0.18233600
H	1.25737300	-0.61990500	1.55930800
Cl	-1.64391400	0.96164900	-0.18233700
Cl	-0.00002400	-1.74058200	-0.31075400
H	-1.25737600	-0.61986300	1.55932800

PCE_p, 7 atoms

atom	X	Y	Z
C	-0.73648800	-0.00000100	0.39738800
C	0.75134400	0.00000000	0.07317400
Cl	-1.56279900	1.48984400	-0.08796000
Cl	1.58148400	1.43553400	-0.03987800
Cl	1.58148900	-1.43553100	-0.03987400
Cl	-1.56279800	-1.48984600	-0.08796500
H	-0.72453800	-0.00000300	1.52314000

MBE_p1, 7 atoms

atom	X	Y	Z
C	2.10857500	-0.28939600	-0.00000300
H	1.93660400	-1.38059400	-0.00002300
H	2.75071400	0.03075500	-0.86567300
C	0.93018600	0.54576900	-0.00000200
H	1.02467900	1.65198000	0.00000300
Br	-0.76272100	-0.05346000	0.00000000
H	2.75066900	0.03071400	0.86571900

MBE_p2, 7 atoms

atom	X	Y	Z
C	2.10857200	-0.28939800	0.00000000
H	1.93659700	-1.38059600	0.00000700
H	2.75068400	0.03072200	-0.86570100
C	0.93018600	0.54577400	0.00000100
H	1.02467800	1.65198700	-0.00000100
Br	-0.76272000	-0.05346000	0.00000000
H	2.75069700	0.03073200	0.86569000

11-DBE_p1, 7 atoms

atom	X	Y	Z
C	-0.00000600	2.06937500	-0.01073700
H	0.91971300	2.48681600	-0.46830800
H	-0.91977700	2.48680100	-0.46821700
C	0.00000100	0.59589800	-0.01884200
Br	1.57482300	-0.33373300	0.00073100
Br	-1.57482200	-0.33373400	0.00073100
H	0.00005100	2.39608700	1.06285800

11-DBE_p2, 7 atoms

atom	X	Y	Z
C	0.63062300	1.34473300	-0.26580600
H	0.38860800	1.47352200	-1.33609000
H	1.14595300	2.20202000	0.20778700
C	-0.32378300	0.61493500	0.57439600
Br	-1.84213500	-0.16943900	-0.05544200
Br	1.75197300	-0.28984500	-0.01310100
H	-0.21991700	0.64139200	1.67579000

***cis*-DBE_p**, 7 atoms

atom	X	Y	Z
C	-0.77499500	1.20999400	-0.00000400
H	-1.35018400	2.15934900	-0.00002700
C	0.67642900	1.27955400	0.00000400
Br	1.74599800	-0.30252200	-0.00000100
Br	-1.74569900	-0.29633200	0.00000100
H	0.96555200	1.93164300	-0.87056600
H	0.96553800	1.93159800	0.87061300

***trans*-DBE_p**, 7 atoms

atom	X	Y	Z
C	-0.32376400	0.61486400	0.57438200
C	0.63061500	1.34471600	-0.26578000
Br	1.75198100	-0.28983600	-0.01310600

H	0.38864900	1.47351400	-1.33606500
H	-0.21991000	0.64130500	1.67577200
Br	-1.84214600	-0.16943000	-0.05544200
H	1.14593100	2.20199500	0.20785600

TBE_p1, 7 atoms

atom	X	Y	Z
C	0.59260600	-1.15079300	0.00001800
C	-0.51305200	-0.15588800	0.00000300
Br	-2.23773200	-0.78602500	-0.00000300
H	0.45201600	-1.81773400	-0.88554900
Br	2.40964900	-0.52395400	-0.00000400
Br	-0.21138500	1.63785100	0.00000100
H	0.45202600	-1.81768200	0.88562700

TBE_p2, 7 atoms

atom	X	Y	Z
C	-0.73737400	-0.18162100	0.84747000
C	0.73733600	-0.18175300	0.84746200
Br	-0.00017300	-1.93993700	-0.17252700
H	-1.23935800	-0.61234400	1.73460700
Br	-1.76643900	1.01875500	-0.10857700
Br	1.76662100	1.01847200	-0.10857500
H	1.23925300	-0.61257800	1.73458100

PBE_p, 7 atoms

atom	X	Y	Z
C	-0.67439600	0.12823600	0.12362800
C	0.63294300	-0.40842300	0.62787000
Br	0.99708400	-1.75785700	-0.77719700
Br	-0.77734100	1.39874900	-1.18945500
Br	1.99323500	0.92055000	0.89114700
Br	-2.22014900	-0.48563600	0.90182800
H	0.49969200	-0.97207300	1.56970200

F. Cartesian Coordinates of Protonated Olefinic radicals

MFE_pr1, 7 atoms

atom	X	Y	Z
C	-1.19978900	-0.16938000	0.01105300
H	-2.01752000	0.54756100	-0.20510000
H	-1.27596300	-1.01498000	-0.70770600
C	0.11495100	0.50876500	-0.09389000
H	0.29811700	1.55037000	0.22584700
F	1.21017500	-0.28018900	0.01722200
H	-1.38717900	-0.59756100	1.02898000

MFE_pr2, 7 atoms

atom	X	Y	Z
C	1.22822600	-0.25239800	-0.03319800
H	2.16782600	0.25514200	-0.30053400
H	1.26396800	-1.28952200	0.33510400
C	-0.03863800	0.51162400	0.05597200
H	-0.09381600	1.29647400	-0.73790600
F	-1.15056500	-0.31907100	-0.05226700
H	-0.12042000	1.05418800	1.03709600

11-DFE_pr1, 7 atoms

atom	X	Y	Z
C	-1.39369800	0.00002400	0.04373000
H	-1.88390700	0.90116200	-0.37250000
H	-1.88394300	-0.90107300	-0.37255900
C	0.05883100	0.00000400	-0.30135900
F	0.73994100	-1.10285100	0.06332900
F	0.73999200	1.10282400	0.06333000
H	-1.54234600	-0.00000900	1.15090100

11-DFE_pr2, 7 atoms

atom	X	Y	Z
C	1.40147200	0.09701600	-0.09195500
H	2.21884400	-0.29852300	0.52841600
H	1.60516800	0.43120000	-1.12099300
C	-0.01021600	-0.00484100	0.35559500
F	-0.73338200	1.07101500	-0.10101000
F	-0.60539400	-1.14092400	-0.17153600
H	-0.12256500	-0.05654400	1.46364900

***cis*-DFE_pr**, 7 atoms

atom	X	Y	Z
C	-0.67824200	0.47081400	-0.30281700
H	-0.89883000	0.87272300	-1.30649500
C	0.65216300	0.47666800	0.33454400
F	1.51571800	-0.50752300	-0.19629500
F	-1.58515000	-0.41628000	0.14186800
H	1.13127100	1.46907000	0.17938000
H	0.54891700	0.28754000	1.42659700

***trans*-DFE_pr**, 7 atoms

atom	X	Y	Z
C	-0.65216600	0.47667600	-0.33454000
C	0.67824700	0.47082100	0.30281300
F	1.58514400	-0.41628400	-0.14186900
H	0.89882900	0.87271900	1.30649600
H	-0.54893200	0.28757200	-1.42659400
F	-1.51571100	-0.50753100	0.19629300
H	-1.13127900	1.46907100	-0.17934800

TFE_pr1, 7 atoms

atom	X	Y	Z
C	0.80808600	-0.55809800	0.29001300
C	-0.47614500	0.00904800	-0.25034300
F	-1.54012700	-0.79246600	-0.08492000
H	0.86206200	-1.63323900	0.01053600
F	1.89271700	0.12945200	-0.21530900
F	-0.76097100	1.26382800	0.11625100
H	0.82171400	-0.47978300	1.40724300

TFE_pr2, 7 atoms

atom	X	Y	Z
C	-0.83046300	-0.41137700	-0.35549400
C	0.43571800	0.00236100	0.30508200
F	1.40556300	-0.92385600	0.02703000
H	-0.88599000	-0.73595300	-1.40815000
F	-1.96871400	0.04685900	0.18058900
F	0.89034900	1.22022200	-0.17409100
H	0.30968200	0.10102900	1.40886900

PFE_pr, 7 atoms

atom	X	Y	Z
C	-0.70890800	-0.00000700	0.31433100
C	0.70134600	-0.00000700	-0.25403000
F	1.40043600	-1.10315800	0.01988600
F	-1.35829000	1.11375400	-0.11973200
F	1.40040200	1.10316300	0.01990700
F	-1.35832300	-1.11375000	-0.11971100
H	-0.71265900	0.00000500	1.43504300

MCE_pr1, 7 atoms

atom	X	Y	Z
C	-0.44919700	0.59759800	0.05216700
H	-0.45578000	1.68261100	-0.13091200
C	-1.65912200	-0.26320800	-0.00603000
H	-2.56713700	0.34209400	0.19518300
H	-1.79588300	-0.74843400	-1.00466200
Cl	1.12259300	-0.12914600	-0.00452000
H	-1.61535800	-1.08713000	0.74040600

MCE_pr2, 7 atoms

atom	X	Y	Z
C	1.64973600	0.36481700	0.00000000
H	1.97267200	0.83219600	-0.94363500
C	0.60408200	-0.66034000	0.00000200
H	0.59691300	-1.29278100	-0.90733200
H	0.59691100	-1.29277400	0.90734200
Cl	-1.09776800	0.15848700	-0.00000100
H	1.97265200	0.83222000	0.94363000

11-DCE_pr1, 7 atoms

atom	X	Y	Z
C	0.00000000	0.32235600	-0.23424400
C	-0.00001000	1.78950200	0.04119000
H	0.90225100	2.25879900	-0.40108600
H	-0.90229500	2.25879700	-0.40104700
Cl	-1.47567200	-0.56483900	0.02426500
Cl	1.47567800	-0.56483000	0.02426500
H	0.00001300	2.01562300	1.13545300

11-DCE_pr2, 7 atoms

atom	X	Y	Z
C	-0.02385500	0.40755300	0.43310500
C	0.01151900	1.74526400	-0.16000500
H	0.43417900	2.58559400	0.41199800
H	-0.21562700	1.87115400	-1.22916300
Cl	-1.50295400	-0.50576300	-0.06162600
Cl	1.49395900	-0.53970800	-0.07710700
H	0.00838400	0.39934700	1.53701400

***cis*-DCE_pr**, 7 atoms

atom	X	Y	Z
C	0.57795800	0.88637100	-0.37087000
C	-0.65195000	0.74495000	0.40777900
H	-0.74522800	1.11471200	1.44062600
Cl	1.85156500	-0.42556100	0.07331200
Cl	-1.86976000	-0.36959700	-0.07620600
H	0.41696300	0.76748100	-1.45853300
H	1.08154800	1.84757000	-0.15436400

***trans*-DCE_pr**, 7 atoms

atom	X	Y	Z
C	0.57795600	0.88636500	0.37087100
C	-0.65195600	0.74496800	-0.40776900
Cl	1.85156200	-0.42556000	-0.07331700
H	1.08154800	1.84757000	0.15439700
H	-0.74526700	1.11476900	-1.44060000
Cl	-1.86975200	-0.36960400	0.07620300
H	0.41695100	0.76745100	1.45853100

TCE_pr1, 7 atoms

atom	X	Y	Z
C	-0.85169100	0.00002100	0.96454500
C	0.51548900	0.00000000	0.42388900
Cl	-2.16827800	0.00001100	-0.36056800
H	-1.03849700	-0.90939800	1.56525500
Cl	1.20457600	1.47311900	-0.15681000
Cl	1.20453500	-1.47314200	-0.15680200
H	-1.03846300	0.90948100	1.56520200

H	0.00004900	2.32360700	1.13700100

TCE_pr2, 7 atoms

atom	X	Y	Z
C	0.79380100	-0.53967700	-0.46879900
C	-0.35477700	-0.09222400	0.32988500
Cl	2.38415900	-0.22939300	0.09717500
H	0.68764500	-0.82127200	-1.52736300
Cl	-0.80190000	1.66964700	-0.06025100
Cl	-1.76876400	-1.16343600	0.01864100
H	-0.15120500	-0.09323200	1.41624700

PCE_pr, 7 atoms

atom	X	Y	Z
C	-0.61927200	-0.36659800	0.50436100
C	0.72000400	0.20518900	0.23365100
Cl	-1.84257900	0.91549500	0.80073900
Cl	0.92824200	1.40722700	-0.97317700
Cl	2.09620400	-0.73085200	0.69390800
Cl	-1.18333800	-1.47539800	-0.86432200
H	-0.57938000	-1.01156200	1.40041400

MBE_pr1, 7 atoms

atom	X	Y	Z
C	2.14240200	-0.29528800	-0.00670200
H	2.27971500	-0.75094100	-1.01902300
H	3.07468700	0.25865900	0.23287100
C	0.97808700	0.62590600	0.05654800
H	1.04023200	1.70591600	-0.14388000
Br	-0.77606300	-0.05877100	-0.00223800
H	2.04465600	-1.14036400	0.70929300

MBE_pr2, 7 atoms

atom	X	Y	Z
C	2.11405900	-0.42749000	0.00000100
H	2.40063200	-0.91908800	0.94303800
H	2.40063300	-0.91907700	-0.94304100
C	1.19751100	0.68678700	0.00000100
H	1.19084300	1.30332100	-0.91552300
Br	-0.77292500	-0.06640800	0.00000000
H	1.19083600	1.30332900	0.91552200

11-DBE_pr1, 7 atoms

atom	X	Y	Z
C	0.00002900	2.09296100	0.04413100
H	0.90212000	2.56353600	-0.39915600
H	-0.90207100	2.56353800	-0.39912700
C	-0.00000300	0.62588600	-0.23386400
Br	1.61221300	-0.33948800	0.01142400
Br	-1.61222000	-0.33947600	0.01142400

11-DBE_pr2, 7 atoms

atom	X	Y	Z
C	0.00864900	2.02233300	-0.18619300
H	-0.44522300	2.87647600	0.34151100
H	0.26494800	2.12151400	-1.25162900
C	0.05710200	0.73032800	0.46305900
Br	-1.64830000	-0.32050700	-0.03584700
Br	1.64202300	-0.31547900	-0.03030900
H	0.00546100	0.74556100	1.56440000

***cis*-DBE_pr**, 7 atoms

atom	X	Y	Z
C	-0.64467100	0.96102000	-0.44463600
H	-0.69799700	1.31577600	-1.48512500
C	0.51975500	1.15678200	0.38773600
Br	2.00214200	-0.25567000	-0.03060100
Br	-2.00064700	-0.23408500	0.03594000
H	1.04289300	2.10576100	0.17047100
H	0.35228900	1.01307900	1.46919500

***trans*-DBE_pr**, 7 atoms

atom	X	Y	Z
C	-0.64466100	0.96104200	0.44462800
C	0.51975500	1.15681200	-0.38773100
Br	2.00211400	-0.25567700	0.03060100
H	0.35230600	1.01312600	-1.46919400
H	-0.69798800	1.31579700	1.48511700
Br	-2.00062200	-0.23409000	-0.03594000
H	1.04289100	2.10578200	-0.17043700

TBE_pr1, 7 atoms

atom	X	Y	Z
C	0.81295200	0.00003100	1.16053000
C	-0.49724100	-0.00000100	0.52641200
Br	-1.24174800	-1.60867700	-0.09784000
H	0.99441000	-0.91479400	1.75240500
Br	2.37262000	0.00002600	-0.19364100
Br	-1.24181600	1.60864300	-0.09784500
H	0.99438800	0.91488600	1.75236600

TBE_pr2, 7 atoms

atom	X	Y	Z
C	-0.85401400	-0.30459500	1.11970800
C	0.52056700	0.08573100	0.85274700
Br	1.52039100	-1.38848300	-0.15299900
H	-1.11733000	-0.79093300	2.07207500
Br	-2.17744600	-0.34442800	-0.18727700

Br	0.71476500	1.78787900	-0.10816800
H	1.09815800	0.18024300	1.78875300

PBE_pr, 7 atoms

atom	X	Y	Z
C	-0.72953900	0.18278500	0.21786600
C	0.57268500	-0.37704800	0.58860200
Br	1.27729500	-1.67088700	-0.81256200
Br	-0.91186000	1.41699100	-1.17393100
Br	1.92026100	1.00584800	0.95852700
Br	-2.27297000	-0.69019900	0.84689500
H	0.49572300	-0.99576000	1.49870200

G. Cartesian Coordinates of Protonated Dehalogenated Olefinic Radical Cations

MFE_rc1, 6 atoms

atom	X	Y	Z
C	0.69670400	0.00000000	0.00000500
H	1.27808700	0.90864300	0.27250700
H	1.27805900	-0.90865500	-0.27253200
C	-0.69670400	0.00000100	-0.00000100
H	-1.27807200	0.90864800	-0.27252100
H	-1.27807900	-0.90863800	0.27252100

MFE_rc2, 6 atoms

atom	X	Y	Z
C	-0.66282700	0.05545300	-0.05363700
H	-1.09764500	0.95472400	0.46992500
H	-1.37077100	-0.79935400	-0.19247600
C	0.69442600	-0.04491100	-0.08950900
H	1.51372300	0.70415000	-0.04441000
H	0.76509700	-0.92277700	0.62583700

11-DFE_rc1, 6 atoms

atom	X	Y	Z
C	-1.21001300	-0.18603200	-0.00000400
H	-2.12880400	0.42796000	0.00001500
H	-1.27481300	-1.29076900	0.00000900
C	0.05903300	0.45642000	-0.00000300
F	1.12071800	-0.25712100	0.00000100
H	0.22303700	1.55457500	0.00000700

11-DFE_rc2, 6 atoms

atom	X	Y	Z
C	1.18988600	0.12165100	0.00000100
H	1.73634500	-0.32864600	-0.87367400
H	1.21141400	1.23583600	0.00000200
C	-0.12713400	-0.42843100	0.00000100
F	-1.22896000	0.14023800	0.00000000
H	1.73636600	-0.32865100	0.87365900

***cis*-DFE_rc**, 6 atoms

atom	X	Y	Z
C	-0.05902800	0.45641400	0.00000300
H	-0.22305700	1.55456800	0.00002500
C	1.21001600	-0.18602900	-0.00000300
F	-1.12072000	-0.25711900	-0.00000400
H	2.12880700	0.42796000	-0.00002800
H	1.27480800	-1.29076500	0.00003800

***trans*-DFE_rc**, 6 atoms

atom	X	Y	Z
C	1.21001200	-0.18602900	-0.00000100
C	-0.05902800	0.45641800	0.00000100
F	-1.12071600	-0.25712100	-0.00000100
H	-0.22305900	1.55457200	0.00000100
H	1.27478800	-1.29076700	0.00000500
H	2.12881400	0.42794400	-0.00000300

TFE_rc1, 6 atoms

atom	X	Y	Z
C	-1.41766800	-0.00002400	-0.00000500
C	0.00742900	0.00000000	-0.00000800
F	0.68731700	1.07549500	0.00000500
H	-1.95530700	0.96448400	-0.00000800
F	0.68736000	-1.07547600	0.00000000
H	-1.95535000	-0.96451300	0.00004700

TFE_rc2, 6 atoms

atom	X	Y	Z
C	-0.57782700	-0.41858900	0.00000800
C	0.57782500	0.41858100	0.00000200
F	1.72690000	-0.14717400	-0.00000300
H	-0.54715600	-1.52832600	-0.00000600
F	-1.72689800	0.14718000	-0.00000400
H	0.54714700	1.52832100	0.00000500

TFE_rc3, 6 atoms

atom	X	Y	Z
C	0.71464600	0.56953700	0.00000300
C	-0.71464700	0.56953700	0.00000300
F	-1.34154900	-0.54622100	-0.00000300
H	1.31979100	1.49876100	0.00000800
F	1.34154900	-0.54622100	-0.00000300
H	-1.31979100	1.49876100	0.00000800

PFE_rc, 6 atoms

atom	X	Y	Z
C	0.80346300	-0.64730400	0.00000400
C	-0.48202800	-0.01469800	-0.00000900
F	-0.61666500	1.25032400	-0.00000100
F	-1.54501500	-0.71629300	0.00000400
F	1.84393300	0.10150700	0.00000200
H	0.93111700	-1.74782300	-0.00002700

MCE_rc1, 6 atoms

atom	X	Y	Z
C	0.69670300	0.00000300	-0.00000500
H	1.27807700	-0.90864600	-0.27251500
H	1.27806100	0.90865400	0.27253300
C	-0.69670600	-0.00000100	0.00000300
H	-1.27808100	0.90864400	-0.27252400
H	-1.27804100	-0.90866400	0.27252100

MCE_rc2, 6 atoms

atom	X	Y	Z
C	0.69670100	0.00000100	0.00000000
H	1.27806700	-0.90864800	0.27253000
C	-0.69670100	0.00000000	-0.00000100
H	-1.27806700	-0.90864700	-0.27252900
H	-1.27807100	0.90864600	0.27253000
H	1.27807400	0.90864400	-0.27252900

11-DCE_rc1, 6 atoms

atom	X	Y	Z
C	1.70914900	0.14076200	0.00000100
H	2.26715400	-0.29558400	-0.87297000
H	1.74625000	1.25385600	0.00000800
C	0.40471300	-0.43569000	0.00000100
H	2.26717400	-0.29560000	0.87295100
Cl	-1.11551500	0.06511100	0.00000000

11-DCE_rc2, 6 atoms

atom	X	Y	Z
C	-0.50018700	0.53336700	0.00001900
C	-1.64430900	-0.28617800	-0.00001000
H	-1.56717000	-1.38853900	0.00001200
H	-2.64382700	0.18587000	0.00000500
Cl	1.03746300	-0.11290800	-0.00000200
H	-0.55888900	1.63897600	-0.00004100

***cis*-DCE_rc**, 6 atoms

atom	X	Y	Z
C	-1.64429000	-0.28618900	-0.00000500
C	-0.50020200	0.53337900	-0.00000800
H	-0.55888700	1.63898200	-0.00001100
Cl	1.03745700	-0.11290800	0.00000300
H	-1.56713800	-1.38854400	-0.00002000
H	-2.64379800	0.18586600	0.00006100

***trans*-DCE_rc**, 6 atoms

atom	X	Y	Z
C	1.64430200	-0.28618100	0.00000000
C	0.50019800	0.53336300	0.00000000
H	2.64380900	0.18587100	-0.00000300
H	0.55889400	1.63896900	0.00000200
Cl	-1.03746100	-0.11290600	0.00000000
H	1.56714300	-1.38853500	0.00000400

TCE_rc1, 6 atoms

atom	X	Y	Z
C	0.00003800	1.75811700	0.00000000
C	0.00000800	0.34365300	0.00000400
H	-0.95581500	2.30987000	-0.00001300
Cl	1.45592200	-0.50679000	-0.00000100
Cl	-1.45594300	-0.50675900	0.00000000
H	0.95590200	2.30984300	0.00000500

TCE_rc2, 6 atoms

atom	X	Y	Z
C	-0.70576200	0.93645900	0.00000100
C	0.70577900	0.93646400	0.00000500
Cl	-1.64061900	-0.44247200	0.00000100
H	-1.24383900	1.90330800	-0.00004200
Cl	1.64061300	-0.44247900	-0.00000200
H	1.24384200	1.90331900	0.00002100

TCE_rc3, 6 atoms

atom	X	Y	Z
C	-0.37817100	0.59269200	0.00001200
C	0.37817100	-0.59269200	0.00001200
Cl	0.37817100	2.08178000	-0.00000500
H	-1.48470000	0.58789700	0.00000900
H	1.48470000	-0.58789700	0.00000900
Cl	-0.37817100	-2.08178000	-0.00000500

PCE_rc, 6 atoms

atom	X	Y	Z
C	-0.67077200	-0.91874500	-0.00000600
C	0.47012300	-0.06910800	0.00000900
Cl	-2.23463500	-0.34416900	0.00000100
Cl	0.34295500	1.60884000	-0.00000100
Cl	1.99381900	-0.79747100	-0.00000100

H	-0.53246100	-2.01528900	0.00000600

MBE_rc1, 6 atoms

atom	X	Y	Z
C	0.69670300	0.00000000	0.00000300
H	1.27806300	-0.90865100	-0.27253300
H	1.27808000	0.90864500	0.27251700
C	-0.69670300	0.00000100	0.00000000
H	-1.27807200	0.90864700	-0.27252700
H	-1.27807300	-0.90864300	0.27252600

MBE_rc2, 6 atoms

atom	X	Y	Z
C	0.67167800	0.02978500	-0.02644600
H	1.38576400	-0.82623100	-0.16640700
H	1.09774300	1.00003500	0.36178300
C	-0.68944400	-0.04633600	-0.07486800
H	-1.39478000	0.81837000	-0.08594000
H	-0.98212900	-0.89286800	0.49844300

11-DBE_rc1, 6 atoms

atom	X	Y	Z
C	-2.21654100	-0.14984300	0.00000100
H	-2.78161000	0.27422800	-0.87434000
H	-2.24338900	-1.26319600	0.00001300
C	-0.92134400	0.44868900	0.00000100
Br	0.76097000	-0.03081000	0.00000000
H	-2.78163200	0.27425200	0.87431600

11-DBE_rc2, 6 atoms

atom	X	Y	Z
C	2.09898100	-0.31927400	-0.00000100
H	3.12376600	0.09636300	-0.00001800
H	1.97099100	-1.41640400	0.00000900
C	1.01373300	0.55708300	0.00000900
Br	-0.71139400	-0.05039100	-0.00000100
H	1.12775100	1.65686300	-0.00001100

***cis*-DBE_rc**, 6 atoms

atom	X	Y	Z
C	1.01370900	0.55708400	-0.00000600
H	1.12767500	1.65688600	0.00004200
C	2.09898300	-0.31926900	-0.00000100
Br	-0.71138900	-0.05039300	0.00000000
H	3.12376500	0.09639900	-0.00002300
H	1.97100500	-1.41641500	0.00003600

***trans*-DBE_rc**, 6 atoms

atom	X	Y	Z
C	-1.01373000	0.55708400	-0.00001600
C	-2.09898500	-0.31927000	0.00000500
H	-1.97100200	-1.41640100	-0.00003800
H	-1.12771500	1.65686600	0.00000400
Br	0.71139400	-0.05039200	0.00000200
H	-3.12377200	0.09636400	0.00004600

TBE_rc1, 6 atoms

atom	X	Y	Z
C	0.00000100	2.02517000	0.00000100
C	0.00000800	0.62365300	-0.00000700
Br	1.60329100	-0.30088000	0.00000100
H	0.95208600	2.58434000	-0.00001300
Br	-1.60329200	-0.30088000	0.00000000
H	-0.95212200	2.58429000	0.00002000

TBE_rc2, 6 atoms

atom	X	Y	Z
C	0.69915800	1.20963400	0.00001600
C	-0.69916800	1.20964100	-0.00001000
H	1.22935800	2.18014200	-0.00001300
Br	1.76818400	-0.26965500	-0.00000100
Br	-1.76818200	-0.26965800	0.00000100
H	-1.22938400	2.18013900	-0.00000900

TBE_rc3, 6 atoms

atom	X	Y	Z
C	0.50602000	-0.47774500	0.00001800
C	-0.50602000	0.47774500	-0.00001800
H	0.30616300	-1.56462800	0.00005900
Br	2.26764500	0.02431100	0.00000000
Br	-2.26764500	-0.02431100	0.00000000
H	-0.30616200	1.56462800	-0.00005900

PBE_rc, 6 atoms

atom	X	Y	Z
C	-0.46072700	-0.14025500	-0.00000100
C	0.62286800	-1.04158900	-0.00000700
Br	-0.25807000	1.69420700	0.00000000
Br	2.38318200	-0.55725400	0.00000100
Br	-2.16505600	-0.87353900	0.00000100
H	0.42521400	-2.12842300	-0.00001900

H. Cartesian Coordinates of Cobalamins

Cob(I)alamin, 179 atoms

atom	X	Y	Z

Co	1.95782100	-1.6376170	1.03266800
N	2.11526400	0.06726500	1.67878300
N	3.60451800	-1.4310720	0.12389400
N	1.58529100	-3.3548330	0.30685900
N	0.38713000	-1.6498010	1.98081800
C	0.84124800	0.73687800	2.07855600
C	1.32699800	1.95983500	2.98338200
C	2.77623700	2.23334800	2.41132200
H	3.45261400	2.42379200	3.27302900
C	3.14595100	0.89959800	1.77865900
C	4.45472100	0.57958600	1.28015300
C	4.60522600	-0.4919170	0.40117100
C	5.87785700	-0.8608810	-0.4035990
C	5.21017200	-1.6014010	-1.6115070
H	5.89393500	-2.3702510	-2.0266390
C	4.02244800	-2.2187950	-0.9157990
C	3.45473800	-3.4467120	-1.2594470
H	3.94899100	-4.0204160	-2.0565170
C	2.33851300	-4.0063660	-0.6374320
C	1.85703200	-5.4448130	-0.8591010
C	0.38861900	-5.3243860	-0.3494720
H	0.07047900	-6.2659360	0.1443340
C	0.49858900	-4.1570510	0.62985500
C	-0.48667900	-3.8741530	1.57680500
C	-0.57678600	-2.5636320	2.14455600
C	-1.79264900	-1.9877470	2.90086700
C	-1.50102600	-0.4490850	2.74661000
H	-1.79932900	-0.1864110	1.71096100
C	0.04232400	-0.4176200	2.74300300
H	0.42111400	-0.5596100	3.77948900
C	0.13047700	1.21279800	0.79417000
H	0.78303900	1.89112900	0.21046800
H	-0.81938300	1.73094500	1.02836400
H	-0.08759800	0.33748400	0.15063900
C	0.37692000	3.17053900	2.91821000
H	-0.67847500	2.88412000	3.10680200
H	0.37726500	3.64459300	1.91884100
H	0.66622100	3.94742700	3.65603300
C	1.48450800	1.51619800	4.47764800
H	2.17552600	0.64834800	4.52931300
H	0.50388700	1.18194700	4.87426000
C	2.05413000	2.59426200	5.40256700
O	3.23854100	2.94231400	5.40305200
N	1.14563700	3.16145000	6.26560700
H	1.46342200	3.92923700	6.86031100
H	0.14814200	2.95641400	6.21836200
C	2.97947100	3.42614000	1.43995500
H	2.15656600	3.48974600	0.69715800
H	3.89357400	3.23891200	0.84205200
C	3.18415400	4.78694000	2.12569700
H	3.84387900	4.65168100	3.01381500
H	2.23403100	5.20705300	2.51657100
C	3.88526700	5.79534000	1.21043400
O	4.77361700	5.48015000	0.41784600
N	3.47908900	7.10171400	1.35750100
H	3.93311700	7.81844800	0.78865800
H	2.71095900	7.36885800	1.97190400
C	5.62390700	1.43925400	1.73242700
H	6.54157400	0.83520000	1.87411800
H	5.40211900	1.90589200	2.71283700
H	5.88146200	2.26662300	1.03642000
C	6.79759600	0.28981100	-0.8546500
H	6.22477900	1.16252900	-1.2216020
H	7.44675900	-0.0617780	-1.6830730
H	7.46576900	0.64264600	-0.0462880
C	6.68951100	-1.8932710	0.45827700
H	6.88909200	-1.4474570	1.45597700
H	6.05509800	-2.7901390	0.62011900
C	7.98982600	-2.3641740	-0.1945630
O	8.02780700	-3.0348220	-1.2271140
N	9.14110500	-1.9802180	0.45539800
H	10.03798900	-2.2436230	0.04307100
H	9.13068400	-1.4017930	1.29386900
C	4.77647900	-0.6243270	-2.7429900
H	4.34379100	0.29469100	-2.2896300
H	5.67666200	-0.3127180	-3.3134260
C	3.75526700	-1.1948930	-3.7461300
H	4.09948300	-2.1892950	-4.1038590
H	2.76772500	-1.3366950	-3.2614010
C	3.66201200	-0.3071630	-4.9945450
O	4.59029700	-0.2485900	-5.8074330
N	2.50662900	0.41106400	-5.1439790
H	2.46999300	1.03375800	-5.9547210
H	1.74273300	0.51030600	-4.4495700
C	2.64500100	-6.3753830	0.10325200
H	3.72824300	-6.3654390	-0.1383240
H	2.27633100	-7.4207830	0.02179500
H	2.52747900	-6.0482590	1.15726800
C	2.03683000	-5.9538800	-2.2983120
H	1.53474500	-5.3065830	-3.0447290
H	1.64033700	-6.9852450	-2.4019280
H	3.11343300	-5.9938470	-2.5660770
C	-0.67971000	-4.9455800	-1.4215780
H	-1.47833800	-4.3583090	-0.9219760
H	-0.22550000	-4.2449130	-2.1551300
C	-1.35476200	-6.1183520	-2.1651330
H	-2.03234300	-5.6982050	-2.9405250
H	-0.61090400	-6.7581960	-2.6762790
C	-2.15369700	-7.0472700	-1.2405270
O	-1.74458400	-8.1716290	-0.9314550
N	-3.34539500	-6.5468730	-0.7851570
H	-3.83367100	-7.1211380	-0.0944040
H	-3.64843500	-5.5605790	-0.8576430
C	-1.49962000	-4.9563110	1.91205500
H	-1.03140300	-5.9589130	1.86624300
H	-2.37245000	-4.9887910	1.22346300
H	-1.89615100	-4.8423180	2.93857200
C	-1.77973700	-2.4425270	4.38176200

H	-2.67315200	-2.0781160	4.93379300
H	-0.87620200	-2.0804730	4.91456000
H	-1.78314500	-3.5482580	4.45553600
C	-2.27790600	0.48898400	3.71411400
H	-2.80984400	-0.0953970	4.49362700
H	-1.57316900	1.15499100	4.25365200
C	-3.24959900	1.40929500	2.95103300
O	-2.80002600	2.34297200	2.26320700
N	-4.57116700	1.12028200	3.03368500
H	-5.31216000	1.63354200	2.46282300
H	-4.88362700	0.35864900	3.63659000
C	-3.16562900	-2.3425010	2.25908100
H	-3.92757400	-1.6615130	2.70055500
H	-3.47090800	-3.3644490	2.56235300
C	-3.21901100	-2.2347670	0.71894300
H	-3.09491500	-1.1784140	0.39738800
H	-2.38344900	-2.8028950	0.26783400
C	-4.51584200	-2.8010700	0.13993800
O	-4.59010800	-3.9160930	-0.4090630
N	-5.59442900	-1.9900600	0.30353700
H	-5.48653600	-1.0742690	0.75709300
C	-6.95817400	-2.2720790	-0.1087290
H	-7.52729300	-2.7546480	0.72174500
H	-6.93878600	-2.9861230	-0.9574050
C	-7.64584500	-0.9479270	-0.4910780
H	-7.17844600	-0.5651130	-1.4264020
C	-9.15409600	-1.0686220	-0.6867000
H	-9.64216700	-1.4278230	0.24367500
H	-9.39653000	-1.7718640	-1.5116970
H	-9.55567200	-0.0666160	-0.9361280
P	-7.02966800	1.57292700	0.24741100
O	-8.04742700	2.16387200	-0.6992000
O	-6.60681300	2.20982700	1.56444900
O	-5.58579000	1.24546400	-0.6513560
O	-7.34732200	-0.0367790	0.58891300
C	-2.76643600	3.02957200	-2.02122100
H	-2.68635200	4.04449700	-1.56414000
C	-3.34712700	2.08231700	-0.95765000
H	-2.98265200	2.32832200	0.06489900
C	-4.85761700	2.37038400	-1.11036100
H	-5.12631000	3.28087700	-0.52690100
C	-5.01003000	2.61365400	-2.63085000
H	-5.25850900	1.65253200	-3.13518000
C	-6.03861300	3.67070400	-3.01780100
H	-7.04361400	3.31776200	-2.70249600
H	-5.82078600	4.60564900	-2.43654700
O	-3.70260200	3.04422400	-3.10308500
O	-3.10724400	0.71671300	-1.27817400
H	-3.97627400	0.28480200	-1.09418000
O	-6.04099000	3.90648000	-4.41683000
H	-5.09887600	4.03883100	-4.64743700
N	-1.43546500	2.72154800	-2.51047300
C	-0.98752600	1.53986900	-3.08545100
H	-1.66063300	0.67945800	-3.17140400
N	0.27906800	1.58564000	-3.46085300
C	1.97487200	3.47468400	-3.28808500
H	2.79962800	2.90203800	-3.74009400
C	2.16717400	4.80228800	-2.86792000
C	1.07607900	5.53859700	-2.29034200
C	-0.18534900	4.93543500	-2.12358700
H	-1.01313800	5.51045000	-1.67823600
C	-0.35206300	3.60379400	-2.53829800
C	0.71298700	2.86779700	-3.12714600
C	3.52956800	5.44713300	-3.00592500
H	4.22843700	4.78366500	-3.55285300
H	3.98441400	5.65942200	-2.01264400
H	3.48135600	6.41226300	-3.55646200
C	1.27725300	6.97277600	-1.85070500
H	2.02491400	7.05179700	-1.03095000
H	0.32964900	7.41784600	-1.48537600
H	1.65075800	7.61171000	-2.68076400

Cob(II)alamin, 179 atoms

atom	X	Y	Z
Co	1.83211000	-1.69475900	1.06162400
N	2.06661400	0.02268600	1.72585600
N	3.48684100	-1.54665500	0.13135500
N	1.34063800	-3.37851200	0.29517600
N	0.24893300	-1.62861100	2.05419100
C	0.81497400	0.74672400	2.10823400
C	1.36519600	1.95846700	2.99223800
C	2.83465300	2.13711200	2.42748800
H	3.51518000	2.29729600	3.29214800
C	3.13950600	0.77951800	1.82226200
C	4.44411300	0.37702300	1.34267100
C	4.54125600	-0.67399800	0.43706900
C	5.78553200	-1.10347300	-0.37954500
C	5.07340600	-1.79514700	-1.59670900
H	5.70553300	-2.60819500	-2.00746000
C	3.84337500	-2.33646900	-0.91969400
C	3.18626600	-3.51351400	-1.29517800
H	3.63777700	-4.09419600	-2.11082900
C	2.04448300	-4.02937600	-0.67995300
C	1.47586200	-5.42458500	-0.95023000
C	0.03745800	-5.26508000	-0.36580400
H	-0.28555100	-6.20667000	0.12295800
C	0.22029200	-4.12722200	0.62919900
C	-0.72035600	-3.81290400	1.60973300
C	-0.74605000	-2.49652200	2.18905300
C	-1.93042700	-1.86710400	2.95672500
C	-1.57584000	-0.34038000	2.79557800
H	-1.85844300	-0.07557300	1.75582600
C	-0.03349500	-0.36580100	2.79512400
H	0.34597200	-0.50869300	3.83105800
C	0.12876400	1.22545000	0.81368500
H	0.80257200	1.87472500	0.22172200
H	-0.80141400	1.77864200	1.04838000

H	-0.14142500	0.35960600	0.17485000
C	0.49245800	3.22226100	2.88811200
H	-0.57801600	3.00252000	3.08068000
H	0.52615000	3.67057200	1.87771000
H	0.83045100	3.99584900	3.60725900
C	1.47869800	1.54591100	4.49825900
H	2.09146300	0.62366500	4.59065900
H	0.47050600	1.31389200	4.89871600
C	2.15176200	2.59973200	5.38697700
O	3.35696700	2.86329800	5.31962900
N	1.32643200	3.23709800	6.27428800
H	1.72873000	3.95588100	6.87984200
H	0.32424400	3.05760000	6.32347100
C	3.11843000	3.29070200	1.43099200
H	2.30158400	3.39288800	0.68646100
H	4.01740300	3.02918400	0.83737400
C	3.42467100	4.64922800	2.08218100
H	3.93130300	4.48911000	3.06162800
H	2.50524500	5.22900600	2.30701000
C	4.39025900	5.47821000	1.22173700
O	5.24521900	4.96309400	0.49862400
N	4.25548300	6.83745600	1.33302500
H	4.91610400	7.43565500	0.83300600
H	3.55708600	7.27086900	1.93624800
C	5.64894600	1.16467100	1.82573100
H	6.55136300	0.52891500	1.88709400
H	5.46561600	1.55592400	2.84620600
H	5.89879900	2.04043500	1.18940000
C	6.75799200	0.00665100	-0.82014500
H	6.23114200	0.91453000	-1.16918400
H	7.38040200	-0.36564200	-1.65892000
H	7.45032200	0.30789100	-0.01199600
C	6.54777500	-2.18183700	0.46828300
H	6.83255100	-1.73644300	1.44491800
H	5.86233600	-3.02883600	0.68328600
C	7.77121100	-2.77133100	-0.24766600
O	7.67860900	-3.42628200	-1.28622600
N	8.97960200	-2.51594000	0.34684100
H	9.82166500	-2.89970300	-0.08783600
H	9.06892400	-1.99730200	1.21932900
C	4.70237000	-0.79202000	-2.72815700
H	4.35170600	0.16194500	-2.27644400
H	5.62156400	-0.56130300	-3.30525300
C	3.63696900	-1.27751400	-3.72658300
H	3.87471000	-2.31186500	-4.05847600
H	2.62874600	-1.29767500	-3.26352700
C	3.66497400	-0.41585400	-5.00158600
O	4.67664800	-0.37385500	-5.70593900
N	2.51659700	0.26515100	-5.28843100
H	2.55164400	0.87244300	-6.11162400
H	1.73197200	0.41842100	-4.62259500
C	2.26587800	-6.43398100	-0.07014300
H	3.33437800	-6.46974000	-0.36610500
H	1.83501900	-7.45012200	-0.18671200
H	2.21462700	-6.16102600	1.00438700
C	1.56598700	-5.86456100	-2.42061000
H	1.07799800	-5.15055300	-3.11281700
H	1.09420700	-6.85911500	-2.55254700
H	2.62447600	-5.96745800	-2.73644500
C	-1.07830600	-4.84086400	-1.37545800
H	-1.80949500	-4.19720700	-0.84341400
H	-0.64058600	-4.19282400	-2.16452700
C	-1.86991800	-5.99862000	-2.01995900
H	-2.60959200	-5.56865300	-2.72788600
H	-1.20324700	-6.67382100	-2.59033800
C	-2.56994400	-6.86569700	-0.96527100
O	-2.02747000	-7.87487300	-0.49999300
N	-3.80270300	-6.43004100	-0.56351300
H	-4.22568100	-6.94503200	0.21289700
H	-4.14958200	-5.46909100	-0.72077900
C	-1.78117300	-4.84389800	1.94932400
H	-1.37906900	-5.86963100	1.84575800
H	-2.67758800	-4.79097800	1.29434200
H	-2.12755800	-4.74182800	2.99437400
C	-1.90224200	-2.32832000	4.43501300
H	-2.75642800	-1.90337200	5.00189800
H	-0.96700000	-2.02571300	4.94966000
H	-1.98068000	-3.43069700	4.51227700
C	-2.32554900	0.63273100	3.74583400
H	-2.91881800	0.07570600	4.50028400
H	-1.60461500	1.25328000	4.31744000
C	-3.20906000	1.60713500	2.93771800
O	-2.65826900	2.46223700	2.22024400
N	-4.54671000	1.43823200	3.01035900
H	-5.24144900	1.98181800	2.39284500
H	-4.93236900	0.74546300	3.65330000
C	-3.32245000	-2.16315600	2.33143000
H	-4.04592400	-1.45558600	2.79334900
H	-3.66580900	-3.17323500	2.63123200
C	-3.39441300	-2.02836700	0.79527000
H	-3.25381200	-0.96922200	0.49144300
H	-2.58021800	-2.60606300	0.31695700
C	-4.71034200	-2.56490400	0.21995300
O	-4.80543400	-3.69002500	-0.30479100
N	-5.75390900	-1.71475000	0.36549000
H	-5.60855100	-0.78400700	0.77952200
C	-7.12367500	-1.91392900	-0.07947700
H	-7.74488400	-2.32892500	0.74870900
H	-7.13650500	-2.64851300	-0.91003900
C	-7.69446600	-0.54764400	-0.51271200
H	-7.19386500	-0.23982200	-1.45847600
C	-9.20642200	-0.54345000	-0.70636000
H	-9.72346100	-0.82166800	0.23559600
H	-9.50881500	-1.25477300	-1.50372100
H	-9.52150000	0.47775200	-0.99770300
P	-6.87266600	1.93874500	0.15011800
O	-7.82369400	2.57558000	-0.83103700
O	-6.41744900	2.58179500	1.45433000

O	-5.43798600	1.48321700	-0.71609000
O	-7.31049500	0.36944700	0.53788800
C	-2.54145100	3.09737100	-2.14017600
H	-2.43249400	4.14612200	-1.77338100
C	-3.17392200	2.25932000	-1.01427100
H	-2.83728500	2.58261800	-0.00444400
C	-4.67333900	2.55509800	-1.24127500
H	-4.94370200	3.51663200	-0.74794900
C	-4.77510000	2.67318900	-2.78020200
H	-5.02536900	1.67833500	-3.21330300
C	-5.77418000	3.70797000	-3.28639600
H	-6.78886600	3.41219100	-2.94485900
H	-5.54035700	4.69223800	-2.80156000
O	-3.44280300	3.04054400	-3.24230800
O	-2.94710900	0.86513600	-1.20381600
H	-3.84324800	0.47528100	-1.05421000
O	-5.76706300	3.79476300	-4.70029600
H	-4.83069100	3.93554400	-4.94567100
N	-1.21142500	2.69479600	-2.56860000
C	-0.84647700	1.49475000	-3.15551000
H	-1.58750000	0.70012600	-3.29751400
N	0.43338600	1.44032700	-3.48879300
C	2.26697100	3.19014600	-3.24229700
H	3.05301400	2.57314400	-3.70416900
C	2.54940500	4.49459100	-2.80141600
C	1.50716500	5.30073300	-2.22535200
C	0.20116300	4.79103400	-2.09057600
H	-0.59011900	5.42110000	-1.65393000
C	-0.05891900	3.48404700	-2.53728400
C	0.96060300	2.67611600	-3.11267100
C	3.95249100	5.04623300	-2.93308500
H	4.60350800	4.34636900	-3.49338200
H	4.42491000	5.21460400	-1.93994400
H	3.96746700	6.01965800	-3.46934700
C	1.80468300	6.71464700	-1.77542400
H	2.59351300	6.74730400	-0.99240600
H	0.89973700	7.20666800	-1.36599600
H	2.17426700	7.34190700	-2.61607500

Cob(III)alamin, 179 atoms

atom	X	Y	Z
Co	1.81007000	-1.69423900	1.03193700
N	2.06570700	-0.00813200	1.68759800
N	3.48927100	-1.57877400	0.16298100
N	1.31524200	-3.36378600	0.26448700
N	0.27167700	-1.66073800	2.02508100
C	0.83703400	0.71226000	2.14505100
C	1.41537300	1.87310500	3.07512400
C	2.85729800	2.08265500	2.46289800
H	3.56624500	2.22205700	3.30850800
C	3.15000700	0.75025400	1.80792400
C	4.44904800	0.36085600	1.32920400
C	4.54473200	-0.70150700	0.42658100
C	5.76161600	-1.09400200	-0.43966300
C	5.00844400	-1.77858800	-1.63769900
H	5.63236500	-2.58195400	-2.08430000
C	3.81507400	-2.33649800	-0.93332900
C	3.15877500	-3.50624800	-1.33249400
H	3.60348000	-4.06966800	-2.16331400
C	2.02382800	-4.02578100	-0.71714600
C	1.45013400	-5.40687100	-1.00341500
C	0.01146600	-5.24258500	-0.42507300
H	-0.32762300	-6.18510200	0.05183100
C	0.20424500	-4.12395300	0.57669000
C	-0.73457200	-3.82739500	1.57984600
C	-0.74350900	-2.52989600	2.16936200
C	-1.91191900	-1.90437000	2.95834500
C	-1.54742300	-0.38064800	2.81333500
H	-1.83274900	-0.09815400	1.77928500
C	-0.00655300	-0.41862000	2.80223900
H	0.37852000	-0.59331000	3.83029500
C	0.12427400	1.26049600	0.89065200
H	0.79480300	1.92934300	0.31738100
H	-0.79303700	1.81131100	1.17643700
H	-0.16178000	0.42518700	0.22034000
C	0.54386500	3.14193800	3.07685800
H	-0.51384900	2.91583500	3.31996000
H	0.52511200	3.64194500	2.09105000
H	0.92077100	3.87608800	3.81742400
C	1.58746600	1.38101300	4.55168400
H	2.18513700	0.44369200	4.56994600
H	0.59415500	1.14573200	4.98639500
C	2.32401000	2.37538500	5.46345800
O	3.51370200	2.66973200	5.30390000
N	1.57852500	2.92008800	6.47079400
H	2.03798500	3.56337900	7.12007300
H	0.60396000	2.67211700	6.63730500
C	3.09545000	3.27163700	1.49424000
H	2.23082800	3.41732200	0.81384400
H	3.94448100	3.02175000	0.82607100
C	3.47416900	4.59851300	2.17180400
H	4.02734000	4.39609200	3.11744500
H	2.58598600	5.19722700	2.46360100
C	4.41291000	5.42676700	1.27884500
O	5.16360500	4.90493300	0.44997600
N	4.37153900	6.77968700	1.47489500
H	5.05296800	7.36315900	0.98415200
H	3.80070200	7.20741600	2.20422400
C	5.64953100	1.15921600	1.79410100
H	6.57136800	0.55084900	1.78948200
H	5.49572800	1.50475500	2.83591300
H	5.84214800	2.06774100	1.18354500
C	6.70169000	0.03743400	-0.89514500
H	6.15412300	0.94655600	-1.20704800
H	7.29975900	-0.31298400	-1.76035200
H	7.41926200	0.32984400	-0.10641800
C	6.57614100	-2.17795700	0.34992400

H	6.92355900	-1.74299700	1.31029700
H	5.90905200	-3.02880300	0.60738600
C	7.75055500	-2.75948900	-0.45518300
O	7.58953000	-3.28150800	-1.56111800
N	8.97703200	-2.66714200	0.13589700
H	9.77895400	-3.08191400	-0.34559700
H	9.11491500	-2.27828400	1.06807100
C	4.60579200	-0.76343100	-2.75782900
H	4.23419200	0.17175200	-2.28511800
H	5.52919500	-0.50748500	-3.31530600
C	3.56195400	-1.26162400	-3.76952000
H	3.82195400	-2.28591300	-4.11215500
H	2.54656600	-1.29816200	-3.32401100
C	3.58287100	-0.39278900	-5.04208500
O	4.57284500	-0.40871000	-5.78081900
N	2.47660600	0.35821700	-5.28636500
H	2.50638300	0.94916500	-6.12202700
H	1.69877600	0.52258800	-4.61276000
C	2.22934200	-6.42777000	-0.11786900
H	3.29857000	-6.47005700	-0.40791100
H	1.78928900	-7.43728500	-0.25007100
H	2.17074000	-6.16269900	0.95772000
C	1.55263000	-5.84199600	-2.47482900
H	1.08403900	-5.11875700	-3.17076700
H	1.06473000	-6.82758800	-2.61214500
H	2.61172500	-5.96652600	-2.77908900
C	-1.09853200	-4.79572700	-1.43772200
H	-1.81232300	-4.12762800	-0.91184700
H	-0.64194600	-4.16837900	-2.23290600
C	-1.91918700	-5.93731200	-2.06809300
H	-2.66801700	-5.49687400	-2.75877400
H	-1.27600600	-6.62290400	-2.65296700
C	-2.60914500	-6.79271600	-0.99726600
O	-2.02761800	-7.76490600	-0.49616700
N	-3.85569700	-6.39480300	-0.61914200
H	-4.28796800	-6.91540600	0.14870400
H	-4.23228800	-5.45421600	-0.81849500
C	-1.78350100	-4.86718400	1.91370400
H	-1.36837700	-5.88889700	1.82278500
H	-2.66677900	-4.82747000	1.23938500
H	-2.15055800	-4.75923900	2.94987900
C	-1.87592900	-2.38520100	4.43120600
H	-2.72461600	-1.96347900	5.00805200
H	-0.93622200	-2.09534000	4.94427300
H	-1.96012900	-3.48762800	4.49717500
C	-2.28276300	0.59026500	3.77724300
H	-2.84474900	0.03515900	4.55586900
H	-1.55417600	1.22820600	4.31871000
C	-3.19758200	1.54335800	2.98143000
O	-2.68399400	2.35939500	2.19758100
N	-4.53447100	1.39839300	3.13272300
H	-5.21665100	1.95007500	2.54093200
H	-4.91237500	0.76887200	3.84149800
C	-3.31279700	-2.18194800	2.34019900
H	-4.02599000	-1.48074800	2.82663600
H	-3.65962600	-3.19508700	2.62460900
C	-3.39882100	-2.01638700	0.80779100
H	-3.26675500	-0.95029600	0.52324800
H	-2.58481100	-2.57637500	0.30898800
C	-4.71174700	-2.54722600	0.21751900
O	-4.77884700	-3.62069800	-0.40640700
N	-5.78010400	-1.74755000	0.45850500
H	-5.64144800	-0.84791700	0.93456900
C	-7.14070300	-1.92778700	-0.02324800
H	-7.79381300	-2.30761200	0.79571800
H	-7.13809400	-2.68363100	-0.83385900
C	-7.67961200	-0.56983000	-0.51676600
H	-7.14393400	-0.29398300	-1.45264900
C	-9.18443700	-0.54989200	-0.74833100
H	-9.72927600	-0.79764100	0.18569900
H	-9.47132000	-1.28145700	-1.53215000
H	-9.48996100	0.46206800	-1.07864500
P	-6.85779500	1.92483200	0.16071900
O	-7.79420600	2.61221000	-0.81242300
O	-6.39357300	2.57148700	1.45827700
O	-5.43949000	1.50861900	-0.73241600
O	-7.30692500	0.37644000	0.52499700
C	-2.54724300	3.14691000	-2.12222100
H	-2.45890600	4.19229700	-1.74224000
C	-3.17201700	2.27921600	-1.01147500
H	-2.83455900	2.57281300	0.00688800
C	-4.67290200	2.59435900	-1.22280300
H	-4.93721100	3.53727200	-0.69323900
C	-4.78259400	2.76119300	-2.75849900
H	-5.08951000	1.80016000	-3.22836200
C	-5.76095800	3.85800500	-3.20350400
H	-6.77308200	3.59781700	-2.82913600
H	-5.45793300	4.81874700	-2.71343000
O	-3.45017700	3.08258300	-3.22620100
O	-2.94245600	0.89536500	-1.24689400
H	-3.82595300	0.48247200	-1.09967400
O	-5.80897600	3.96616700	-4.60817500
H	-4.89261400	4.14202200	-4.90446200
N	-1.21919400	2.76533200	-2.55836700
C	-0.84888800	1.57120000	-3.16738300
H	-1.58794100	0.77842100	-3.32757300
N	0.43046500	1.52699500	-3.48964600
C	2.25563600	3.27967800	-3.21023300
H	3.04572500	2.67803300	-3.68481300
C	2.53307600	4.58086400	-2.74523200
C	1.48686200	5.37346900	-2.15271100
C	0.18354100	4.85674600	-2.03257100
H	-0.61071100	5.47659600	-1.58731200
C	-0.07013900	3.55504300	-2.50441100
C	0.95448000	2.75958300	-3.08944500
C	3.93154800	5.13710800	-2.86662500
H	4.57945400	4.46528700	-3.46290800
H	4.40861000	5.26009200	-1.86825400

H	3.93926500	6.13477600	-3.35497200
C	1.78133300	6.77679700	-1.67278900
H	2.57854800	6.79259200	-0.89850300
H	0.87954700	7.25586200	-1.24307100
H	2.13981200	7.42333300	-2.50290700

I. Cartesian Coordinates of PBE-Cobalamin Complexes

PBE-Cob(I)alamin, 185 atoms

Co···Br distance = 2.15 Å

atom	X	Y	Z
Co	-1.66458400	-0.25146000	0.52843800
N	-1.28391100	1.01726400	-0.77458700
N	-2.46122600	1.13774200	1.57459300
N	-1.58553300	-1.52327000	1.96908500
N	-0.62261500	-1.35795300	-0.53711600
C	-0.11385400	0.74404700	-1.65966000
C	-0.39929900	1.67569100	-2.92317900
C	-1.26502500	2.83687100	-2.28245000
H	-2.09282600	3.06570300	-2.98753100
C	-1.85371600	2.17248400	-1.04919300
C	-2.89293100	2.75402200	-0.23172100
C	-3.06539000	2.29565600	1.06856800
C	-3.98530900	2.88887600	2.16657700
C	-3.21114200	2.38072400	3.43375300
H	-3.89525900	2.24663900	4.29536600
C	-2.69028500	1.06491500	2.91280100
C	-2.52660600	-0.08308700	3.69659300
H	-2.83002500	-0.01116700	4.75034300
C	-2.05364200	-1.31107000	3.23541100
C	-2.08106200	-2.60777300	4.05237300
C	-1.04370100	-3.46005300	3.25800000
H	-1.34746600	-4.52679400	3.24408900
C	-1.11275100	-2.81966900	1.87450600
C	-0.59277200	-3.42562600	0.73127000
C	-0.23779200	-2.62139500	-0.40400700
C	0.69067700	-3.05050400	-1.56128800
C	1.10379200	-1.63497500	-2.11329900
H	1.86448600	-1.24538200	-1.40585100
C	-0.16573100	-0.80144000	-1.83655300
H	-0.95975300	-1.04596700	-2.57626700
C	1.16579500	1.15714800	-0.90376200
H	1.12702900	2.22508200	-0.61365800
H	2.06609800	0.98103700	-1.52353900
H	1.25998000	0.56629000	0.02940000
C	0.88781700	2.15047700	-3.62220300
H	1.57542200	1.30900400	-3.84470600
H	1.47028400	2.84863200	-2.99194800
H	0.65557500	2.67235200	-4.57332000
C	-1.30431600	0.93605700	-3.96307800
H	-2.24365100	0.59948500	-3.47132800
H	-0.78741900	0.02485400	-4.32757600
C	-1.70576200	1.79428400	-5.16750400
O	-2.41226200	2.80415000	-5.08996700
N	-1.21920900	1.36124200	-6.37603700
H	-1.47543900	1.88450400	-7.21544600
H	-0.63961800	0.52841900	-6.46908300
C	-0.58996600	4.19560200	-1.96535400
H	0.40498100	4.05635900	-1.49205700
H	-1.20020400	4.72263500	-1.20427200
C	-0.47985900	5.14993900	-3.16490600
H	-1.40589400	5.07602200	-3.78029500
H	0.35306700	4.87499300	-3.84484600
C	-0.35200600	6.61283300	-2.72791700
O	-0.87736000	7.05988700	-1.70772800
N	0.37729500	7.41350900	-3.57542900
H	0.43308700	8.41279900	-3.37108000
H	0.80405700	7.05754300	-4.43000300
C	-3.72709200	3.87437600	-0.82639300
H	-4.78037200	3.80971600	-0.49438500
H	-3.73990600	3.79954100	-1.93126600
H	-3.36120300	4.89230000	-0.57341800
C	-4.20449600	4.41275900	2.18264600
H	-3.26384600	4.97429300	2.02268600
H	-4.63397500	4.69409600	3.16337400
H	-4.92760600	4.73694100	1.41106500
C	-5.33808900	2.12878400	2.01711800
H	-5.84186000	2.47705800	1.08797100
H	-5.14863700	1.04634100	1.84343000
C	-6.34908700	2.26920200	3.16481100
O	-6.25793700	3.08406700	4.08639500
N	-7.40905800	1.40606100	3.05494400
H	-8.10539100	1.41367100	3.80223600
H	-7.41610800	0.63461700	2.37881000
C	-2.05181000	3.33075500	3.85426900
H	-1.54006900	3.70954400	2.94232600
H	-2.48496400	4.21108500	4.37231200
C	-0.99327600	2.70235500	4.78084000
H	-1.49626200	2.19493000	5.63281200
H	-0.39871500	1.93657700	4.24126100
C	-0.09788700	3.78183000	5.40670600
O	-0.55254300	4.59428400	6.21704300
N	1.21312900	3.78071200	5.01467900
H	1.79508500	4.52779900	5.40178500
H	1.62509400	3.22400700	4.24176500
C	-3.48900200	-3.24042300	3.87438100
H	-4.27004300	-2.59562600	4.32722800
H	-3.52518800	-4.23510100	4.36742000
H	-3.74017900	-3.36836300	2.80146800
C	-1.79926400	-2.41878700	5.55107900
H	-0.82574900	-1.92625100	5.74554200
H	-1.80972800	-3.39723300	6.07372100
H	-2.58774100	-1.79501500	6.02108800
C	0.43594400	-3.37451500	3.74719200
H	1.10110200	-3.50660400	2.86837900
H	0.64160400	-2.34504300	4.11238000

C	0.86351900	-4.40480100	4.81400200
H	1.91646900	-4.19387500	5.10171500
H	0.24053500	-4.32877000	5.72507600
C	0.73990300	-5.85618000	4.32936600
O	-0.18882500	-6.58609900	4.69129800
N	1.71881900	-6.27590700	3.46835300
H	1.59071800	-7.20778700	3.06738900
H	2.39969100	-5.65733200	2.99482300
C	-0.30745200	-4.91622400	0.76963800
H	-1.06491600	-5.44048400	1.38391100
H	0.68340600	-5.17513000	1.20290900
H	-0.35600800	-5.36610900	-0.23920600
C	-0.11511000	-3.87239500	-2.59778600
H	0.52846700	-4.20537200	-3.43963000
H	-0.96262700	-3.29209000	-3.01636600
H	-0.54225500	-4.78477200	-2.13672000
C	1.73472500	-1.61744600	-3.53384100
H	1.64506500	-2.60997700	-4.02241300
H	1.19568200	-0.90049800	-4.18693200
C	3.20147100	-1.14612900	-3.48310300
O	3.45067800	0.04268800	-3.21601500
N	4.16306500	-2.07805400	-3.68616300
H	5.20409000	-1.86648200	-3.56825700
H	3.89760700	-3.03059700	-3.93817600
C	1.94854500	-3.84604100	-1.11212900
H	2.66026600	-3.85499500	-1.96749400
H	1.68152700	-4.90786900	-0.93795200
C	2.66422200	-3.28924800	0.13815300
H	3.10265500	-2.29095200	-0.07592800
H	1.93970300	-3.14660700	0.96232200
C	3.75236000	-4.22979700	0.65973800
O	3.60177900	-4.95691700	1.65932800
N	4.88905000	-4.22258500	-0.08250100
H	4.97700000	-3.58672900	-0.88548300
C	6.08852600	-5.00564100	0.15927600
H	6.06907800	-5.94600100	-0.44153000
H	6.12235900	-5.29330800	1.22988000
C	7.31588400	-4.16805500	-0.24898800
H	7.42631400	-3.32865400	0.47431400
C	8.61525900	-4.96472800	-0.31075100
H	8.53165200	-5.79416800	-1.04405000
H	8.87197900	-5.39046700	0.68256300
H	9.42797600	-4.28437200	-0.63327200
P	7.47332200	-2.07157700	-1.94261400
O	8.92130100	-1.82081400	-1.59603400
O	6.84532200	-1.76724400	-3.29619200
O	6.49304700	-1.30380900	-0.73707300
O	6.98991300	-3.62695200	-1.54773500
C	5.38575300	2.01630000	0.13765200
H	5.55664300	2.72029500	-0.71132100
C	5.08165500	0.63094300	-0.45698500
H	4.48750800	0.69711300	-1.39552200
C	6.51297100	0.11286600	-0.72215900
H	6.88187400	0.51405000	-1.69395000
C	7.31620400	0.69664700	0.46460300
H	7.32912800	-0.03933800	1.30007800
C	8.74502500	1.11519300	0.13557200
H	9.31756700	0.21143400	-0.16324600
H	8.71761700	1.79616500	-0.75590400
O	6.57912300	1.86966100	0.91152200
O	4.45314800	-0.22584300	0.49107200
H	4.93990700	-1.07816700	0.37932400
O	9.37844000	1.72502300	1.24852300
H	8.74291900	2.40242400	1.55716600
N	4.33919700	2.62504500	0.93824200
C	3.73010200	2.11565000	2.07616900
H	3.99570900	1.11799200	2.44365100
N	2.83328500	2.93271900	2.60254400
C	2.08671300	5.24919100	1.85676300
H	1.35439400	5.37930100	2.66850000
C	2.28111600	6.25865700	0.89811700
C	3.25088500	6.07926000	-0.14800400
C	4.00247600	4.89135900	-0.23052100
H	4.74286500	4.76659400	-1.03697700
C	3.78575300	3.89195800	0.73271000
C	2.83875900	4.05938700	1.78025600
C	1.45485800	7.52498400	0.95951000
H	0.83588600	7.55030900	1.87813600
H	0.76219700	7.60322600	0.09209300
H	2.08973300	8.43786300	0.95580000
C	3.47035000	7.17006400	-1.17385900
H	2.55503300	7.36146300	-1.77602000
H	4.28556200	6.90339900	-1.87642100
H	3.74097300	8.13722700	-0.69637700
Br	-3.52733000	-0.91516900	-0.31546300
Br	-5.52605100	-1.47086800	-3.17348100
C	-5.56348200	-1.49078000	-1.27374000
C	-6.70173400	-1.73460300	-0.61013400
Br	-6.71921400	-1.78001100	1.31662000
Br	-8.46753800	-2.09416900	-1.35837000

PBE-Cob(I)alamin, 185 atoms

Co···Br distance = 2.65 Å

atom	X	Y	Z
Co	-1.58827600	-0.19540500	0.59406800
N	-1.29047000	1.03418300	-0.74569400
N	-2.43355600	1.16138100	1.61337300
N	-1.57713900	-1.48836200	1.99623600
N	-0.65246400	-1.33670900	-0.51574400
C	-0.13401500	0.75473500	-1.64792100
C	-0.42012200	1.68682700	-2.91085100
C	-1.27814600	2.85186000	-2.26846000
H	-2.11447600	3.07780800	-2.96485300
C	-1.85027400	2.19981100	-1.01960200
C	-2.86494700	2.79363600	-0.18701900
C	-3.03970700	2.32130700	1.10885900
C	-3.97266800	2.90291500	2.20326600

C	-3.20403300	2.40073100	3.47354000
H	-3.89570500	2.26500300	4.32866400
C	-2.67544700	1.08795000	2.95398600
C	-2.51951300	-0.06125700	3.73395700
H	-2.83066300	0.00556400	4.78602300
C	-2.05413400	-1.28853300	3.26396500
C	-2.11105900	-2.59520000	4.06261800
C	-1.07218200	-3.44768500	3.27217700
H	-1.38176900	-4.51270800	3.24803900
C	-1.12588500	-2.79527300	1.89349800
C	-0.61370100	-3.40447100	0.74905600
C	-0.27014900	-2.60657200	-0.39115300
C	0.64866400	-3.04175900	-1.55342000
C	1.06692500	-1.62857400	-2.10519000
H	1.83172100	-1.24420800	-1.39957700
C	-0.19700700	-0.78873600	-1.82240700
H	-0.99088400	-1.02989500	-2.56290600
C	1.15511000	1.16122100	-0.90357700
H	1.12030700	2.22791400	-0.60788400
H	2.05100800	0.98522900	-1.52952200
H	1.25075300	0.56650700	0.02687100
C	0.86721000	2.15532500	-3.61443300
H	1.55196000	1.31098300	-3.83564300
H	1.45374200	2.85265600	-2.98708900
H	0.63567400	2.67599500	-4.56646100
C	-1.33077600	0.94963300	-3.94936100
H	-2.26750300	0.62052700	-3.45024200
H	-0.81815700	0.03724800	-4.31714600
C	-1.73882700	1.80995000	-5.14908700
O	-2.51223900	2.76939600	-5.07477500
N	-1.18022500	1.43864100	-6.34794200
H	-1.40448200	1.99191300	-7.17716300
H	-0.50673300	0.67801700	-6.42769500
C	-0.59518200	4.21151600	-1.97071300
H	0.40589600	4.07224000	-1.51064200
H	-1.19337800	4.74453800	-1.20458100
C	-0.49980700	5.15851500	-3.17754300
H	-1.44402900	5.09834900	-3.76643700
H	0.30964000	4.86551000	-3.87799600
C	-0.33747300	6.62120700	-2.75173200
O	-0.85496800	7.08835900	-1.73667800
N	0.41059200	7.39877200	-3.60474500
H	0.50317100	8.39500100	-3.39894700
H	0.85072900	7.02207100	-4.44339100
C	-3.69407300	3.92692500	-0.76645800
H	-4.75275100	3.85194700	-0.45263100
H	-3.69078500	3.88066300	-1.87290300
H	-3.33669300	4.93972100	-0.48317200
C	-4.21734200	4.42300900	2.22641000
H	-3.28685800	5.00052100	2.06524100
H	-4.64092800	4.69629400	3.21255800
H	-4.94948300	4.74112500	1.46043000
C	-5.31128700	2.12660900	2.03651000
H	-5.74770200	2.36875300	1.04293900
H	-5.10042800	1.03467700	1.98702700
C	-6.39578300	2.33499500	3.10044000
O	-6.25154800	2.96963000	4.14656300
N	-7.58511100	1.72511500	2.77670100
H	-8.32490100	1.71946000	3.48086100
H	-7.66350800	1.09851400	1.97190400
C	-2.05165000	3.35921500	3.89346800
H	-1.54336900	3.74101000	2.98065000
H	-2.48709300	4.23754700	4.41342100
C	-0.98629200	2.73593600	4.81571700
H	-1.48270200	2.23625700	5.67601000
H	-0.40008500	1.96433500	4.27549000
C	-0.08128900	3.81761700	5.42204200
O	-0.52022900	4.63349900	6.23793700
N	1.22219200	3.81802000	5.00442600
H	1.81133400	4.56556300	5.37935800
H	1.62399400	3.25235100	4.23340700
C	-3.52213600	-3.21305300	3.85906800
H	-4.30503900	-2.55836800	4.29480100
H	-3.58092700	-4.20680700	4.35231800
H	-3.75114400	-3.34298600	2.78126600
C	-1.84854600	-2.42802000	5.56751600
H	-0.87364300	-1.94597800	5.78071500
H	-1.87451500	-3.41240200	6.07866800
H	-2.63750800	-1.80222400	6.03430200
C	0.40324800	-3.37347000	3.77519300
H	1.07519500	-3.50273400	2.90097700
H	0.61036600	-2.34694600	4.14778100
C	0.81731400	-4.41116500	4.84030600
H	1.86655300	-4.20197400	5.14316700
H	0.18315900	-4.34165800	5.74414800
C	0.70416100	-5.86109800	4.34877700
O	-0.21241200	-6.60392100	4.71547600
N	1.68111800	-6.26780500	3.47878200
H	1.55909900	-7.19954000	3.07574800
H	2.35482100	-5.64341700	3.00285300
C	-0.34133400	-4.89816700	0.78517000
H	-1.10623900	-5.41838200	1.39396500
H	0.64446200	-5.16691800	1.22395600
H	-0.38680000	-5.34601800	-0.22486100
C	-0.15436700	-3.86403600	-2.59133600
H	0.49082400	-4.20636700	-3.42859600
H	-0.99535200	-3.28048500	-3.01860600
H	-0.59010200	-4.77085300	-2.12726000
C	1.69234400	-1.61222700	-3.52861400
H	1.59768100	-2.60444000	-4.01711700
H	1.15210800	-0.89378700	-4.17915400
C	3.16123000	-1.14696700	-3.48807100
O	3.41896500	0.04324900	-3.23539300
N	4.11728700	-2.08617900	-3.68537000
H	5.15963700	-1.87921900	-3.57502600
H	3.84562300	-3.04044400	-3.92383500
C	1.90629800	-3.84078200	-1.10639400
H	2.61601000	-3.85201600	-1.96360900

H	1.63681200	-4.90191300	-0.93145600
C	2.62735500	-3.28759100	0.14260300
H	3.06846300	-2.29047300	-0.07159300
H	1.90517500	-3.14352000	0.96848400
C	3.71405300	-4.23237000	0.65861400
O	3.56464700	-4.96320400	1.65560300
N	4.85002500	-4.22529600	-0.08566400
H	4.93675700	-3.58922800	-0.88845400
C	6.04520400	-5.01661200	0.14947000
H	6.01629000	-5.95714300	-0.45088800
H	6.08270500	-5.30458100	1.21992000
C	7.27646600	-4.18833000	-0.26525800
H	7.39582800	-3.34854600	0.45611800
C	8.57021800	-4.99394100	-0.33086600
H	8.47800000	-5.82408500	-1.06236200
H	8.82808300	-5.41972800	0.66215100
H	9.38622700	-4.31968300	-0.65788900
P	7.43844300	-2.09489000	-1.96199200
O	8.88954300	-1.85117600	-1.62289200
O	6.80590600	-1.78823100	-3.31302500
O	6.46793100	-1.32137100	-0.75276600
O	6.94942200	-3.64742000	-1.56378200
C	5.37650700	2.00616300	0.11423700
H	5.54560700	2.70374800	-0.74038000
C	5.06357100	0.61832800	-0.46991000
H	4.46275400	0.68107400	-1.40457600
C	6.49133800	0.09525000	-0.74349400
H	6.85357700	0.49150100	-1.71987400
C	7.30514000	0.68227700	0.43441300
H	7.32285900	-0.05011900	1.27292700
C	8.73224600	1.09658500	0.09248800
H	9.30175600	0.19032600	-0.20454200
H	8.69943100	1.77197200	-0.80309700
O	6.57435100	1.85894500	0.88169800
O	4.43991700	-0.23023700	0.48817500
H	4.91983100	-1.08627600	0.37688400
O	9.37398600	1.71309900	1.19710000
H	8.73936600	2.39067900	1.50737000
N	4.33818300	2.62526900	0.91715200
C	3.72946000	2.12519900	2.05988800
H	3.98687400	1.12596600	2.42898100
N	2.84303500	2.95223700	2.58784400
C	2.11230000	5.27164800	1.83653900
H	1.38338500	5.40967000	2.65009900
C	2.31034200	6.27561100	0.87286600
C	3.27440400	6.08465600	-0.17638000
C	4.01619800	4.89050600	-0.25750900
H	4.75173300	4.75642700	-1.06691700
C	3.79540000	3.89649600	0.71030100
C	2.85476500	4.07579300	1.76170300
C	1.49340600	7.54820300	0.93157700
H	0.87537600	7.58046000	1.85062700
H	0.80069000	7.62945000	0.06446700
H	2.13491000	8.45652700	0.92509800
C	3.49720400	7.16910400	-1.20823200
H	2.58149900	7.36083500	-1.80975500
H	4.30979000	6.89475400	-1.91094200
H	3.77309100	8.13775200	-0.73683800
Br	-3.97489000	-0.97595700	-0.25287400
C	-5.91070200	-1.51904600	-0.83655600
C	-6.27637500	-2.77189100	-1.18028900
Br	-8.05548900	-3.31144500	-1.70123300
Br	-5.02512800	-4.20770200	-1.18388600
Br	-7.17491700	-0.09189600	-0.84171000

PBE-Cob(I)alamin, 185 atoms

Co···Br distance = 3.15 Å

atom	X	Y	Z
Co	-1.56526400	-0.20655700	0.57986900
N	-1.28518500	1.01372600	-0.76289700
N	-2.46126300	1.12850200	1.57806500
N	-1.59809400	-1.50899600	1.96642100
N	-0.63992900	-1.34904400	-0.52804900
C	-0.12395800	0.74101200	-1.66217000
C	-0.40878700	1.66892500	-2.92923300
C	-1.27846200	2.82894700	-2.29469000
H	-2.11132000	3.05060400	-2.99678300
C	-1.85308600	2.17638000	-1.04657500
C	-2.87291000	2.76819100	-0.22152100
C	-3.06030300	2.29187900	1.07234000
C	-3.98414200	2.89029900	2.16697300
C	-3.22156500	2.37988300	3.43759700
H	-3.91522700	2.25495900	4.29284100
C	-2.70763400	1.06004900	2.92073200
C	-2.55851300	-0.08879100	3.70114200
H	-2.87394600	-0.02208300	4.75208900
C	-2.08987300	-1.31505200	3.23153700
C	-2.14873000	-2.62317200	4.02784000
C	-1.09662700	-3.46861300	3.24739100
H	-1.39934400	-4.53569700	3.21986600
C	-1.13828800	-2.81465800	1.86846100
C	-0.60362700	-3.41976200	0.73128700
C	-0.25395800	-2.62108500	-0.40493800
C	0.67657500	-3.05154400	-1.55937200
C	1.09237400	-1.63684500	-2.10885100
H	1.85275900	-1.24891700	-1.40036000
C	-0.17691100	-0.80258700	-1.83388300
H	-0.96094100	-1.04955000	-2.58317200
C	1.16102400	1.15571500	-0.91537300
H	1.11808900	2.22172600	-0.61824800
H	2.05961700	0.98629800	-1.53927000
H	1.25640200	0.56076600	0.01481000
C	0.87986400	2.14530900	-3.62558600
H	1.57136000	1.30539100	-3.84335300
H	1.45853000	2.84555800	-2.99436400
H	0.65106100	2.66592900	-4.57838600
C	-1.30679700	0.92351500	-3.97346600

H	-2.24385200	0.58900100	-3.47949400
H	-0.78435700	0.01505300	-4.33723900
C	-1.71594800	1.77842400	-5.17617200
O	-2.52537800	2.70830100	-5.11328400
N	-1.11709300	1.43570400	-6.36486500
H	-1.32589900	2.00101400	-7.19003100
H	-0.39640000	0.71775100	-6.42775200
C	-0.60212400	4.19196400	-1.99458400
H	0.39994600	4.05638600	-1.53567300
H	-1.20193300	4.72005200	-1.22653600
C	-0.51197500	5.14205300	-3.19948300
H	-1.46061900	5.08557500	-3.78169400
H	0.29217100	4.84865800	-3.90595900
C	-0.34508000	6.60350800	-2.77145600
O	-0.86934300	7.07292300	-1.76097200
N	0.41358300	7.37811300	-3.61806600
H	0.51698700	8.37189900	-3.40573800
H	0.86997200	6.99710300	-4.44597100
C	-3.69870200	3.90171200	-0.80648500
H	-4.75607800	3.83820500	-0.48555800
H	-3.70217200	3.84482700	-1.91275000
H	-3.33367000	4.91561600	-0.53664600
C	-4.19889300	4.41561700	2.18082900
H	-3.25880500	4.97209200	2.00291500
H	-4.60378800	4.70734100	3.16946100
H	-4.93345900	4.74248100	1.42062800
C	-5.34117300	2.14223200	2.02078600
H	-5.76629600	2.35215400	1.01508000
H	-5.15548100	1.04440500	2.02609000
C	-6.42275500	2.42122700	3.07213600
O	-6.24506900	3.02967900	4.12812300
N	-7.65232000	1.90618500	2.72988900
H	-8.39088100	1.93686400	3.43496900
H	-7.76794800	1.28832700	1.92303200
C	-2.05980300	3.32670400	3.85802800
H	-1.54067700	3.69581300	2.94616800
H	-2.48833400	4.21370700	4.36914000
C	-1.00892800	2.69697500	4.79269900
H	-1.51865100	2.20233200	5.64795300
H	-0.42294900	1.92053200	4.25928800
C	-0.10388800	3.77312000	5.40835700
O	-0.54190700	4.58037300	6.23356500
N	1.19865200	3.78152300	4.98769000
H	1.78651700	4.52650100	5.36958900
H	1.60316000	3.22232700	4.21361800
C	-3.55317500	-3.25249800	3.81603200
H	-4.34450200	-2.60077400	4.24111600
H	-3.61035200	-4.24421000	4.31397800
H	-3.77240100	-3.39081500	2.73726600
C	-1.90058300	-2.45415600	5.53527100
H	-0.93089000	-1.96533400	5.75644500
H	-1.92475800	-3.43811500	6.04755600
H	-2.69738500	-1.83261600	5.99448600
C	0.37236200	-3.38628600	3.76750000
H	1.05494100	-3.50875100	2.90061600
H	0.56831200	-2.35915000	4.14421400
C	0.78137300	-4.42350900	4.83528000
H	1.82369200	-4.20469000	5.15491900
H	0.13282300	-4.36381600	5.72959400
C	0.69167300	-5.87287800	4.33772100
O	-0.22141000	-6.62785100	4.68846000
N	1.68639400	-6.26648400	3.48167200
H	1.57913200	-7.19759500	3.07304900
H	2.35781600	-5.63331400	3.01422700
C	-0.31954600	-4.91161400	0.77200000
H	-1.08386100	-5.43817300	1.37617800
H	0.66505600	-5.17213300	1.21852700
H	-0.35259100	-5.36204400	-0.23760700
C	-0.10848100	-3.88105500	-2.60565200
H	0.55074700	-4.23426300	-3.42759400
H	-0.93734500	-3.29737200	-3.05633900
H	-0.55721200	-4.78161900	-2.14144600
C	1.72191700	-1.61855600	-3.53077300
H	1.63110700	-2.61088000	-4.01983700
H	1.18116500	-0.90132100	-4.18220600
C	3.18940400	-1.14998000	-3.48917800
O	3.44491400	0.04314100	-3.24828500
N	4.14748900	-2.09007600	-3.67338900
H	5.18923900	-1.88172400	-3.56288300
H	3.87752600	-3.04721800	-3.90199400
C	1.93529700	-3.84278200	-1.10042300
H	2.65266200	-3.85100500	-1.95137100
H	1.67054900	-4.90530000	-0.92640200
C	2.64226500	-3.28418100	0.15418100
H	3.07832000	-2.28418100	-0.05688300
H	1.91210700	-3.14444500	0.97376000
C	3.73141300	-4.22178400	0.67751700
O	3.58063500	-4.95447100	1.67290200
N	4.87291100	-4.20724400	-0.05894800
H	4.95924000	-3.57429400	-0.86414100
C	6.06757700	-4.99806900	0.18018500
H	6.03818200	-5.94193000	-0.41507100
H	6.10487600	-5.28071900	1.25209400
C	7.29985100	-4.17358700	-0.23833000
H	7.41827700	-3.32861800	0.47712700
C	8.59336600	-4.98040300	-0.29500000
H	8.50238300	-5.81585600	-1.02061300
H	8.84872200	-5.39907100	0.70169700
H	9.41048300	-4.30895100	-0.62505800
P	7.46608600	-2.09189600	-1.94846600
O	8.91625600	-1.84573100	-1.60680400
O	6.83739500	-1.79350500	-3.30316300
O	6.49146500	-1.31255000	-0.74698200
O	6.97646800	-3.64212000	-1.54163000
C	5.38312800	2.01264200	0.10628600
H	5.54503100	2.70824700	-0.75129300
C	5.07761200	0.62067800	-0.47212200
H	4.47515300	0.67773700	-1.40616100

C	6.50787400	0.10411900	-0.74578800
H	6.86634200	0.49659600	-1.72507400
C	7.32043700	0.70130100	0.42782400
H	7.34297400	-0.02700800	1.26979900
C	8.74498200	1.12077100	0.08159400
H	9.31880100	0.21551200	-0.21025600
H	8.70763700	1.79045500	-0.81811300
O	6.58485400	1.87656800	0.87022900
O	4.46031800	-0.22800900	0.48964000
H	4.94378000	-1.08225700	0.37976300
O	9.38473100	1.74767800	1.18159100
H	8.74571100	2.42227300	1.48941600
N	4.34275900	2.62731500	0.90970700
C	3.73317700	2.12296900	2.05038800
H	3.99282000	1.12377900	2.41791400
N	2.84249500	2.94561800	2.57747200
C	2.10312300	5.26249100	1.82796100
H	1.37103400	5.39515500	2.63960300
C	2.29869000	6.26862800	0.86602400
C	3.26658200	6.08382100	-0.18073100
C	4.01428400	4.89334000	-0.26173000
H	4.75258800	4.76397100	-1.06940800
C	3.79553300	3.89680700	0.70388200
C	2.85160900	4.07044500	1.75332300
C	1.47476600	7.53681600	0.92354700
H	0.85227700	7.56379300	1.83975100
H	0.78562400	7.61641000	0.05341400
H	2.11140700	8.44863500	0.92201000
C	3.48682700	7.17074300	-1.21055300
H	2.57220400	7.35727000	-1.81537900
H	4.30374300	6.90199400	-1.91044800
H	3.75495900	8.14067100	-0.73729400
Br	-4.48261000	-1.06845500	-0.23788700
C	-6.35371100	-1.52844200	-0.68104200
C	-6.79048600	-2.79354900	-0.90056000
Br	-8.60153100	-3.25042000	-1.32576700
Br	-5.62206300	-4.28616700	-0.80375300
Br	-7.54638900	-0.04404600	-0.79114900

PBE-Cob(I)alamin, 185 atoms

Co···Br distance = 3.65 Å

atom	X	Y	Z
Co	-1.56050700	-0.22473800	0.56183200
N	-1.28445700	0.99786400	-0.77662400
N	-2.48596600	1.09468000	1.55210500
N	-1.60857500	-1.53381600	1.93958500
N	-0.62660000	-1.35912300	-0.54296900
C	-0.11788600	0.73482600	-1.67194400
C	-0.40320000	1.66289500	-2.93931400
C	-1.28268900	2.81637500	-2.30700500
H	-2.11226300	3.03716000	-3.01332300
C	-1.86041700	2.15725300	-1.06341700
C	-2.88771200	2.74177000	-0.24337300
C	-3.08241000	2.26008800	1.04813900
C	-4.00046500	2.86520400	2.14487000
C	-3.23923800	2.34870100	3.41400200
H	-3.93288700	2.22781000	4.26985100
C	-2.73271500	1.02630300	2.89589500
C	-2.58325800	-0.12310600	3.67482600
H	-2.89983700	-0.05877600	4.72566400
C	-2.10778200	-1.34638800	3.20362600
C	-2.15976600	-2.65614500	3.99815400
C	-1.09852200	-3.49283500	3.22048400
H	-1.39401000	-4.56197800	3.18992200
C	-1.13764700	-2.83616400	1.84233700
C	-0.58906600	-3.43480200	0.70782200
C	-0.23636400	-2.63158900	-0.42373700
C	0.70188300	-3.05412100	-1.57474300
C	1.11321300	-1.63605300	-2.11899800
H	1.86976200	-1.24633800	-1.40735300
C	-0.16093300	-0.80857000	-1.84631400
H	-0.93985500	-1.05828700	-2.60022700
C	1.16264100	1.15570800	-0.92101900
H	1.11155900	2.22019500	-0.61975700
H	2.06373000	0.99474200	-1.54359400
H	1.25943500	0.55824300	0.00732100
C	0.88518700	2.14857100	-3.62982400
H	1.58234300	1.31330200	-3.84784000
H	1.45766100	2.84984800	-2.99418600
H	0.65693500	2.67143400	-4.58159100
C	-1.29186600	0.91274700	-3.98851100
H	-2.22755000	0.57011800	-3.49777500
H	-0.76067100	0.00946100	-4.35257000
C	-1.70519900	1.76602800	-5.19059700
O	-2.53760800	2.67559200	-5.13217600
N	-1.08344700	1.44519200	-6.37413300
H	-1.28742900	2.01821900	-7.19520500
H	-0.33628900	0.75398300	-6.42884000
C	-0.61286300	4.18101700	-1.99823400
H	0.38889900	4.04708400	-1.53825400
H	-1.21616200	4.70214500	-1.22826200
C	-0.52423200	5.13810700	-3.19777900
H	-1.47423400	5.08535600	-3.77817200
H	0.27856100	4.84827100	-3.90731300
C	-0.35694700	6.59712900	-2.76183100
O	-0.88816400	7.06317700	-1.75345700
N	0.40941600	7.37418000	-3.59943700
H	0.51837500	8.36543500	-3.37823400
H	0.87853600	6.99420900	-4.42066100
C	-3.71405800	3.87409000	-0.83054100
H	-4.76995100	3.81637500	-0.50358500
H	-3.72339400	3.81035400	-1.93664100
H	-3.34532500	4.88920800	-0.56984400
C	-4.19968900	4.39295500	2.15571400
H	-3.25535500	4.93843300	1.96708300
H	-4.59183900	4.69383200	3.14672500
H	-4.93720800	4.72507400	1.40046100

C	-5.36779800	2.13268300	2.01195600
H	-5.78817700	2.32269500	1.00030200
H	-5.19555500	1.03322200	2.05099100
C	-6.44455600	2.45335400	3.05695100
O	-6.24420700	3.03444900	4.12398400
N	-7.69786100	2.00956800	2.69942600
H	-8.43519700	2.06397700	3.40455700
H	-7.84212500	1.40759000	1.88528600
C	-2.07261100	3.28937500	3.83515300
H	-1.55080300	3.65626900	2.92398100
H	-2.49733900	4.17804200	4.34666100
C	-1.02583300	2.65379100	4.77049300
H	-1.53962900	2.15286400	5.61959900
H	-0.43728600	1.88139000	4.23413300
C	-0.12525100	3.72603600	5.39919700
O	-0.56815400	4.52537400	6.22968800
N	1.17920700	3.74089600	4.98473600
H	1.76350800	4.48368100	5.37624100
H	1.58916000	3.18965500	4.20786300
C	-3.55792200	-3.29834300	3.78469600
H	-4.35645900	-2.65142500	4.20376200
H	-3.60912600	-4.28860500	4.28639200
H	-3.77156200	-3.44401800	2.70579700
C	-1.91715800	-2.48565900	5.50649600
H	-0.95219800	-1.98867300	5.72999900
H	-1.93462400	-3.46964100	6.01912500
H	-2.72008100	-1.87031000	5.96346300
C	0.36720800	-3.40256200	3.74802000
H	1.05448100	-3.51955100	2.88414500
H	0.55516900	-2.37472900	4.12678800
C	0.77755700	-4.43898000	4.81624400
H	1.81647600	-4.21353200	5.14234000
H	0.12350600	-4.38571800	5.70696700
C	0.70123600	-5.88786500	4.31532900
O	-0.20848800	-6.65039800	4.65877300
N	1.70418500	-6.27282300	3.46490800
H	1.60515900	-7.20336300	3.05292800
H	2.37299100	-5.63385900	3.00157100
C	-0.29502700	-4.92496300	0.74723200
H	-1.05592900	-5.45778500	1.35026000
H	0.69098600	-5.17994700	1.19395200
H	-0.32410300	-5.37453200	-0.26305500
C	-0.07194700	-3.88608100	-2.62760000
H	0.59424800	-4.23737700	-3.44489900
H	-0.89882800	-3.30456500	-3.08499300
H	-0.52130700	-4.78812100	-2.16669000
C	1.74609300	-1.61121900	-3.53948200
H	1.65981600	-2.60232500	-4.03186000
H	1.20415400	-0.89387700	-4.18979300
C	3.21180000	-1.13793400	-3.49459700
O	3.46351000	0.05640900	-3.25588600
N	4.17299000	-2.07596600	-3.67421700
H	5.21387800	-1.86543200	-3.56235600
H	3.90592400	-3.03441600	-3.90069400
C	1.96260800	-3.83988900	-1.11153900
H	2.68425100	-3.84278000	-1.95895000
H	1.70236300	-4.90411000	-0.94095000
C	2.66053700	-3.28055000	0.14778700
H	3.09244600	-2.27782300	-0.05877700
H	1.92544400	-3.14625500	0.96386700
C	3.75198900	-4.21411700	0.67314900
O	3.60094600	-4.95098600	1.66540800
N	4.89688400	-4.19180400	-0.05825800
H	4.98266100	-3.55807800	-0.86284100
C	6.09217600	-4.98146000	0.18144100
H	6.06411200	-5.92544800	-0.41377500
H	6.12915200	-5.26426300	1.25334300
C	7.32411600	-4.15616800	-0.23605300
H	7.44042300	-3.31028900	0.47867700
C	8.61865100	-4.96165000	-0.28940700
H	8.52994300	-5.79803700	-1.01424500
H	8.87264500	-5.37893000	0.70823000
H	9.43561600	-4.28963400	-0.61871500
P	7.49028900	-2.07543300	-1.94701700
O	8.93945400	-1.82665700	-1.60272400
O	6.86359300	-1.77812000	-3.30285800
O	6.51185600	-1.29846800	-0.74745800
O	7.00279500	-3.62653200	-1.54058300
C	5.38882900	2.02108000	0.10823400
H	5.54627200	2.71863800	-0.74855200
C	5.08987700	0.62831400	-0.47178900
H	4.48720600	0.68444400	-1.40580500
C	6.52247300	0.11818700	-0.74573600
H	6.87956800	0.51258700	-1.72474800
C	7.33205000	0.71784700	0.42862600
H	7.35617200	-0.01079600	1.27030400
C	8.75555400	1.14195500	0.08387800
H	9.33271300	0.23853800	-0.20716000
H	8.71698100	1.81146200	-0.81591000
O	6.59242300	1.89057400	0.87052700
O	4.47644800	-0.22436400	0.48873200
H	4.96275600	-1.07675300	0.37694400
O	9.39198700	1.77120700	1.18454300
H	8.74976400	2.44289300	1.49210400
N	4.34589600	2.62905400	0.91330500
C	3.73579900	2.11748000	2.05062700
H	3.99765000	1.11729900	2.41378900
N	2.84141300	2.93467700	2.57958300
C	2.09457100	5.25171500	1.83875200
H	1.35997500	5.37748500	2.64923900
C	2.28793200	6.26263900	0.88139600
C	3.25890900	6.08628700	-0.16391500
C	4.01164300	4.89921900	-0.24847000
H	4.75214300	4.77628400	-1.05515700
C	3.79473100	3.89759300	0.71222500
C	2.84811500	4.06313100	1.76057000
C	1.45811500	7.52688000	0.94206800
H	0.83320000	7.54717700	1.85679200

H	0.77066200	7.60704100	0.07063000
H	2.09051500	8.44166400	0.94589700
C	3.47664500	7.17835200	-1.18883100
H	2.56259600	7.36262200	-1.79525200
H	4.29662700	6.91623200	-1.88767900
H	3.73884700	8.14777400	-0.71121200
Br	-4.99185800	-1.16319500	-0.25525400
C	-6.85221900	-1.54884900	-0.60124600
C	-7.34532500	-2.80604100	-0.75805900
Br	-9.18380200	-3.18640100	-1.09766200
Br	-6.23715700	-4.33914500	-0.65220800
Br	-7.98612500	-0.02099200	-0.72272600

PBE-Cob(I)alamin, 185 atoms

Co···Br distance = 4.15 Å

atom	X	Y	Z
Co	-1.59417000	-0.22748800	0.72271300
N	-1.36062900	0.97873300	-0.63607600
N	-2.50063000	1.09649200	1.72350400
N	-1.61088500	-1.52442900	2.11231800
N	-0.69168200	-1.37213200	-0.39481300
C	-0.22181500	0.70760500	-1.56449800
C	-0.54638000	1.62011400	-2.83383300
C	-1.41140100	2.77820600	-2.19056000
H	-2.26103600	2.98821800	-2.87609300
C	-1.94917100	2.13336300	-0.92188300
C	-2.94909200	2.72714500	-0.07675100
C	-3.10304000	2.25924300	1.22660300
C	-3.96183300	2.89708200	2.34827500
C	-3.17153600	2.38053100	3.59829000
H	-3.84728900	2.27151700	4.47124600
C	-2.70195200	1.04547700	3.07668800
C	-2.53730500	-0.09723800	3.86147600
H	-2.82450300	-0.02236800	4.91999700
C	-2.07826500	-1.32603500	3.38684100
C	-2.11605700	-2.63072900	4.19057000
C	-1.07085700	-3.47280300	3.39744300
H	-1.36449100	-4.54281900	3.38345500
C	-1.14241800	-2.82807400	2.01475100
C	-0.62102100	-3.43674200	0.87279400
C	-0.29912300	-2.64465100	-0.27553400
C	0.60393100	-3.07942600	-1.44937400
C	0.99780600	-1.66729500	-2.02161600
H	1.77552100	-1.27039400	-1.33741100
C	-0.26785000	-0.83735600	-1.71909200
H	-1.07029700	-1.09615900	-2.44481600
C	1.08067100	1.13924000	-0.85810800
H	1.03662000	2.20677600	-0.56623800
H	1.96212000	0.97411500	-1.50714900
H	1.20772000	0.55196200	0.07299000
C	0.72074900	2.10221000	-3.56550600
H	1.41253500	1.26608400	-3.79712100
H	1.31034700	2.80993000	-2.95313000
H	0.46360500	2.61601500	-4.51486300
C	-1.45940400	0.85679100	-3.85209000
H	-2.38307300	0.51439700	-3.33890200
H	-0.93485400	-0.04894800	-4.21944300
C	-1.90307000	1.69561800	-5.05339500
O	-2.72603400	2.61349100	-4.98452700
N	-1.32049800	1.35214500	-6.25024300
H	-1.54929800	1.91009500	-7.07506700
H	-0.58709500	0.64766600	-6.31880400
C	-0.73654400	4.14827900	-1.91843100
H	0.27708700	4.02260200	-1.48276500
H	-1.32084600	4.67835100	-1.14008600
C	-0.68177200	5.09049200	-3.13194400
H	-1.64179400	5.01907300	-3.69360700
H	0.11071500	4.80054800	-3.85287700
C	-0.52364100	6.55669400	-2.71803400
O	-1.04652500	7.03191100	-1.70925000
N	0.22360300	7.32995200	-3.57623300
H	0.33146700	8.32376100	-3.36626300
H	0.69179700	6.94161900	-4.39409100
C	-3.79183200	3.85555900	-0.64809100
H	-4.83613500	3.80778400	-0.28231900
H	-3.84256800	3.77641800	-1.75214800
H	-3.41043100	4.87366700	-0.41786800
C	-4.12059800	4.42936900	2.34463600
H	-3.17304400	4.94702100	2.10275900
H	-4.44352800	4.76684300	3.35107800
H	-4.88656300	4.77567700	1.62520000
C	-5.37239100	2.20904600	2.29898400
H	-5.78997200	2.32249100	1.27601300
H	-5.23990500	1.12109300	2.47846400
C	-6.35675000	2.72929700	3.34792600
O	-6.18831200	2.59903200	4.56125500
N	-7.46286100	3.37168700	2.84055300
H	-8.14998500	3.74251100	3.49945100
H	-7.62131300	3.48529600	1.84069200
C	-1.97843700	3.30754700	3.97289400
H	-1.47781500	3.65561600	3.04258800
H	-2.37183500	4.20909100	4.48772800
C	-0.91244400	2.66983700	4.88458900
H	-1.40695400	2.18096900	5.75175200
H	-0.34576500	1.88829700	4.33829400
C	0.01147000	3.74286800	5.47709700
O	-0.40361200	4.55007800	6.31484000
N	1.30192600	3.75158600	5.02177500
H	1.89905200	4.49686100	5.38851300
H	1.68474400	3.19847800	4.23208600
C	-3.51866600	-3.27258700	4.00613500
H	-4.30953200	-2.62026000	4.43130000
H	-3.56419900	-4.25856800	4.51692200
H	-3.74681000	-3.42842500	2.93126800
C	-1.84527200	-2.45263700	5.69308100
H	-0.87545700	-1.95583100	5.89510000
H	-1.85379300	-3.43382700	6.21143700

H	-2.63854500	-1.83349300	6.16168100
C	0.40612100	-3.37428800	3.89124200
H	1.07408300	-3.49555900	3.01284700
H	0.59905000	-2.34293400	4.25784800
C	0.84374200	-4.40072600	4.95835600
H	1.88835300	-4.16826500	5.26071100
H	0.20853300	-4.34332100	5.86238200
C	0.76424200	-5.85419200	4.47139300
O	-0.13058000	-6.62014500	4.84512700
N	1.74753400	-6.24023900	3.59865000
H	1.64317000	-7.17456300	3.19667600
H	2.39967000	-5.60185200	3.11160300
C	-0.32485100	-4.92634900	0.91851900
H	-1.06638900	-5.45374100	1.54968400
H	0.67465100	-5.17615600	1.33725200
H	-0.38433500	-5.38610200	-0.08583900
C	-0.19980600	-3.92378300	-2.46919300
H	0.44062800	-4.28010700	-3.30478200
H	-1.04439500	-3.35001400	-2.90297500
H	-0.63015000	-4.82330800	-1.98579200
C	1.58600000	-1.65745400	-3.46143800
H	1.48200200	-2.65298200	-3.94128600
H	1.02524800	-0.94518300	-4.10116800
C	3.05306000	-1.18730000	-3.46879800
O	3.31567000	0.00945900	-3.25455800
N	4.00602000	-2.13039200	-3.66639300
H	5.04989500	-1.92217600	-3.58966400
H	3.72951100	-3.09162400	-3.86845800
C	1.87875900	-3.85881500	-1.01378300
H	2.57670300	-3.86902600	-1.88079400
H	1.62464400	-4.92159000	-0.82580100
C	2.61063500	-3.28683300	0.22062100
H	3.03605200	-2.28587900	-0.00708700
H	1.89838300	-3.14511200	1.05550100
C	3.71685800	-4.21468200	0.72437700
O	3.59522400	-4.94056500	1.72867600
N	4.84021100	-4.20110400	-0.04048300
H	4.90173700	-3.57783200	-0.85530500
C	6.03907900	-4.99370800	0.16940100
H	5.98638300	-5.94555100	-0.41157500
H	6.11099700	-5.26255400	1.24315000
C	7.26050800	-4.18102700	-0.30019600
H	7.40498800	-3.32615500	0.39850100
C	8.54853900	-4.99426500	-0.38521300
H	8.43174700	-5.83965000	-1.09548600
H	8.83317900	-5.39974700	0.60902200
H	9.35756500	-4.33111100	-0.75018700
P	7.37853200	-2.12318000	-2.04169600
O	8.83828800	-1.87495300	-1.74457300
O	6.71144500	-1.83968300	-3.38106600
O	6.43928900	-1.32839900	-0.82249700
O	6.89945600	-3.66744200	-1.60081300
C	5.33258900	2.00107700	0.01421900
H	5.45075900	2.68295500	-0.86123100
C	5.01939000	0.59606900	-0.52690400
H	4.38102100	0.63197600	-1.43794900
C	6.44303800	0.08784400	-0.84672100
H	6.75967100	0.46556400	-1.84605500
C	7.29365700	0.71300200	0.28449000
H	7.35109300	0.00156200	1.13915900
C	8.70181400	1.13412500	-0.12121100
H	9.27147800	0.22647700	-0.41389600
H	8.62760100	1.78417400	-1.03294900
O	6.56688700	1.89271900	0.72956100
O	4.44863800	-0.24128500	0.47270100
H	4.93287700	-1.09431200	0.35640900
O	9.37570200	1.78896900	0.94173800
H	8.74174100	2.46401700	1.25892900
N	4.31839000	2.61817600	0.84891400
C	3.75119700	2.12071500	2.01422900
H	4.02742000	1.12526200	2.37969700
N	2.87518300	2.94357800	2.56479900
C	2.09705900	5.24930800	1.82089100
H	1.39243000	5.38489100	2.65601100
C	2.25305400	6.24739800	0.84338700
C	3.18608000	6.05892000	-0.23379500
C	3.93795200	4.87216600	-0.32950600
H	4.64911400	4.73954900	-1.16067000
C	3.75809700	3.88312500	0.65164400
C	2.84999900	4.06116200	1.73157600
C	1.42299800	7.51093300	0.91712000
H	0.83055600	7.54168300	1.85296200
H	0.70517900	7.57980300	0.06950200
H	2.05300800	8.42691200	0.88739400
C	3.36437500	7.13769000	-1.28023900
H	2.42853000	7.31326000	-1.85529100
H	4.15866100	6.86726400	-2.00510400
H	3.64258300	8.11357200	-0.82527500
Br	-4.61418400	-1.68824900	-1.72027500
C	-5.92979200	-2.24804700	-2.98745100
C	-6.63302500	-3.40709500	-2.86198300
Br	-7.94751100	-3.96374300	-4.12023700
Br	-6.37668500	-4.59726800	-1.41135400
Br	-6.19278300	-1.06210900	-4.44382100

PBE-Cob(I)alamin, 185 atoms

Co···C distance = 2.15 Å

atom	X	Y	Z
Co	-1.95289000	-0.52560700	-0.16580300
N	-1.43421900	0.97853000	-1.14606100
N	-3.00648500	0.65308400	0.91827500
N	-1.81432900	-1.90686100	1.17978600
N	-0.57917800	-1.35327200	-1.13701600
C	-0.06304600	0.94151100	-1.74314200
C	-0.10309200	2.11559900	-2.82820400
C	-1.24967200	3.05393900	-2.26079900
H	-1.90232500	3.34347900	-3.11306400

C	-2.03575400	2.12682700	-1.35075900
C	-3.27869200	2.48790400	-0.70089500
C	-3.62627700	1.83476500	0.47283500
C	-4.69936100	2.25696000	1.50618400
C	-4.05937400	1.62362400	2.79532300
H	-4.83397600	1.31645500	3.52911300
C	-3.35491800	0.42439600	2.20837800
C	-3.08141000	-0.75337400	2.91893400
H	-3.47120500	-0.81401200	3.94429800
C	-2.38613100	-1.85390600	2.42737900
C	-2.20985100	-3.17313500	3.19050000
C	-1.00651100	-3.78811100	2.41313000
H	-1.12530600	-4.88652800	2.32451200
C	-1.12331200	-3.09266300	1.05976300
C	-0.46173400	-3.54349400	-0.09082400
C	-0.05604900	-2.56875600	-1.07177800
C	1.09449100	-2.73506500	-2.08837300
C	1.43901400	-1.22379600	-2.35194700
H	2.02244400	-0.88572600	-1.47156600
C	0.06286400	-0.54115100	-2.20725900
H	-0.55228600	-0.68157500	-3.12329100
C	0.94648000	1.23999600	-0.61377000
H	0.73707300	2.22136600	-0.14499100
H	1.98301300	1.23972100	-1.00040400
H	0.87004400	0.47082900	0.18027400
C	1.25918200	2.81346600	-3.00152600
H	2.07180000	2.08224800	-3.19436100
H	1.56326300	3.37706600	-2.09947400
H	1.22820800	3.53146100	-3.84637600
C	-0.56734000	1.58462500	-4.22206700
H	-1.55992900	1.09778200	-4.11799600
H	0.13897600	0.80883300	-4.58076100
C	-0.71009000	2.67183900	-5.28956800
O	-1.56039400	3.56782900	-5.24459600
N	0.17697300	2.58674700	-6.33287900
H	0.12754400	3.29355100	-7.06918900
H	0.91443100	1.88423000	-6.37022000
C	-0.85027600	4.37780300	-1.56034000
H	0.00210700	4.22677100	-0.86484800
H	-1.69091000	4.70826100	-0.91769200
C	-0.55840700	5.54280600	-2.51856300
H	-1.23962800	5.47970700	-3.39836700
H	0.46886200	5.49534100	-2.93583900
C	-0.79728100	6.90724500	-1.86362800
O	-1.59629000	7.08692900	-0.94374500
N	-0.06538500	7.94248200	-2.39656000
H	-0.24595000	8.88917500	-2.05807000
H	0.57320000	7.81084900	-3.18031800
C	-4.09947300	3.61250200	-1.30245200
H	-5.18119700	3.44902800	-1.14157400
H	-3.94092900	3.65040700	-2.39856200
H	-3.84921500	4.61867600	-0.90367800
C	-4.97903800	3.76212100	1.66854000
H	-4.04982600	4.36066600	1.72770200
H	-5.57435800	3.91491600	2.58939500
H	-5.58895200	4.15914300	0.83665600
C	-6.00986300	1.49516400	1.11525600
H	-6.48794900	2.03550500	0.26985900
H	-5.75707400	0.48436100	0.73926000
C	-7.05650400	1.39251800	2.23220300
O	-7.47375800	2.35995000	2.87188800
N	-7.49993300	0.11454300	2.45196700
H	-8.22790900	-0.03313700	3.15356900
H	-7.14250300	-0.68067600	1.91375500
C	-3.05771200	2.57963300	3.50948300
H	-2.44064600	3.09831000	2.74372600
H	-3.63876100	3.36069300	4.04158600
C	-2.11366100	1.91524800	4.52902900
H	-2.69693200	1.24987300	5.20265600
H	-1.35174300	1.28870800	4.02186400
C	-1.47006800	2.96468700	5.44926900
O	-2.16015300	3.64064400	6.21730300
N	-0.10965500	3.08217200	5.37163600
H	0.30772400	3.80981100	5.95766400
H	0.49741200	2.67847600	4.63177300
C	-3.44693000	-4.07877600	2.94033400
H	-4.37351700	-3.60938100	3.33327600
H	-3.29804800	-5.04681300	3.46341600
H	-3.58545100	-4.28601000	1.85944700
C	-2.02635500	-2.99042700	4.70601800
H	-1.18546300	-2.31413000	4.95905700
H	-1.85005400	-3.97292500	5.18827100
H	-2.94545200	-2.56644700	5.16202100
C	0.41091500	-3.48402000	2.98684300
H	1.13737100	-3.55534000	2.15230700
H	0.45262100	-2.42414600	3.32136300
C	0.92342600	-4.40796800	4.11352400
H	1.96491200	-4.10525400	4.35751400
H	0.31954500	-4.31041000	5.03434100
C	0.88527100	-5.89310500	3.72902600
O	0.00068300	-6.64834600	4.14623000
N	1.87977100	-6.30109800	2.88394300
H	1.81297300	-7.25859100	2.53203900
H	2.54378800	-5.66059800	2.41493100
C	0.07394100	-4.96141500	-0.09319800
H	-0.68662600	-5.63851300	0.33628600
H	1.01325000	-5.08088700	0.49035200
H	0.24005900	-5.31945800	-1.12312600
C	0.54324600	-3.45786700	-3.34415100
H	1.36032700	-3.70305700	-4.05633500
H	-0.21480100	-2.84263900	-3.86915800
H	0.01842500	-4.39281800	-3.06281000
C	2.30518000	-0.95042800	-3.61252000
H	2.39936900	-1.86577200	-4.23290700
H	1.82094900	-0.18913600	-4.25818900
C	3.68264200	-0.37749300	-3.22709700
O	3.74771300	0.75508500	-2.71543700
N	4.76905800	-1.15944600	-3.42714000

H	5.74846500	-0.86362300	-3.11253300
H	4.66141000	-2.06658500	-3.88217200
C	2.35421100	-3.47581500	-1.56129900
H	3.15658000	-3.33437600	-2.31924500
H	2.16515400	-4.56627900	-1.53189900
C	2.87103000	-3.00289000	-0.18600400
H	3.25376000	-1.96170600	-0.24747700
H	2.04435500	-2.98958000	0.54896300
C	3.96211400	-3.91034000	0.38471800
O	3.75596500	-4.73703000	1.29260000
N	5.17474200	-3.75206700	-0.20570200
H	5.31052500	-3.01280300	-0.90680600
C	6.40745500	-4.42975400	0.15653000
H	6.62547300	-5.25254900	-0.56476900
H	6.28182500	-4.88479400	1.15989200
C	7.56383000	-3.41089700	0.12783200
H	7.42860400	-2.70076800	0.97478800
C	8.94921000	-4.04474800	0.20517800
H	9.10768600	-4.74384200	-0.64268100
H	9.08213400	-4.60187300	1.15689200
H	9.70758100	-3.23903000	0.14843600
P	7.74969400	-1.05694700	-1.18802700
O	9.09171600	-0.72796100	-0.57931100
O	7.29405200	-0.59744000	-2.56703900
O	6.52319600	-0.58714300	-0.05679100
O	7.40158200	-2.69313700	-1.11470900
C	4.95729300	2.44731200	1.10763600
H	5.18372500	3.29336500	0.41575500
C	4.89359400	1.15945400	0.27046300
H	4.44873800	1.32657400	-0.73548500
C	6.39412500	0.80385700	0.17747300
H	6.86660500	1.39011400	-0.64391600
C	6.93710600	1.24237700	1.55852600
H	6.89156200	0.38228500	2.26407000
C	8.34971200	1.81575100	1.54712700
H	9.05073800	1.02027000	1.21608800
H	8.39381300	2.63185300	0.77824500
O	6.02306200	2.26828600	2.04250500
O	4.21718700	0.11450900	0.96161200
H	4.79069000	-0.67189000	0.79281900
O	8.73554800	2.27705400	2.83184800
H	7.99511500	2.84536900	3.12618800
N	3.73984100	2.83230300	1.80057000
C	3.02068400	2.09572100	2.73005800
H	3.33212800	1.07642300	2.98483600
N	1.97007400	2.73953300	3.21183700
C	1.10610600	5.07946900	2.70417200
H	0.24889400	5.01680500	3.39197400
C	1.33767100	6.24562600	1.95451900
C	2.46850500	6.31847100	1.06988700
C	3.34543400	5.22421900	0.93892100
H	4.20986800	5.29368900	0.25925200
C	3.09200800	4.06602100	1.69314000
C	1.98217500	3.98232700	2.57860800
C	0.38274400	7.41411700	2.07086300
H	-0.34663100	7.24940900	2.88851300
H	-0.20193900	7.56034300	1.13541400
H	0.91315800	8.36848300	2.27945600
C	2.72575800	7.57770700	0.27072700
H	1.88701800	7.80518700	-0.42354300
H	3.65055600	7.48852300	-0.33425700
H	2.83982000	8.46719900	0.92858900
C	-3.59241900	-1.09840400	-1.43322300
C	-4.82645700	-1.55662600	-1.12039700
Br	-5.25687200	-2.23288200	0.61112300
Br	-6.32132000	-1.74551000	-2.31973800
Br	-2.72377700	-4.60425100	-1.77159200
Br	-3.33167500	-0.72540900	-3.29928400

PBE-Cob(I)alamin, 185 atoms

Co···C distance = 2.65 Å

atom	X	Y	Z
Co	-1.82044500	-0.82844700	-0.17179100
N	-1.52032700	0.72172900	-1.14241100
N	-3.01984400	0.17360700	0.94848200
N	-1.66774100	-2.30466300	1.05127900
N	-0.42386600	-1.49332000	-1.20387800
C	-0.14893700	0.85867700	-1.72137900
C	-0.29894500	2.06161900	-2.76004000
C	-1.50800000	2.87740700	-2.13832300
H	-2.19543200	3.15250100	-2.96818500
C	-2.20258200	1.84696200	-1.25782700
C	-3.42015600	2.10461400	-0.53186400
C	-3.68282500	1.36098700	0.61600400
C	-4.68432000	1.72612600	1.74365100
C	-3.98812000	1.00582300	2.95145600
H	-4.74745100	0.65724300	3.68136000
C	-3.32142600	-0.14753200	2.24045800
C	-3.05211700	-1.38197300	2.83830100
H	-3.45200300	-1.54164400	3.84914100
C	-2.30769700	-2.40835400	2.25922000
C	-2.11415000	-3.79153600	2.89180300
C	-0.81135900	-4.24954000	2.16509000
H	-0.85276900	-5.33788200	1.95150200
C	-0.85119300	-3.41106400	0.88855800
C	-0.02728200	-3.67282200	-0.20611700
C	0.26474700	-2.63296700	-1.14913400
C	1.43745800	-2.63737900	-2.15343600
C	1.60174500	-1.09059200	-2.37505600
H	2.13750600	-0.71322000	-1.48039900
C	0.15211000	-0.57992000	-2.23270100
H	-0.41659800	-0.74808900	-3.17275800
C	0.81393400	1.22442600	-0.56876600
H	0.49017400	2.15553300	-0.06410300
H	1.85015900	1.35696100	-0.93459100
H	0.80981800	0.42014900	0.19366300
C	0.99890200	2.87575500	-2.92568100

H	1.87136100	2.22600700	-3.14634800
H	1.26588000	3.43341500	-2.00853800
H	0.90087400	3.61623900	-3.74609400
C	-0.74405400	1.54265300	-4.16591200
H	-1.69228500	0.97566000	-4.06085000
H	0.01570900	0.83946400	-4.56453700
C	-0.99325900	2.64879700	-5.19292000
O	-1.94790900	3.43082300	-5.14081200
N	-0.07451000	2.71654600	-6.21307900
H	-0.17081100	3.46857600	-6.89818400
H	0.76743500	2.14203800	-6.22748800
C	-1.19572500	4.19805700	-1.38810100
H	-0.30452600	4.09210100	-0.73445100
H	-2.03268500	4.42069300	-0.69760400
C	-1.04515500	5.42935300	-2.29485200
H	-1.79306000	5.37309400	-3.11932100
H	-0.05455500	5.46404600	-2.79459600
C	-1.30896100	6.73880400	-1.54532500
O	-2.09577600	6.83260100	-0.60228300
N	-0.62172500	7.83133000	-2.02180400
H	-0.80392200	8.74303600	-1.59892900
H	0.03559000	7.76658000	-2.79818600
C	-4.32890200	3.21781300	-1.02155200
H	-5.39322200	2.97302800	-0.83686100
H	-4.21978000	3.33890200	-2.11813000
H	-4.13181700	4.21247200	-0.56740300
C	-4.91562300	3.22877700	1.99405200
H	-3.97585000	3.81189400	1.95504000
H	-5.36263000	3.36973500	2.99932200
H	-5.61792900	3.67115700	1.26256500
C	-6.05242200	1.02532300	1.45046400
H	-6.39734200	1.31156300	0.43582400
H	-5.89719600	-0.07410200	1.42923900
C	-7.13563000	1.31040300	2.49184700
O	-7.04159000	0.99587100	3.67979200
N	-8.24821600	1.95884300	2.00774000
H	-9.01968000	2.13894200	2.65298400
H	-8.36571500	2.17712100	1.01956500
C	-2.96399400	1.91218500	3.69283400
H	-2.33873200	2.45526200	2.95051600
H	-3.53194200	2.67660500	4.26300700
C	-2.03543100	1.18606500	4.68656300
H	-2.63108100	0.47325600	5.29604700
H	-1.25838700	0.60281600	4.15126400
C	-1.42814200	2.17517700	5.69271300
O	-2.12231700	2.68565600	6.57744800
N	-0.09614500	2.45246500	5.54928300
H	0.28230100	3.15153500	6.19340600
H	0.50887300	2.19038900	4.74758300
C	-3.28757300	-4.70311200	2.44115700
H	-4.25284800	-4.32589200	2.83801700
H	-3.13228800	-5.73716100	2.81708300
H	-3.36723900	-4.73800500	1.33544200
C	-2.06389700	-3.77702400	4.42844800
H	-1.27421500	-3.10882000	4.82590000
H	-1.89189400	-4.80011500	4.82126700
H	-3.03244000	-3.43162900	4.84605700
C	0.53095000	-3.94728700	2.89935400
H	1.31995600	-3.80517200	2.13201200
H	0.45223500	-2.96654700	3.41649100
C	1.03169400	-5.02181000	3.88902000
H	1.96796900	-4.65216500	4.36129200
H	0.29657900	-5.20784300	4.69438700
C	1.29144400	-6.38037200	3.22374600
O	0.50971100	-7.32906800	3.35056700
N	2.43915000	-6.46293400	2.48099600
H	2.56830100	-7.32993900	1.95464600
H	3.02110800	-5.65660200	2.19541000
C	0.59953800	-5.05115000	-0.32600800
H	-0.08160400	-5.82277100	0.08289700
H	1.56384400	-5.16730100	0.21510200
H	0.77951700	-5.32185400	-1.38368900
C	1.00027900	-3.37855100	-3.44197000
H	1.81659200	-3.41021600	-4.19529500
H	0.11211500	-2.90363000	-3.90635000
H	0.72641600	-4.42859600	-3.21648100
C	2.42901900	-0.67184800	-3.62273900
H	2.58538000	-1.53206700	-4.30645900
H	1.87586100	0.09097800	-4.20849200
C	3.76497600	-0.01674700	-3.22397300
O	3.75439500	1.09856400	-2.67344700
N	4.90204600	-0.71340200	-3.46218500
H	5.86435300	-0.36834500	-3.15070400
H	4.85101000	-1.61045300	-3.94587500
C	2.76460300	-3.24909200	-1.62421800
H	3.56881300	-2.96389200	-2.33852700
H	2.71237600	-4.35546500	-1.66673500
C	3.17704000	-2.81492900	-0.20021600
H	3.43541100	-1.73444200	-0.17612600
H	2.33280600	-2.95439100	0.50150600
C	4.34956300	-3.63731500	0.33656700
O	4.21664000	-4.55090400	1.17218600
N	5.55228400	-3.30797100	-0.20379900
H	5.62031100	-2.53921100	-0.88246700
C	6.82861500	-3.93964800	0.08387000
H	7.03861200	-4.74976100	-0.65492900
H	6.77941600	-4.40861000	1.08774800
C	7.94256000	-2.87876800	0.00200300
H	7.82293500	-2.17578500	0.85700000
C	9.35239600	-3.46180900	0.01355600
H	9.49906600	-4.14944400	-0.84577000
H	9.54855000	-4.01893600	0.95432700
H	10.0770350	-2.62790600	-0.07000600
P	7.94075900	-0.50663500	-1.28423200
O	9.27331500	-0.10233300	-0.70046800
O	7.42127200	-0.05163300	-2.64183000
O	6.71313200	-0.14989200	-0.11662500
O	7.70093700	-2.16450600	-1.22939300

C	4.89267800	2.67984700	1.17571700
H	4.99760600	3.56366900	0.50248500
C	4.93354800	1.41563600	0.30169200
H	4.43681400	1.56674900	-0.68232200
C	6.45850800	1.21751400	0.14867900
H	6.84103600	1.86019800	-0.67718800
C	7.00511900	1.68088500	1.52009500
H	7.07549100	0.80483100	2.20373000
C	8.35051600	2.39656400	1.47184400
H	9.11713900	1.68214200	1.10307000
H	8.28348100	3.22528200	0.71811600
O	6.01160400	2.59573500	2.06278600
O	4.39476600	0.28578300	0.98002700
H	5.04271900	-0.43070600	0.77178700
O	8.73249500	2.87507300	2.75149000
H	7.94454100	3.35114800	3.08410900
N	3.66927900	2.90784300	1.92301100
C	3.04587100	2.05139300	2.81945200
H	3.46030300	1.05491000	3.00828100
N	1.94704400	2.55806800	3.35170800
C	0.83875400	4.81958500	2.98907900
H	0.00471400	4.62785700	3.68179400
C	0.93432000	6.04125600	2.30037100
C	2.03737300	6.28005500	1.40997800
C	3.02035600	5.29209000	1.20771400
H	3.86106800	5.48783000	0.52283400
C	2.89958600	4.07414100	1.89727800
C	1.82154700	3.82881500	2.79184900
C	-0.13681500	7.09470300	2.48453400
H	-0.84661200	6.80256900	3.28362200
H	-0.73054900	7.24224700	1.55489100
H	0.29163200	8.08321300	2.75954900
C	2.14848100	7.59973300	0.67747800
H	1.28855100	7.76419100	-0.00867900
H	3.07622000	7.64662700	0.07207000
H	2.16153300	8.46234400	1.37934100
C	-3.65883100	-1.89751800	-1.75290600
C	-4.96727000	-1.60634400	-1.37074000
Br	-5.81284700	-2.52579600	0.05537400
Br	-5.99488000	-0.18711500	-2.10711200
Br	-3.14447000	-3.78849500	-1.60993100
Br	-3.16207200	-1.23533300	-3.52747800

PBE-Cob(I)alamin, 185 atoms

Co···C distance = 3.15 Å

atom	X	Y	Z
Co	-1.74159300	-0.73393700	-0.04335000
N	-1.46483100	0.77521300	-1.05930400
N	-2.96166200	0.26170300	1.03564200
N	-1.65592200	-2.22772200	1.14718400
N	-0.41496300	-1.45288200	-1.10795100
C	-0.11621100	0.88111800	-1.69479500
C	-0.29490500	2.04919600	-2.76877000
C	-1.47066800	2.89864600	-2.13203300
H	-2.17942600	3.16487000	-2.94673600
C	-2.14785000	1.90208400	-1.20061600
C	-3.34945000	2.18465200	-0.46230000
C	-3.62072700	1.44829800	0.68911900
C	-4.64208900	1.81317000	1.79873200
C	-3.96272700	1.10183500	3.01929400
H	-4.72910000	0.76188400	3.74617300
C	-3.29353600	-0.05871700	2.32328300
C	-3.04409500	-1.29427400	2.92503300
H	-3.45766600	-1.44956900	3.93141900
C	-2.30796600	-2.32940700	2.35085600
C	-2.14848200	-3.72034900	2.97634800
C	-0.85905000	-4.20799700	2.24499500
H	-0.92669400	-5.29501500	2.03068100
C	-0.88043000	-3.36366500	0.97166600
C	-0.07124300	-3.64786600	-0.12985600
C	0.23774900	-2.61882500	-1.07716800
C	1.39169100	-2.65709600	-2.10174900
C	1.58465800	-1.11579600	-2.34146200
H	2.14470000	-0.74189100	-1.46031600
C	0.14905100	-0.57448600	-2.17327200
H	-0.44246900	-0.75808300	-3.09674300
C	0.89562700	1.27256500	-0.59473300
H	0.59835800	2.22021400	-0.10472700
H	1.91687500	1.38448900	-1.00684800
H	0.91256300	0.49098900	0.19051400
C	1.00249100	2.84375100	-3.01389800
H	1.86142200	2.17921400	-3.24329800
H	1.30891400	3.42840200	-2.12636100
H	0.87960400	3.55784000	-3.85427800
C	-0.80279400	1.48348600	-4.13570700
H	-1.75143400	0.93256600	-3.96882400
H	-0.06630600	0.75866900	-4.53951000
C	-1.08714400	2.55155200	-5.19350100
O	-2.05417900	3.31824700	-5.15077500
N	-0.18569700	2.60071400	-6.23096800
H	-0.29718500	3.33928800	-6.92838400
H	0.67328400	2.05151000	-6.23077400
C	-1.11536000	4.23267200	-1.42453500
H	-0.20381800	4.12962200	-0.79915700
H	-1.92572900	4.48151300	-0.71155900
C	-0.98114100	5.44170100	-2.36384000
H	-1.76643300	5.38204100	-3.15263900
H	-0.01263900	5.44667800	-2.90628700
C	-1.19191300	6.77110000	-1.63273400
O	-1.96426000	6.90484400	-0.68265000
N	-0.47713500	7.83374000	-2.13573400
H	-0.61367700	8.75449800	-1.71523700
H	0.18446000	7.73202000	-2.90441400
C	-4.24784300	3.30689000	-0.95363800
H	-5.31548000	3.07690800	-0.76784600
H	-4.13832900	3.42827300	-2.05017000
H	-4.03996700	4.29989800	-0.50027700

C	-4.88890200	3.31405600	2.04552200
H	-3.95234700	3.90287500	2.01834000
H	-5.34862400	3.45335000	3.04556400
H	-5.58402000	3.75383200	1.30553100
C	-5.99937100	1.09846600	1.47994900
H	-6.32919200	1.38496900	0.45993400
H	-5.82846600	0.00191400	1.46410300
C	-7.10300000	1.37096500	2.50256600
O	-7.05563300	0.99145000	3.67401000
N	-8.17692600	2.08570900	2.02329800
H	-8.94059600	2.29982900	2.66725400
H	-8.23644200	2.40331400	1.05727900
C	-2.93763600	2.01259000	3.75504400
H	-2.31694600	2.55328800	3.00712100
H	-3.50061500	2.77922700	4.32756400
C	-1.99964900	1.28867700	4.74126200
H	-2.59140400	0.59034400	5.37102000
H	-1.24073900	0.68998600	4.19716700
C	-1.36016500	2.28449800	5.71953600
O	-2.02606200	2.81050500	6.61709400
N	-0.03132200	2.55387000	5.53529900
H	0.37025900	3.25602700	6.16165600
H	0.55509100	2.26734800	4.72884400
C	-3.34443500	-4.60402300	2.53052200
H	-4.29953600	-4.20256700	2.92857100
H	-3.21609400	-5.64245000	2.90512100
H	-3.42699400	-4.63826800	1.42500500
C	-2.09267300	-3.71139100	4.51325900
H	-1.28450900	-3.06437200	4.90843100
H	-1.94611600	-4.73907000	4.90494000
H	-3.04995900	-3.34047800	4.93509100
C	0.49180400	-3.94010700	2.97733400
H	1.28101200	-3.80623300	2.20863800
H	0.43462300	-2.96278600	3.50342300
C	0.97275000	-5.03434300	3.95521300
H	1.91171100	-4.68479200	4.43748800
H	0.23038600	-5.22052900	4.75399100
C	1.21783100	-6.38781300	3.27433800
O	0.42572500	-7.32960200	3.38895300
N	2.36644000	-6.47613700	2.53310200
H	2.48416200	-7.33832000	1.99622200
H	2.95547200	-5.67386800	2.25079200
C	0.52544000	-5.04030200	-0.24961900
H	-0.16144900	-5.79724900	0.17679200
H	1.49568700	-5.17046100	0.27768500
H	0.68615400	-5.32282200	-1.30755000
C	0.93186900	-3.40291500	-3.37948700
H	1.74332100	-3.46457700	-4.13656100
H	0.05474200	-2.91123100	-3.84775300
H	0.63308500	-4.44317500	-3.14032700
C	2.39451000	-0.72418600	-3.60972300
H	2.53183900	-1.59687500	-4.28170500
H	1.83851700	0.03438100	-4.19839700
C	3.74434200	-0.07772800	-3.24505400
O	3.75908800	1.05438900	-2.73003000
N	4.86694400	-0.80187400	-3.47110300
H	5.83725100	-0.46728600	-3.17517100
H	4.79562600	-1.71322000	-3.92451000
C	2.71369500	-3.28825500	-1.57966600
H	3.51731900	-3.02078300	-2.30163600
H	2.64267700	-4.39400400	-1.61468900
C	3.14329100	-2.85242800	-0.16121100
H	3.41534400	-1.77518800	-0.14577800
H	2.30269700	-2.97634000	0.54771200
C	4.30972700	-3.68617300	0.37058500
O	4.17275100	-4.59627600	1.20934000
N	5.51281000	-3.37046300	-0.17774100
H	5.58358600	-2.60678400	-0.86174300
C	6.78363000	-4.01672900	0.10103600
H	6.97357000	-4.83798900	-0.63097200
H	6.74107700	-4.47399100	1.11066300
C	7.91068300	-2.97225200	-0.00659400
H	7.81033000	-2.25696600	0.84067500
C	9.31264900	-3.57415000	-0.00305100
H	9.44063300	-4.27410000	-0.85540700
H	9.51162500	-4.12242200	0.94233000
H	10.0473280	-2.75110100	-0.10464300
P	7.92659600	-0.61644500	-1.32191900
O	9.26761200	-0.22323200	-0.74977400
O	7.40651100	-0.17158600	-2.68256600
O	6.70954300	-0.22849800	-0.15318700
O	7.66538200	-2.27023400	-1.24430400
C	4.93140900	2.64065700	1.11117500
H	5.04098200	3.51097500	0.42127300
C	4.94994800	1.36146500	0.25833000
H	4.44484400	1.50304200	-0.72303600
C	6.47126600	1.14556800	0.09253400
H	6.85098900	1.77055100	-0.74809600
C	7.03715200	1.62603100	1.45030400
H	7.10743000	0.76053400	2.14725200
C	8.38814900	2.32897000	1.37578100
H	9.14504100	1.60146600	1.01252300
H	8.32055400	3.14472900	0.60804400
O	6.05804400	2.55834500	1.98906400
O	4.40716800	0.24874000	0.96083000
H	5.04594200	-0.47779600	0.75950700
O	8.78655200	2.82716000	2.64291100
H	8.00471600	3.31357600	2.97514200
N	3.71843100	2.89778100	1.86556900
C	3.08615200	2.06348600	2.77723800
H	3.48229800	1.06082500	2.97272600
N	2.00265100	2.59760500	3.31378200
C	0.93429800	4.87527400	2.93387600
H	0.10166400	4.70636700	3.63425400
C	1.04715000	6.08689900	2.23016500
C	2.14811400	6.29527400	1.32971400
C	3.11060200	5.28668800	1.13096200
H	3.94979500	5.45902200	0.43794300

C	2.97172900	4.07875100	1.83442300
C	1.89695200	3.86414400	2.74076400
C	-0.00372200	7.16166000	2.40784900
H	-0.71683600	6.88968500	3.21110000
H	-0.59650400	7.31214000	1.47805000
H	0.44366400	8.14446400	2.67330700
C	2.27889500	7.60451500	0.58185200
H	1.42049700	7.77442900	-0.10488700
H	3.20603900	7.62941200	-0.02581700
H	2.30697100	8.47506500	1.27335300
C	-3.86646800	-2.07507800	-1.94302000
C	-5.08324700	-1.64661500	-1.46977700
Br	-5.94522400	-2.48614200	-0.01146100
Br	-5.97551400	-0.12747700	-2.16917600
Br	-3.22896100	-3.82362200	-1.54405100
Br	-3.21255900	-1.39526700	-3.60978900

PBE-Cob(I)alamin, 185 atoms

Co···C distance = 3.65 Å

atom	X	Y	Z
Co	-1.65991300	-0.64455400	0.10495200
N	-1.39801800	0.83115100	-0.95091800
N	-2.86743200	0.36306400	1.16829200
N	-1.62039500	-2.14561500	1.27971100
N	-0.40436800	-1.41704900	-0.99496600
C	-0.07906300	0.89740200	-1.64865700
C	-0.28842400	2.03510300	-2.75034800
C	-1.42771100	2.91820900	-2.09548500
H	-2.16130500	3.17454400	-2.89107300
C	-2.08204300	1.95688300	-1.11282900
C	-3.26912500	2.25994100	-0.36113800
C	-3.53483100	1.53913900	0.80181400
C	-4.57372800	1.89744500	1.89623700
C	-3.88822800	1.21995100	3.13166000
H	-4.64995600	0.88872000	3.86734900
C	-3.21085500	0.05251900	2.45643700
C	-2.97525700	-1.18135000	3.06637100
H	-3.39057400	-1.32652000	4.07381200
C	-2.26611800	-2.23344400	2.48843900
C	-2.15321900	-3.63498100	3.10002300
C	-0.88916700	-4.16257800	2.35311800
H	-0.99120900	-5.24740300	2.14141400
C	-0.90140000	-3.31544800	1.08138600
C	-0.12443400	-3.62805300	-0.03714400
C	0.20279300	-2.60959800	-0.98927600
C	1.32718100	-2.68824500	-2.04348000
C	1.55343000	-1.15463700	-2.30658600
H	2.14708000	-0.78619800	-1.44529100
C	0.13785100	-0.57480300	-2.09975700
H	-0.49076300	-0.76771300	-2.99710300
C	0.98818400	1.30090000	-0.60798800
H	0.72633600	2.26503000	-0.12990500
H	1.99058700	1.38525200	-1.06988700
H	1.02711800	0.53971400	0.19617800
C	1.00699800	2.80459800	-3.07281300
H	1.84824600	2.12224500	-3.31537000
H	1.35581500	3.41096000	-2.21600400
H	0.85837500	3.49491400	-3.92878500
C	-0.85932900	1.43202400	-4.07644000
H	-1.80606600	0.89827300	-3.85199300
H	-0.14785400	0.68617800	-4.48663000
C	-1.17659000	2.46760600	-5.15698800
O	-2.14344700	3.23393500	-5.10936900
N	-0.30590800	2.48566300	-6.22199700
H	-0.43453200	3.20865700	-6.93272600
H	0.55790700	1.94391200	-6.22532600
C	-1.03022200	4.26462600	-1.43485700
H	-0.10206300	4.16309600	-0.83398500
H	-1.81572800	4.54415400	-0.70528300
C	-0.90658800	5.44694100	-2.40927500
H	-1.72364100	5.38496800	-3.16498300
H	0.04002000	5.41689300	-2.98819300
C	-1.06166400	6.79834800	-1.70508800
O	-1.80783300	6.97604300	-0.74155300
N	-0.32884900	7.82816400	-2.24921600
H	-0.42321600	8.76015700	-1.84206700
H	0.31955000	7.68775900	-3.02301000
C	-4.16768800	3.38011200	-0.85835800
H	-5.23553800	3.15509800	-0.66813100
H	-4.06176000	3.49567600	-1.95572300
H	-3.95634000	4.37515500	-0.41079900
C	-4.86423000	3.39302500	2.12613800
H	-3.94386000	4.00678600	2.09951600
H	-5.33336700	3.52871500	3.12243900
H	-5.56635300	3.80755800	1.37811800
C	-5.90559300	1.13903600	1.56521800
H	-6.22405500	1.40105900	0.53455800
H	-5.70121000	0.04796800	1.57172200
C	-7.03515200	1.39583500	2.56302200
O	-6.99969400	1.03330900	3.74014100
N	-8.11808600	2.07641600	2.05441300
H	-8.89500100	2.28685000	2.68355500
H	-8.16366600	2.38792200	1.08567100
C	-2.86582200	2.15677700	3.83838700
H	-2.27246800	2.70152000	3.07139200
H	-3.42655400	2.91891500	4.41922200
C	-1.88871800	1.45629000	4.80282500
H	-2.45245600	0.76494200	5.46561000
H	-1.14745700	0.85194100	4.24099800
C	-1.21820000	2.47314000	5.73700900
O	-1.85912500	3.03749000	6.62953300
N	0.11126700	2.71553000	5.52083200
H	0.53638700	3.42857500	6.11863600
H	0.67870100	2.39133500	4.71553700
C	-3.38444500	-4.46904500	2.65441100
H	-4.32122100	-4.03394400	3.06069000
H	-3.29597200	-5.51553500	3.01827800

H	-3.47340400	-4.49056200	1.54877700
C	-2.08502000	-3.64348900	4.63628700
H	-1.24991100	-3.03057300	5.02982600
H	-1.97357800	-4.67945600	5.01799900
H	-3.02398300	-3.24028100	5.06969200
C	0.47776700	-3.93219400	3.06859500
H	1.26017000	-3.81390000	2.29033900
H	0.45143100	-2.95612400	3.59940000
C	0.94316500	-5.04297000	4.03519300
H	1.89286000	-4.71684700	4.51295000
H	0.20278500	-5.21925800	4.83810900
C	1.15562000	-6.39668600	3.34395100
O	0.34879100	-7.32531700	3.46351500
N	2.29352500	-6.50189500	2.58821500
H	2.38855900	-7.36338500	2.04575500
H	2.89298400	-5.70951300	2.30010900
C	0.43159500	-5.03732900	-0.16140100
H	-0.26580200	-5.77505300	0.28125600
H	1.40709800	-5.18914900	0.35041600
H	0.56888600	-5.32946400	-1.22006500
C	0.82579200	-3.43703100	-3.30356800
H	1.62169700	-3.52992900	-4.07401700
H	-0.04518700	-2.92738000	-3.76431300
H	0.50373100	-4.46614100	-3.04706500
C	2.33657400	-0.79739700	-3.60185900
H	2.44506200	-1.68423800	-4.26054500
H	1.77756800	-0.04151400	-4.19112200
C	3.70551800	-0.16735300	-3.28237000
O	3.75444700	0.97921100	-2.80262100
N	4.80802700	-0.92290300	-3.50554900
H	5.78987400	-0.60402900	-3.23256400
H	4.70883600	-1.84617500	-3.92855100
C	2.64436800	-3.34520100	-1.53906500
H	3.44225700	-3.10087200	-2.27557000
H	2.54820400	-4.44946600	-1.56398800
C	3.10476900	-2.90842400	-0.13050500
H	3.39632900	-1.83619500	-0.12753200
H	2.27325700	-3.01155400	0.59234300
C	4.26418100	-3.75937900	0.38885800
O	4.12383500	-4.66409000	1.23287900
N	5.46473700	-3.46463700	-0.17646300
H	5.53750600	-2.70696000	-0.86687300
C	6.72849900	-4.13128500	0.08535400
H	6.88871200	-4.96532600	-0.63933700
H	6.69859300	-4.57487200	1.10157000
C	7.87167300	-3.10902900	-0.05877400
H	7.80078900	-2.38018100	0.77991800
C	9.26253500	-3.73599800	-0.07357000
H	9.36150400	-4.44976900	-0.91829300
H	9.46999800	-4.27474000	0.87546300
H	10.0094990	-2.92769100	-0.20072600
P	7.90567400	-0.77282500	-1.40809600
O	9.26213500	-0.39744000	-0.86069800
O	7.37499700	-0.33819200	-2.76789200
O	6.71269300	-0.34384100	-0.22876400
O	7.61484800	-2.42007400	-1.30150300
C	5.01022400	2.58315300	1.00868700
H	5.12506000	3.43516000	0.29712700
C	4.98908200	1.28542500	0.18429400
H	4.46845900	1.41645500	-0.79054000
C	6.50286200	1.03875300	-0.00514700
H	6.87734500	1.64052700	-0.86487700
C	7.10228500	1.53563600	1.33220200
H	7.16855200	0.68334800	2.04567100
C	8.46481900	2.21080900	1.21977600
H	9.20168200	1.46150200	0.85968600
H	8.39933300	3.01129600	0.43594800
O	6.15089500	2.49756200	1.86831400
O	4.43982300	0.19847900	0.92105500
H	5.06097200	-0.54425000	0.72438900
O	8.89387600	2.72816300	2.46916900
H	8.12656900	3.23555500	2.80394800
N	3.81690500	2.88281800	1.77826600
C	3.18213800	2.08312900	2.71920000
H	3.55678400	1.07459200	2.92679300
N	2.12363500	2.65533000	3.26618900
C	1.10465500	4.95090200	2.85967500
H	0.28145800	4.81674100	3.57848800
C	1.23341500	6.14488900	2.12906000
C	2.32126900	6.30747300	1.20367500
C	3.25443900	5.27125000	1.00730000
H	4.08380300	5.40850000	0.29487300
C	3.09955100	4.08155600	1.73791300
C	2.03815400	3.91230100	2.66929000
C	0.21253700	7.24861100	2.30425400
H	-0.49168800	7.01007400	3.12576800
H	-0.39394100	7.39519900	1.38270100
H	0.68856800	8.22516600	2.54160100
C	2.46953500	7.59753700	0.42628300
H	1.60403400	7.77273200	-0.25016800
H	3.38683800	7.58830100	-0.19660000
H	2.52869400	8.48150500	1.09850900
C	-4.12817400	-2.15978800	-2.11636600
C	-5.27496700	-1.68085200	-1.55471200
Br	-6.06296400	-2.47789100	-0.03286700
Br	-6.18660500	-0.16448200	-2.23572100
Br	-3.26709400	-3.72326700	-1.51877000
Br	-3.43414200	-1.43272800	-3.72686000

PBE-Cob(I)alamin, 185 atoms

Co···C distance = 4.15 Å

atom	X	Y	Z
Co	-1.52113500	-0.50166700	0.23748500
N	-1.24848800	0.94490900	-0.85134500
N	-2.67701300	0.54359600	1.30974600
N	-1.54513200	-2.01199000	1.39789200
N	-0.35792500	-1.34205000	-0.90651500

C	0.02832500	0.94584100	-1.62665400
C	-0.21565700	2.05093000	-2.75341000
C	-1.28167300	2.99368400	-2.06126400
H	-2.04947200	3.25594400	-2.82165500
C	-1.91237800	2.08239000	-1.01833600
C	-3.06996000	2.42760000	-0.23925800
C	-3.33449300	1.72255700	0.93326500
C	-4.38273700	2.07941900	2.01797100
C	-3.69255000	1.42381400	3.26210600
H	-4.45076600	1.10785800	4.00763200
C	-3.02301000	0.24502500	2.59991400
C	-2.81457700	-0.99191900	3.21396600
H	-3.22248800	-1.12103400	4.22673700
C	-2.16402900	-2.07367100	2.62161500
C	-2.12590600	-3.48754300	3.21412000
C	-0.92631700	-4.08992200	2.41938000
H	-1.10463800	-5.16397300	2.20400600
C	-0.92732100	-3.22991500	1.15648400
C	-0.21806000	-3.58399100	0.00337400
C	0.15845700	-2.57551900	-0.94249000
C	1.24000500	-2.71503000	-2.03468700
C	1.54472000	-1.19472400	-2.30429200
H	2.18517800	-0.86107000	-1.46225100
C	0.16918700	-0.54299900	-2.04815900
H	-0.50408700	-0.73087600	-2.91341900
C	1.16945900	1.34271000	-0.66632200
H	0.97175300	2.33038600	-0.20568400
H	2.14376600	1.37348200	-1.19094400
H	1.22979700	0.60540700	0.15853200
C	1.07977000	2.76359500	-3.18602300
H	1.88304200	2.04508400	-3.45083800
H	1.49989600	3.38868100	-2.37599100
H	0.90038200	3.42568100	-4.05834300
C	-0.89217500	1.41699100	-4.01535300
H	-1.83220100	0.91108400	-3.70909200
H	-0.22622000	0.64227200	-4.44775000
C	-1.26134800	2.42224700	-5.10813600
O	-2.20739800	3.21092800	-5.02395700
N	-0.46287100	2.38609200	-6.22790000
H	-0.62683300	3.08423300	-6.95591900
H	0.38256100	1.81813200	-6.27410900
C	-0.80204800	4.34077000	-1.45903400
H	0.15293000	4.22091700	-0.90525900
H	-1.53790600	4.66587600	-0.69684700
C	-0.69018200	5.49367400	-2.46974100
H	-1.56141500	5.45619800	-3.16390900
H	0.21060800	5.40293600	-3.11182600
C	-0.73103300	6.86560300	-1.78979900
O	-1.42203500	7.10618700	-0.79931000
N	0.03823800	7.83793900	-2.38680900
H	0.02314200	8.77989800	-1.99202200
H	0.64840800	7.64171400	-3.17931000
C	-3.94975600	3.56648700	-0.72823600
H	-5.02073300	3.36451400	-0.53132400
H	-3.84996100	3.68553300	-1.82545900
H	-3.71418100	4.55421600	-0.27664500
C	-4.70546700	3.56933900	2.23983900
H	-3.79845100	4.20261700	2.21397100
H	-5.17981700	3.69656800	3.23471700
H	-5.41538700	3.96557200	1.48926300
C	-5.69477800	1.29179800	1.67201300
H	-5.99702100	1.53756000	0.63214600
H	-5.47039200	0.20416200	1.69378800
C	-6.85001300	1.53843000	2.64326700
O	-6.80405900	1.26007400	3.84262800
N	-7.96727600	2.11375100	2.08195100
H	-8.78024400	2.27106300	2.68042800
H	-8.04244800	2.29913900	1.08305200
C	-2.66011800	2.37177600	3.93920100
H	-2.09163600	2.91703700	3.15389100
H	-3.20751000	3.13352800	4.53307500
C	-1.64957500	1.67981900	4.87431600
H	-2.19017600	1.00539500	5.57331500
H	-0.93931400	1.05766600	4.29231500
C	-0.92677700	2.70639000	5.75693100
O	-1.52772600	3.32249600	6.64291500
N	0.40496900	2.89486300	5.50313200
H	0.86938300	3.61104000	6.06693400
H	0.94146100	2.51979400	4.69885600
C	-3.42481900	-4.23008200	2.79939600
H	-4.31619300	-3.73668700	3.23976300
H	-3.39767800	-5.28468400	3.14932100
H	-3.54888400	-4.23250900	1.69672600
C	-2.00859000	-3.51938500	4.74708000
H	-1.12054200	-2.97029400	5.11836000
H	-1.95722700	-4.56496500	5.11534200
H	-2.90250900	-3.05679500	5.21506900
C	0.47686500	-3.95109000	3.08746300
H	1.23836900	-3.87109700	2.28384100
H	0.52811600	-2.98142500	3.62793400
C	0.90648300	-5.09926000	4.02632400
H	1.88719200	-4.83430200	4.47855200
H	0.18123100	-5.24364000	4.84919100
C	1.02047500	-6.45333800	3.31293000
O	0.16600700	-7.33629900	3.44593500
N	2.12732100	-6.61197300	2.52113600
H	2.15804800	-7.47055200	1.96676100
H	2.76441400	-5.85139400	2.22746900
C	0.24219700	-5.02498700	-0.14752100
H	-0.49440300	-5.72174300	0.29796600
H	1.21355100	-5.24356000	0.34803800
H	0.34558200	-5.31267900	-1.21098200
C	0.66328100	-3.43034700	-3.28175300
H	1.43355500	-3.57022000	-4.07086000
H	-0.18479000	-2.86764400	-3.72314000
H	0.28519200	-4.43836800	-3.01847900
C	2.30170700	-0.87926400	-3.62594000
H	2.36526100	-1.77867500	-4.27341500

H	1.75082600	-0.11485000	-4.21186700
C	3.69947100	-0.29258100	-3.35172600
O	3.80338700	0.86335400	-2.90458700
N	4.76618900	-1.09855600	-3.57379500
H	5.76497100	-0.81615100	-3.32463200
H	4.62219100	-2.02708600	-3.97169300
C	2.53100200	-3.44656700	-1.56577300
H	3.32322100	-3.24520900	-2.32132700
H	2.37226000	-4.54378300	-1.58923400
C	3.04806000	-3.03982500	-0.16816200
H	3.38614700	-1.98134300	-0.16906100
H	2.23196600	-3.11004800	0.57589900
C	4.18234500	-3.94324800	0.31670100
O	4.02310300	-4.85103400	1.15404100
N	5.38110200	-3.68972500	-0.27120800
H	5.46967000	-2.92622400	-0.95340100
C	6.62464600	-4.40365200	-0.03949900
H	6.74139100	-5.23614800	-0.77413300
H	6.59861900	-4.85491200	0.97345500
C	7.79965500	-3.42048900	-0.19786800
H	7.76908200	-2.69538200	0.64661100
C	9.16767800	-4.09445400	-0.24264700
H	9.22601100	-4.80619600	-1.09285200
H	9.37444700	-4.64553400	0.69942500
H	9.93903900	-3.31109100	-0.37990500
P	7.90249900	-1.08126000	-1.53867000
O	9.28235300	-0.76756800	-1.01103800
O	7.37089800	-0.62003600	-2.88929700
O	6.74696400	-0.60174500	-0.34115200
O	7.54273200	-2.71469500	-1.43118400
C	5.19867400	2.41354300	0.89114900
H	5.34620500	3.24973600	0.16699400
C	5.10366800	1.10856500	0.08327500
H	4.57579400	1.25449000	-0.88569400
C	6.60142800	0.79041600	-0.12427300
H	6.99048700	1.36900700	-0.99344800
C	7.24146600	1.26943700	1.20050500
H	7.27471700	0.42175000	1.92179600
C	8.63395400	1.87583900	1.06529700
H	9.32886100	1.08845400	0.70311900
H	8.59787600	2.67174000	0.27497800
O	6.34493600	2.28199600	1.73760300
O	4.51427100	0.05759700	0.84091300
H	5.09666800	-0.71591200	0.64561200
O	9.10329100	2.38227800	2.30469600
H	8.36655700	2.93071200	2.64337300
N	4.03325800	2.78263600	1.67278900
C	3.38171800	2.03428000	2.64399800
H	3.71186500	1.01310800	2.86540700
N	2.36516700	2.66887600	3.20186400
C	1.45040300	5.00327700	2.76789000
H	0.63821200	4.92500700	3.50713500
C	1.62051800	6.17421600	2.00898700
C	2.69307700	6.26362800	1.05624800
C	3.56998200	5.17901400	0.86232400
H	4.38794800	5.26017200	0.12847500
C	3.37426200	4.01397700	1.62222100
C	2.32734900	3.91605400	2.57978500
C	0.65948400	7.33058200	2.18302300
H	-0.03822600	7.14262700	3.02301500
H	0.04191700	7.49039100	1.27109300
H	1.18843500	8.28622900	2.39198700
C	2.88525700	7.52771900	0.24648300
H	2.01487000	7.72832000	-0.41649400
H	3.78770200	7.46126000	-0.39435300
H	2.99967700	8.42271200	0.89655700
C	-4.58767100	-2.01831900	-2.11169100
C	-5.76901700	-1.74136500	-1.49040500
Br	-6.28798300	-2.57744300	0.12478800
Br	-7.02334200	-0.49086900	-2.17685800
Br	-3.32972100	-3.24702000	-1.43866300
Br	-4.10661300	-1.18408100	-3.74826600

References

1. L. Adrian and F. E. Löffler, Organohalide Respiring Bacteria, Springer-Verlag Berlin Heidelberg, Heidelberg, 2016.
2. H. Scholz-Muramatsu, A. Neumann, M. Meßmer, E. Moore and G. Diekert, Arch. Microbiol., 1995, 163, 48-56.
3. E. Miller, G. Wohlfarth and G. Diekert, Arch. Microbiol., 1996, 166, 379-387.
4. L. Ye, A. Schilhabel, S. Bartram, W. Boland and G. Diekert, Environ. Microbiol., 2010, 12, 501-509.
5. X. Maymo-Gatell, Y.-t. Chien, J. M. Gossett and S. H. Zinder, Science, 1997, 276, 1568-1571.
6. X. Maymó-Gatell, T. Anguish and S. H. Zinder, Appl. Environ. Microbiol., 1999, 65, 3108-3113.
7. E. Miller, G. Wohlfarth and G. Diekert, Arch. Microbiol., 1997, 168, 513-519.
8. J. Im, E. E. Mack, E. S. Seger and F. E. Löffler, Environ. Sci. Technol., 2019, 53, 11941-11948.
9. R. A. Marcus, Angew. Chem. Int. Ed., 1993, 32, 1111-1121.
10. J. N. Schrauben, M. Cattaneo, T. C. Day, A. L. Tenderholt and J. M. Mayer, J. Am. Chem. Soc., 2012, 134, 16635-16645.
11. S. F. Nelsen, S. C. Blackstock and Y. Kim, J. Am. Chem. Soc., 1987, 109, 677-682.
12. O. López-Estrada, H. G. Laguna, C. Barrueta-Flores and C. Amador-Bedolla, ACS omega, 2018, 3, 2130-2140.
13. S. Zhang, L. Adrian and G. Schüürmann, Environ. Sci. Technol., 2020, 54, 15751-15758.
14. J. M. Saveant, J. Am. Chem. Soc., 1987, 109, 6788-6795.
15. J. M. Mayer, Annu. Rev. Phys. Chem., 2004, 55, 363-390.
16. S. S. Kristjansdottir and J. R. Norton, J. Am. Chem. Soc., 1991, 113, 4366-4367.
17. J. M. Mayer, J. Phys. Chem. Lett., 2011, 2, 1481-1489.