Two Pathways of Proton Transfer Reaction to (triphos)Cu(η1-BH4) via Dihydrogen Bond [triphos = 1,1,1-tris (diphenylphosphinomethyl)ethane]

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Supplementary Information

Figure S1. IR spectra of **1** (0.06 M) at the presence PNP at ν_{OH} region in CH_2Cl_2 at 260–200 K, *l* =1.0 mm.

Figure S2. IR spectra of **1** (0.06 M) at the presence PNP in the ν_{OH} region in CH_2Cl_2 at 200 K, *l* =1.0 mm with band deconvolution.

Figure S3. Optimized geometries (DFT/M06) of DHB complexes **2**·HFIP (**IIbc, Icb, IIab, IIa, IIIab**).

Figure S4. Optimized geometry (DFT/M06) of DHB complex of **IIa** type for **1**·MeOH.

Figure S5. Optimized geometry (DFT/M06) of DHB complex of **IIa** type for **1**·TFE.

Figure S6. Optimized geometry (DFT/M06) of DHB complex of **IIab** type for **1**·HFIP.

Table S1. Structural parameters (bond length, ***l*** in Å and ∠ in °) of **1** and **2**(DFT/M06).

Table S2. Structural parameters (bond length, ***l*** in Å and ∠ in °) of **2**·ROH DHB complexes (DFT/M06).

Table S3. Bond length changes (in Å) upon **2**·ROH DHB complexes (DFT/M06).

Table S4. M06-optimized **2**·ROH DHB complex formation energies (in kcal/mol).

Table S5. Frequency shifts (Δν, cm^{-1}) and intensity changes (ΔA, Km/mol) calculated for M06-optimized **2**·ROH DHB complexes.

Table S6. Structural parameters, frequencies and formation enthalpies for M06-optimized DHB complexes **IIa** type of **2** with alcohols.

Table S7. Structural parameters, frequencies and formation enthalpies for M06-optimized DHB complexes **IIab** type of **2** with alcohols.

Figure S7. The dependence of complex formation enthalpy from alcohol acidity −ΔH°=f(P*i*).

Figure S1. IR spectra of **1** (0.06 M) at the presence PNP at ν_{OH} region in CH_2Cl_2 at 260–200 K, *l* =1.0 mm.

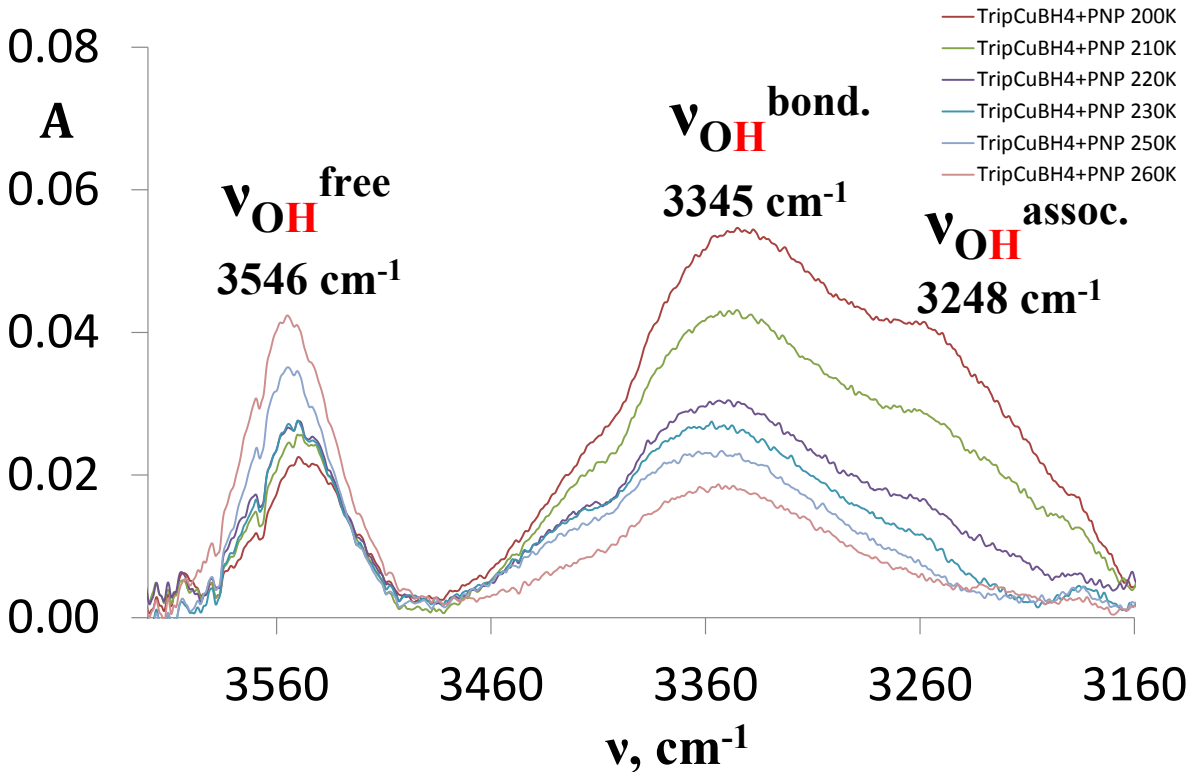


Figure S2. IR spectra of **1** (0.06 M) at the presence PNP in the ν_{OH} region in CH_2Cl_2 at 200 K, *l* =1.0 mm with band deconvolution.

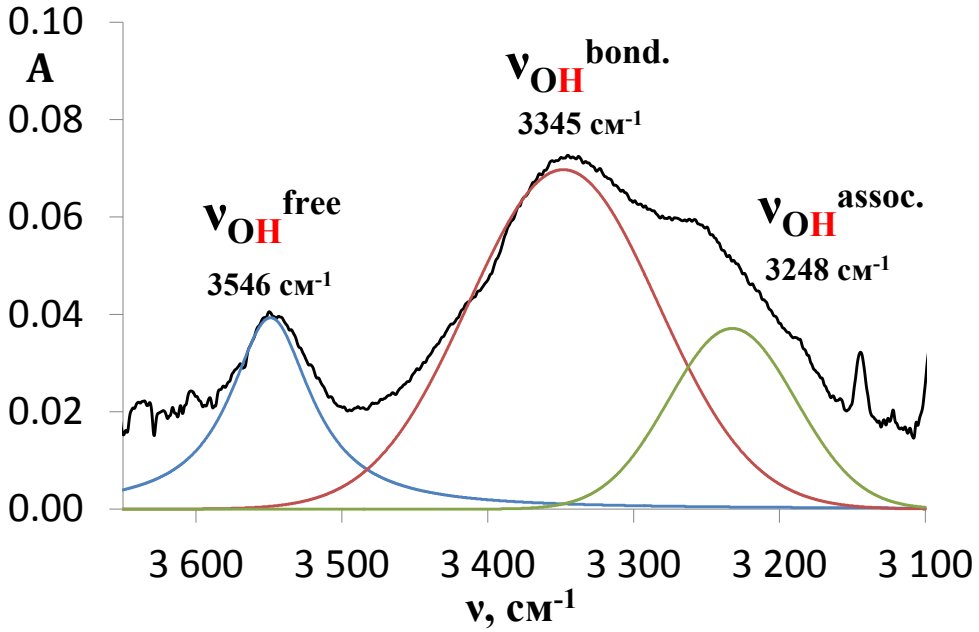


Figure S3. Optimized geometries (DFT/M06) of DHB complexes **2**·HFIP (**IIbc, Icb, IIab, IIa, IIIab**).

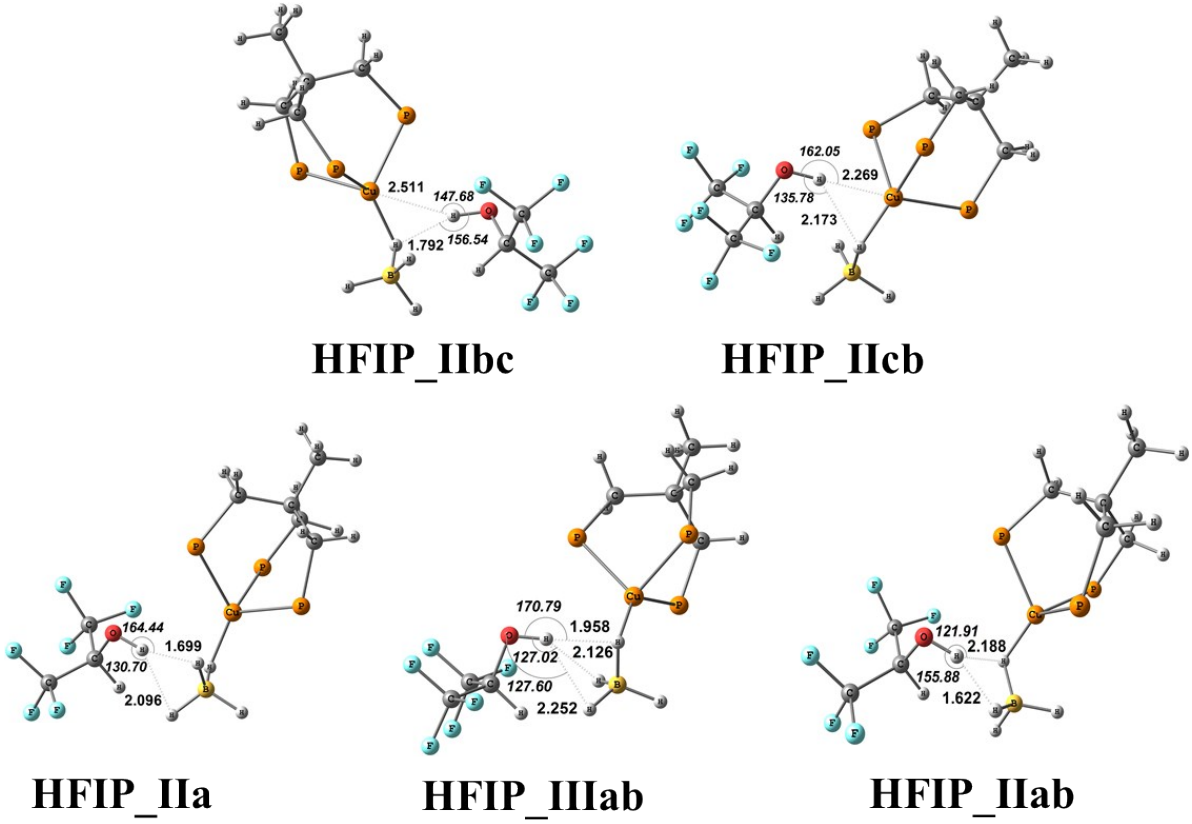


Figure S4. Optimized geometry (DFT/M06) of DHB complex of **IIa** type for **1**·MeOH.

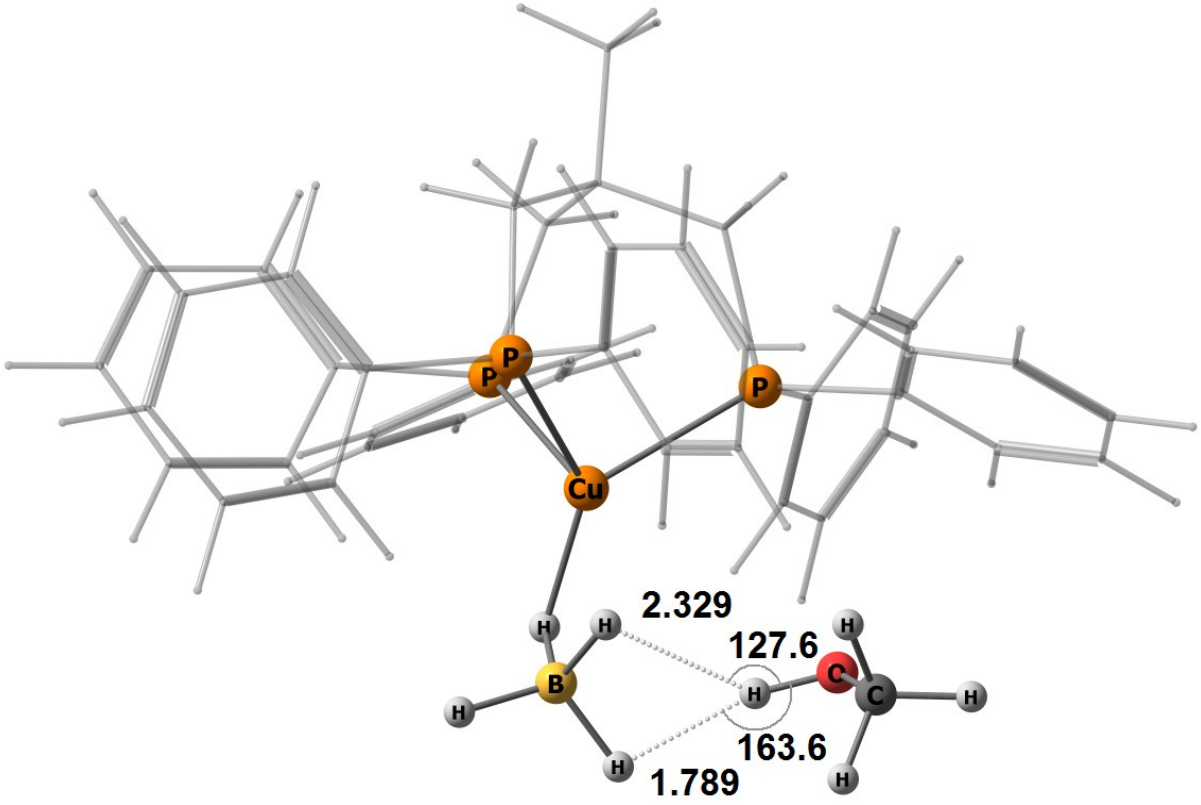


Figure S5. Optimized geometry (DFT/M06) of DHB complex of **IIa** type for **1**·TFE.

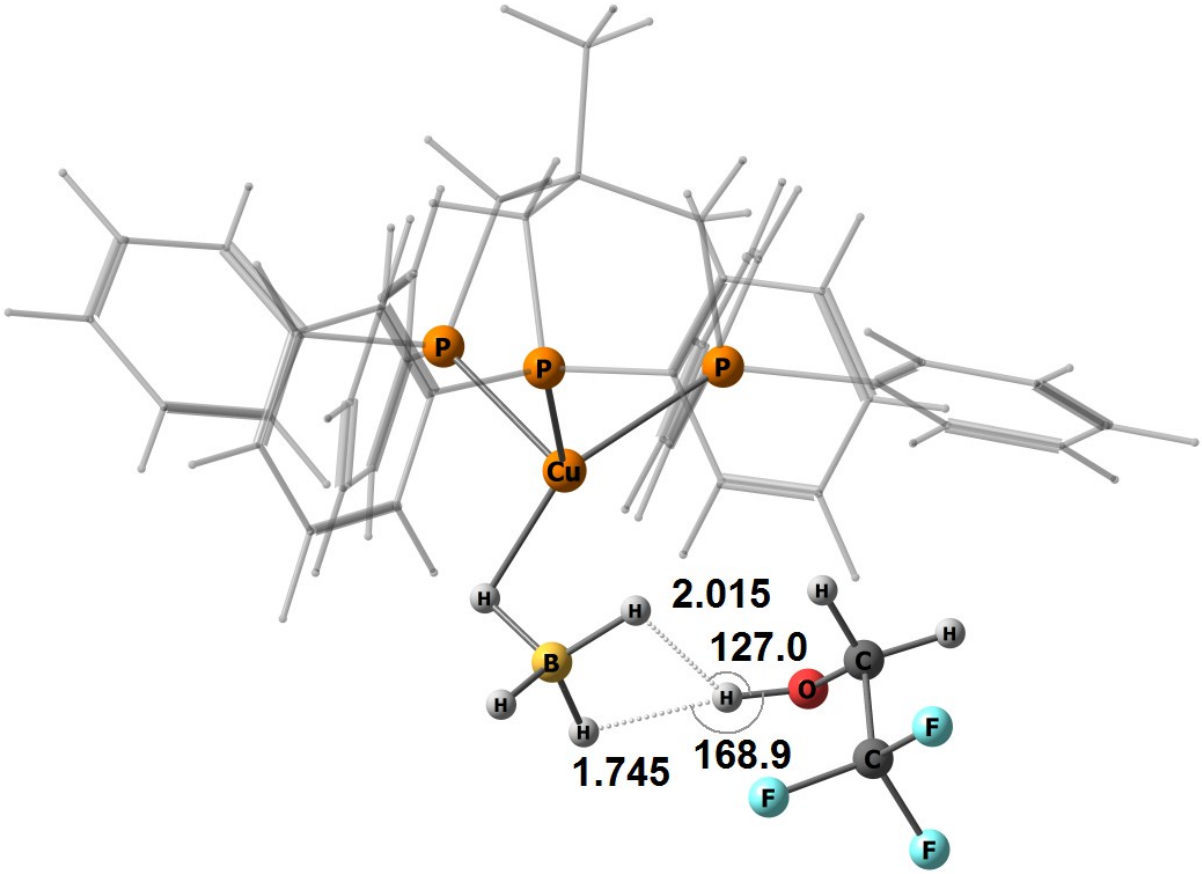


Figure S6. Optimized geometry (DFT/M06) of DHB complex of **IIab** type for **1**·HFIP.

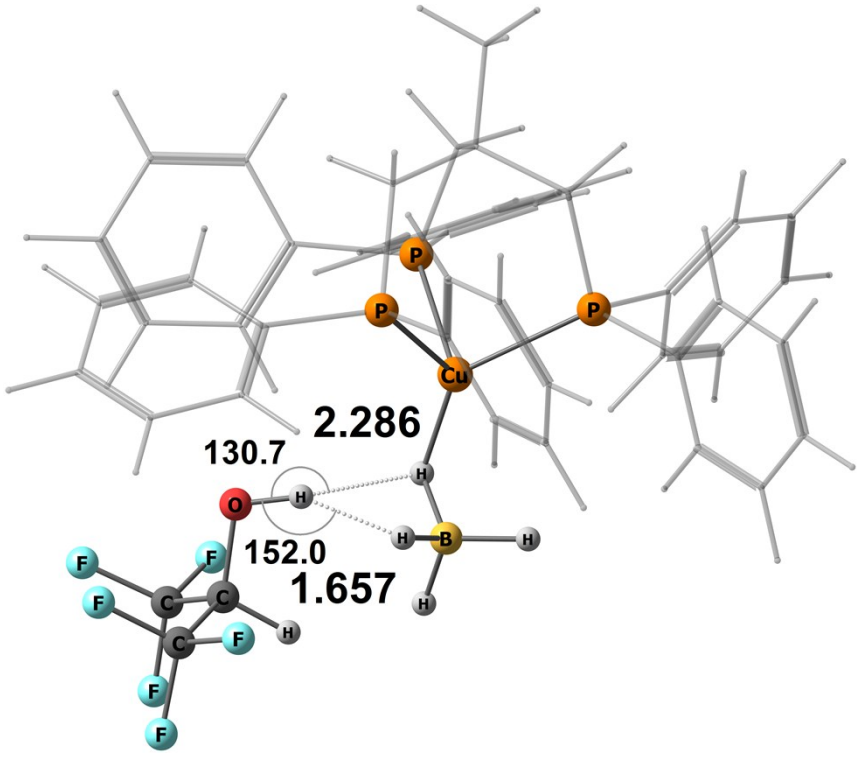


Table S1. Structural parameters (bond length, ***l*** in Å and ∠ in °) of **1** and **2**(DFT/M06).

(triphos)Cu(η^1-BH$_4$) (1)			
B–H1	***l***		∠
B–H2	1.242	B–H–B	108
B–H3	1.224		110
B–H4(Cu)	1.214		112
Cu–H4(B)	1.271		114
Cu–H3(B)	1.787	Cu–H–B	104
Cu–P1	2.049		108
Cu–P2	2.410	P–Cu–P	88
Cu–P3	2.338		92
B–H1	2.341		94

(triphos^{Me})Cu(η^1-BH$_4$) (2)			
Bond	***l***	Angle	∠
B–H1	1.226	B–H–B	111
B–H2	1.221		111
B–H3	1.211		112
B–H4(Cu)	1.298		113
Cu–H4(B)	1.680	Cu–H–B	99
Cu–H3(B)	2.411		109
Cu–P1	2.316	P–Cu–P	92
Cu–P2	2.318		93
Cu–P3	2.332		93

Table S2. Structural parameters (bond length, ***l*** in Å and ∠ in °) of **2**·ROH DHB complexes (DFT/M06).

	MeOH			TFE			HFIP		
	l	∠	***contact***	***l***	∠	***contact***	***l***	∠	***contact***
IIbc				1.824	155	**BH_{br}···HO**	1.792	157	**BH_{br}···HO**
				2.514	153	**Cu···HO**	2.511	148	**Cu···HO**
IIcb	2.401	152	**Cu···HO**	2.337	164	**Cu···HO**	2.269	162	**Cu···HO**
	2.144	148	**BH_{br}···HO**	2.005	147	**BH_{br}···HO**	2.173	136	**BH_{br}···HO**
IIa	1.851	155	**BH_{t1}···HO**	1.775	162	**BH_{t1}···HO**	1.699	164	**BH_{t1}···HO**
	2.068	141	**BH_{t2}···HO**	2.062	135	**BH_{t2}···HO**	2.096	131	**BH_{t2}···HO**
IIab	1.985	140	**BH_{t2}···HO**	1.911	167	**BH_{br}···HO**	1.622	156	**BH_{t1}···HO**
	2.07	160	**BH_{br}···HO**	2.154	132	**BH_{t2}···HO**	2.188	122	**BH_{br}···HO**
IIIab	1.896	145	**BH_{t1}···HO**	1.845	139	**BH_{t1}···HO**	1.958	171	**BH_{br}···HO**
	2.308	158	**BH_{br}···HO**	2.257	129	**BH_{t2}···HO**	2.126	127	**BH_{t1}···HO**
	2.382	122	**BH_{t2}···HO**	2.324	161	**BH_{br}···HO**	2.252	128	**BH_{t2}···HO**

Table S3. Bond length changes (in Å) upon **2**·ROH DHB complexes (DFT/M06).

HFIP

	contact	r(OH)	r(BH1)	r(BH2)	r(BH3)	r(BHbr)	r(CuH)
IIbc	**BH^{br}···HO** **Cu···HO**	0.011	−0.002	0.004	−0.012	0.003	0.009
IIcb	**Cu···HO** **BH^{br}···HO**	0.012	0.001	0.004	−0.012	0.004	0.008
IIa	**BH^{t}_{1}···HO** **BH^{t}_{2}···HO**	0.020	0.011	0.007	−0.016	−0.020	0.030
IIab	**BH^{t}_{1}···HO** **BH^{br}···HO**	0.018	0.010	0.001	−0.011	−0.019	0.010
IIIab	**BH^{br}···HO** **BH^{t}_{1}···HO** **BH^{t}_{2}···HO**	0.013	0.020	0.006	−0.016	−0.006	0.013

TFE

	contact	r(OH)	r(BH1)	r(BH2)	r(BH3)	r(BHbr)	r(CuH)
IIbc	**BH^{br}···HO** **Cu···HO**	0.008	−0.003	0.003	−0.009	0.004	0.007
IIcb	**Cu···HO** **BH^{br}···HO**	0.009	0.003	0.002	−0.011	0.000	0.032
IIa	**BH^{t}_{1}···HO** **BH^{t}_{2}···HO**	0.015	0.010	0.007	−0.014	−0.020	0.026
IIab	**BH^{br}···HO** **BH^{t}_{2}···HO**	0.010	−0.009	0.006	−0.002	−0.010	0.038
IIIab	**BH^{t}_{1}···HO** **BH^{t}_{2}···HO** **BH^{br}···HO**	0.011	0.005	0.004	−0.014	−0.010	0.017

MeOH

	contact	r(OH)	r(BH1)	r(BH2)	r(BH3)	r(BHbr)	r(CuH)
IIcb	**Cu···HO** **BH^{br}···HO**	0.010	0.004	0.001	−0.009	0.005	0.011
IIa	**BH^{t}_{1}···HO** **BH^{t}_{2}···HO**	0.014	0.008	0.006	−0.010	−0.011	0.012
IIab	**BH^{t}_{2}···HO** **BH^{br}···HO**	0.012	−0.009	0.006	0.002	−0.012	0.032
IIIab	**BH^{t}_{1}···HO** **BH^{br}···HO** **BH^{t}_{2}···HO**	0.012	0.004	0.008	−0.014	−0.010	0.014

Table S4. M06-optimized **2**·ROH DHB complex formation energies (in kcal/mol).

HFIP

	ΔE	ΔE_{ZPVE}	ΔE_{BSSE}	ΔH_{DCM}	ΔH_{THF}	$\Delta H^{theor}(\Delta\nu_{OH})$	$E_{H\cdots H}$, kcal/mol
IIbc	−23.4	−19.8	−17.2	−5.2	−5.9	−3.7	−3.2
IIcb	−23.7	−21.6	−17.3	−5.9	−6.5	−3.9	−3.0
IIa	−25.9	−23.4	−20.4	−8.8	−9.3	−6.0	−5.0
IIab	−25.3	−22.8	−19.0	−8.8	−9.4	−5.7	−5.6
IIIab	−23.8	−20.7	−18.4	−6.8	−7.3	−4.4	−3.2

TFE

	ΔE	ΔE_{ZPVE}	ΔE_{BSSE}	ΔH_{DCM}	ΔH_{THF}	$\Delta H^{theor}(\Delta\nu_{OH})$	$E_{H\cdots H}$, kcal/mol
IIbc	−18.6	−15.6	−13.4	−4.9	−5.3	−3.1	−2.8
IIcb	−18.4	−17.0	−13.7	−6.3	−6.7	−3.6	−2.5
IIa	−21.3	−18.4	−16.5	−6.3	−6.8	−4.8	−4.1
IIab	−18.0	−16.8	−13.9	−5.6	−6.0	−3.7	−2.8
IIIab	−19.0	−16.1	−14.7	−4.8	−5.2	−4.0	−3.8

MeOH

	ΔE	ΔE_{ZPVE}	ΔE_{BSSE}	ΔH_{DCM}	ΔH_{THF}	$\Delta H^{theor}(\Delta\nu_{OH})$	$E_{H\cdots H}$, kcal/mol
IIcb	−11.6	−9.6	−10.1	−4.6	−4.8	−3.0	−2.3
IIa	−14.6	−12.8	−13.2	−3.6	−3.8	−4.3	−3.3
IIab	−11.7	−10.1	−8.2	−2.3	−2.6	−3.7	−2.7
IIIab	−13.7	−12.3	−12.4	−4.4	−4.6	−5.5	−4.0

Table S5. Frequency shifts (Δν, cm^{-1}) and intensity changes (ΔA, Km/mol) calculated for M06-optimized **2**·ROH DHB complexes.

HFIP

M06	$\Delta\nu_{OH}$	ΔA	$\Delta\nu_{BHt}^{as1}$	ΔA	$\Delta\nu_{BHt}^{as2}$	ΔA	$\Delta\nu_{BHt}^{s}$	ΔA	$\Delta\nu_{BHbr}$	ΔA
IIbc	−184	361	−11	−86	55	−12	50	−15	−26	−15
IIcb	−211	453	−16	−52	46	−11	33	−26	−26	−1
IIa	−367	544	8	−102	30	52	−34	16	106	−42
IIab	−342	496	−7	−56	44	−74	−42	77	128	−18
IIIab	−240	453	9	−112	50	−9	46	7	46	−20

TFE

M06	$\Delta\nu_{OH}$	ΔA	$\Delta\nu_{BHt}^{as1}$	ΔA	$\Delta\nu_{BHt}^{as2}$	ΔA	$\Delta\nu_{BHt}^{s}$	ΔA	$\Delta\nu_{BHbr}$	ΔA
IIbc	−152	302	−17	−75	59	−9	45	−5	−31	35
IIcb	−183	387	−10	−26	43	28	17	−18	−13	19
IIa	−263	445	−9	−80	29	55	−25	13	109	−46
IIab	−184	389	−11	−56	41	82	22	−32	49	−41
IIIab	−205	409	−4	−92	47	24	35	−5	64	−13

MeOH

M06	$\Delta\nu_{OH}$	ΔA	$\Delta\nu_{BHt}^{as1}$	ΔA	$\Delta\nu_{BHt}^{as2}$	ΔA	$\Delta\nu_{BHt}^{s}$	ΔA	$\Delta\nu_{BHbr}$	ΔA
IIcb	−144	170	−4	−40	31	14	12	−5	−39	26
IIa	−229	309	−15	−77	36	38	−13	5	62	−5
IIab	−183	228	−6	−68	34	64	−11	4	64	−27
IIIab	−190	222	−16	−78	24	77	10	−22	56	−8

Table S6. Structural parameters, frequencies and formation enthalpies for M06-optimized DHB complexes **IIa** type of **2** with alcohols.

ROH	P_i	$r(BH^t_1\cdots HO)$ $\angle OH\cdots H$	$r(BH^t_2\cdots HO)$ $\angle NH\cdots H$	ν_{OH}^{free} $A(\nu_{OH}^{free})$	ν_{OH}^{bond} $A(\nu_{OH}^{bond})$	Δν	−ΔH°, kcal/mol
MeOH	0.63	1.851 155	2.068 141	3920 41	3692 350	−229	4.3
TFE	0.89	1.775 162	2.062 135	3882 68	3619 513	−263	4.8
PhOH	1.00	1.799 161	1.996 136	3898 79	3588 693	−310	5.4
HFIP	1.05	1.699 164	2.096 131	3892 109	3525 653	−367	6.1
PNAP	1.23	1.741 158	1.959 137	3884 199	3489 1749	−395	6.4
PNP	1.27	1.718 158	1.955 136	3882 130	3473 1128	−409	6.5
PFTB	1.33	1.567 164	2.056 130	3848 132	3259 1148	−589	8.1

Table S7. Structural parameters, frequencies and formation enthalpies for M06-optimized DHB complexes **IIab** type of **2** with alcohols.

ROH	P_i	$r(BH^t_1\cdots HO)$ $\angle OH\cdots H$	r(BHbr···HO) $\angle NH\cdots H$	ν_{OH}^{free} $A(\nu_{OH}^{free})$	ν_{OH}^{bond} $A(\nu_{OH}^{bond})$	Δν	−ΔH°, kcal/mol
MeOH	0.63	1.985 140	2.070 160	3920 41	3737 269	−183	3.7
TFE	0.89	2.154 132	1.911 167	3882 68	3697 457	−184	3.7
PhOH	1.00	1.677 165	2.373 136	3898 79	3572 682	−326	5.6
HFIP	1.05	1.622 156	2.188 122	3892 109	3550 605	−342	5.8
PNDP	1.23	1.753 149	2.007 141	3884 199	3547 1739	−337	5.7
PNP	1.27	1.600 164	2.257 134	3882 130	3471 1109	−411	6.5
PFTB	1.33	1.508 167	2.121 124	3848 132	3214 1252	−634	8.4

Figure S7. The dependence of complex formation enthalpy from alcohol acidity $-\Delta H°=f(P_i)$.

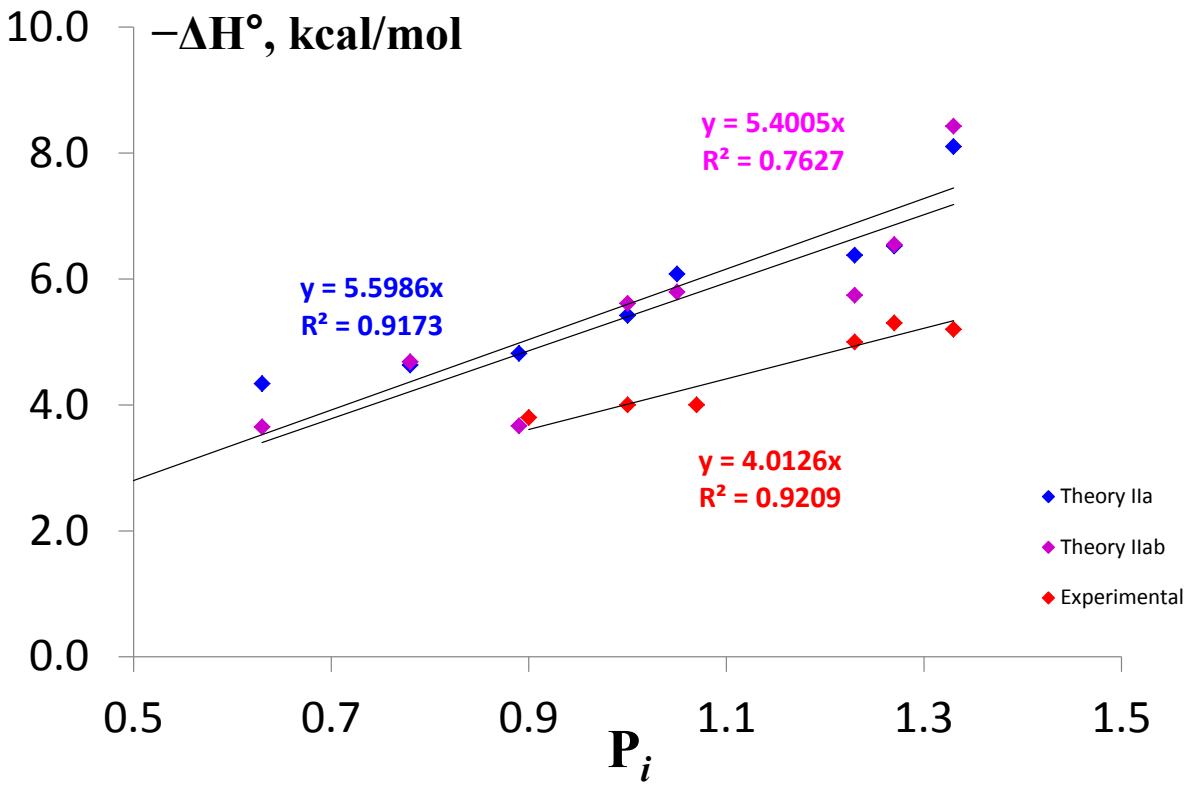


Table S8. Changes in NPA charges for **2**·ROH DHB complexes.

HFIP

	contact	Δq[H(O)]	Δq[H^{t1}(B)]	Δq[H^{t2}(B)]	Δq[H^{t3}(B)]	Δq[H^{br}(B)]
IIbc	**BH^{br}···HO** **Cu···HO**	0.047	0.013	0.001	0.026	-0.043
IIcb	**Cu···HO** **BH^{br}···HO**	0.036	0.024	0.000	0.015	-0.017
IIa	**BH^{t}_1···HO** **BH^{t}_2···HO**	0.077	0.009	-0.018	0.029	-0.002
IIab	**BH^{t}_1···HO** **BH^{br}···HO**	0.069	-0.014	0.006	0.028	-0.012
IIIab	**BH^{br}···HO** **BH^{t}_1···HO** **BH^{t}_2···HO**	0.074	0.019	-0.006	0.034	-0.003

TFE

	contact	Δq[H(O)]	Δq[H^{t1}(B)]	Δq[H^{t2}(B)]	Δq[H^{t3}(B)]	Δq[H^{br}(B)]
IIbc	**BH^{br}···HO** **Cu···HO**	0.034	0.016	-0.001	0.017	-0.043
IIcb	**Cu···HO** **BH^{br}···HO**	0.029	0.027	-0.019	0.009	-0.022
IIa	**BH^{t}_1···HO** **BH^{t}_2···HO**	0.074	0.013	-0.017	0.025	0.003
IIab	**BH^{t}_1···HO** **BH^{br}···HO**	0.051	0.033	-0.027	0.023	-0.002
IIIab	**BH^{br}···HO** **BH^{t}_1···HO** **BH^{t}_2···HO**	0.031	0.028	-0.019	0.009	-0.022

MeOH

	contact	Δq[H(O)]	Δq[H^{t1}(B)]	Δq[H^{t2}(B)]	Δq[H^{t3}(B)]	Δq[H^{br}(B)]
IIcb	**Cu···HO** **BH^{br}···HO**	0.028	0.014	-0.004	0.000	-0.020
IIa	**BH^{t}_1···HO** **BH^{t}_2···HO**	0.061	0.008	-0.011	0.016	-0.001
IIab	**BH^{t}_1···HO** **BH^{br}···HO**	0.050	0.031	-0.022	0.012	0.001
IIIab	**BH^{br}···HO** **BH^{t}_1···HO** **BH^{t}_2···HO**	0.059	0.022	-0.021	0.021	-0.005

Table S9. Wiberg bond indexes (WBI) and its changes (ΔWBI) of BH, CuH and OH bonds upon **2**·ROH DHB complexes formation.

HFIP

	contact	WBI(H···H)	ΔWBI(OH)	ΔWBI(BH1)	ΔWBI(BH2)	ΔWBI(BH3)	ΔWBI(BHbr)	ΔWBI(CuH)
IIbc	**BH^{br}···HO**	0.012	−0.062	−0.016	−0.006	0.021	−0.006	−0.017
	Cu···HO	0.016						
IIcb	**Cu···HO**	0.031	−0.065	−0.022	−0.008	0.025	−0.006	−0.008
	BH^{br}···HO	0.006						
IIa	**BH^{t}_{1}···HO**	0.018	−0.113	−0.049	−0.012	0.030	0.038	−0.037
	BH^{t}_{2}···HO	0.004						
IIab	**BH^{t}_{1}···HO**	0.058	−0.118	−0.041	−0.001	0.013	0.031	−0.035
	BH^{br}···HO	0.002						
IIIab	**BH^{br}···HO**	0.002	−0.092	−0.026	−0.006	0.028	0.013	−0.021
	BH^{t}_{1}···HO	0.005						
	BH^{t}_{2}···HO	0.001						

TFE

	contact	WBI(H···H)	WBI(OH)	WBI(BH1)	WBI(BH2)	WBI(BH3)	WBI(BHbr)	WBI(CuH)
IIbc	**BH^{br}···HO**	0.010	−0.062	−0.012	−0.002	0.019	−0.007	−0.014
	Cu···HO	0.016						
IIcb	**Cu···HO**	0.024	−0.066	−0.040	−0.003	0.034	0.001	−0.013
	BH^{br}···HO	0.008						
IIa	**BH^{t}_{1}···HO**	0.011	−0.102	−0.045	−0.008	0.032	0.038	−0.037
	BH^{t}_{2}···HO	0.003						
IIab	**BH^{br}···HO**	0.002	−0.077	0.006	−0.006	−0.014	0.020	−0.026
	BH^{t}_{2}···HO	0.005						
IIIab	**BH^{t}_{1}···HO**	0.009	−0.093	−0.038	0	0.028	0.019	−0.020
	BH^{t}_{2}···HO	0.001						
	BH^{br}···HO	0.001						

MeOH

	contact	WBI(H···H)	WBI(OH)	WBI(BH1)	WBI(BH2)	WBI(BH3)	WBI(BHbr)	WBI(CuH)
IIcb	**Cu···HO**	0.020	−0.053	−0.005	0.002	0.004	−0.006	−0.003
	BH^{br}···HO	0.004						
IIa	**BH^{t}_{1}···HO**	0.006	−0.083	−0.011	−0.002	0.008	0.018	−0.018
	BH^{t}_{2}···HO	0.003						
IIab	**BH^{t}_{2}···HO**	0.004	−0.067	0.037	−0.003	−0.044	0.024	−0.024
	BH^{br}···HO	0.001						
IIIab	**BH^{t}_{1}···HO**	0.007	−0.078	−0.007	−0.006	0.009	0.019	−0.018
	BH^{br}···HO	0						
	BH^{t}_{2}···HO	0						

Table S10. Natural bond orbital analysis (E^2 in kcal/mol) for **2**·ROH adducts .

	Donor NBOs	HFIP	TFE	MeOH
IIbc	τ(Cu-H-B)	4.7	3.9	
	n1(Cu)	-	0.5	
	n2(Cu)	-	0.5	
IIcb	τ(Cu-H-B)	2.5	3.0	1.5
	n1(Cu)	3.1	2.1	0.5
IIa	σ(B-Ht^1)	8.0	5.1	2.9
	σ(B-Ht^2)	2.0	2.0	1.6
IIab	σ(B-Ht^1)	9.6	0.9	1.8
	τ(Cu-H-B)	1.6	3.6	1.3
IIIab	τ(Cu-H-B)	4.4	3.4	0.5
	σ(B-Ht^1)	0.9	0.5	3.0
	σ(B-Ht^2)	0.9	0.5	-

Table S11. Energy of H···X bond derived from critical point ($E_{H\cdots X}$), Laplacian of electron density at critical point ($\nabla^2\rho_c$), electron densities at the H···H bond critical point (ρ_c) and bond ellipticity (ε) for **2**·ROH DHB complexes.

HFIP

	$E_{H\cdots X}$, kcal/mol	$\nabla^2\rho_c$, au	ρ_c, au	ε	*contact*
IIbc	−3.2	0.05	0.02	0.25	**BH^{br}···HO**
IIcb	−3.0	0.05	0.02	0.17	**Cu···HO**
IIa	−5.0	0.06	0.03	0.35	**BH^{t}_{1}···HO**
IIab	−5.6	0.07	0.03	0.20	**BH^{t}_{1}···HO**
IIIab	−3.2	0.05	0.02	1.39	**BH^{br}···HO**

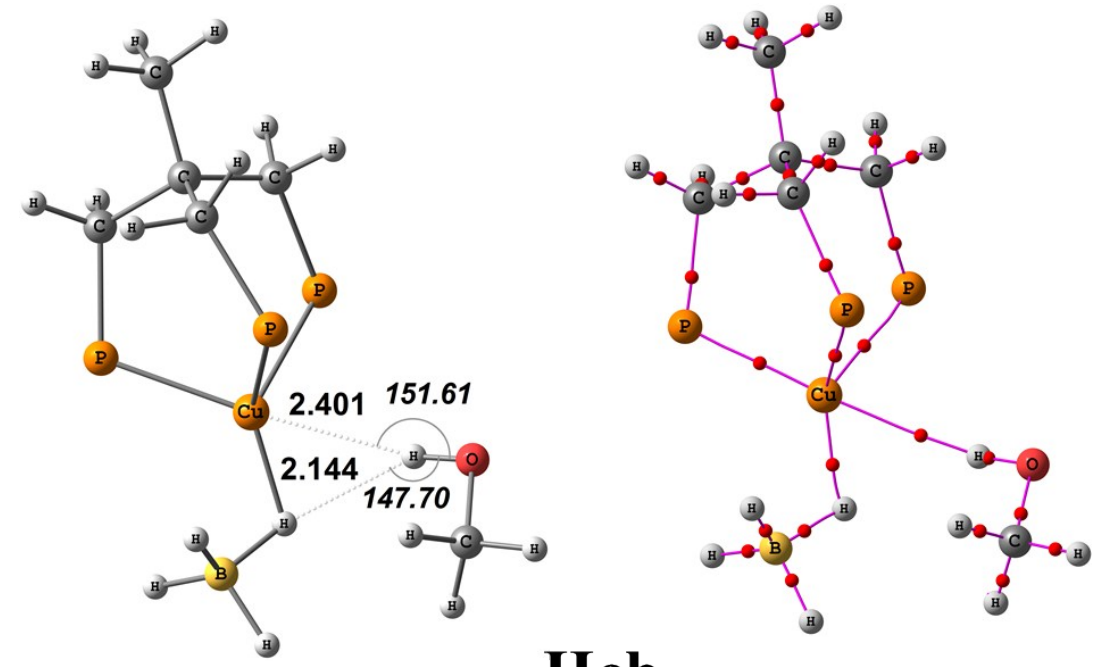
TFE

	$E_{H\cdots X}$, kcal/mol	$\nabla^2\rho_c$, au	ρ_c, au	ε	*contact*
IIbc	−2.8	0.04	0.02	0.33	**BH^{br}···HO**
IIcb	−2.5	0.04	0.02	1.03	**Cu···HO**
IIa	−4.1	0.06	0.02	0.52	**BH^{t}_{1}···HO**
IIab	−2.8	0.05	0.02	0.49	**BH^{t}_{1}···HO**
IIIab	−3.8	0.06	0.02	0.28	**BH^{br}···HO**

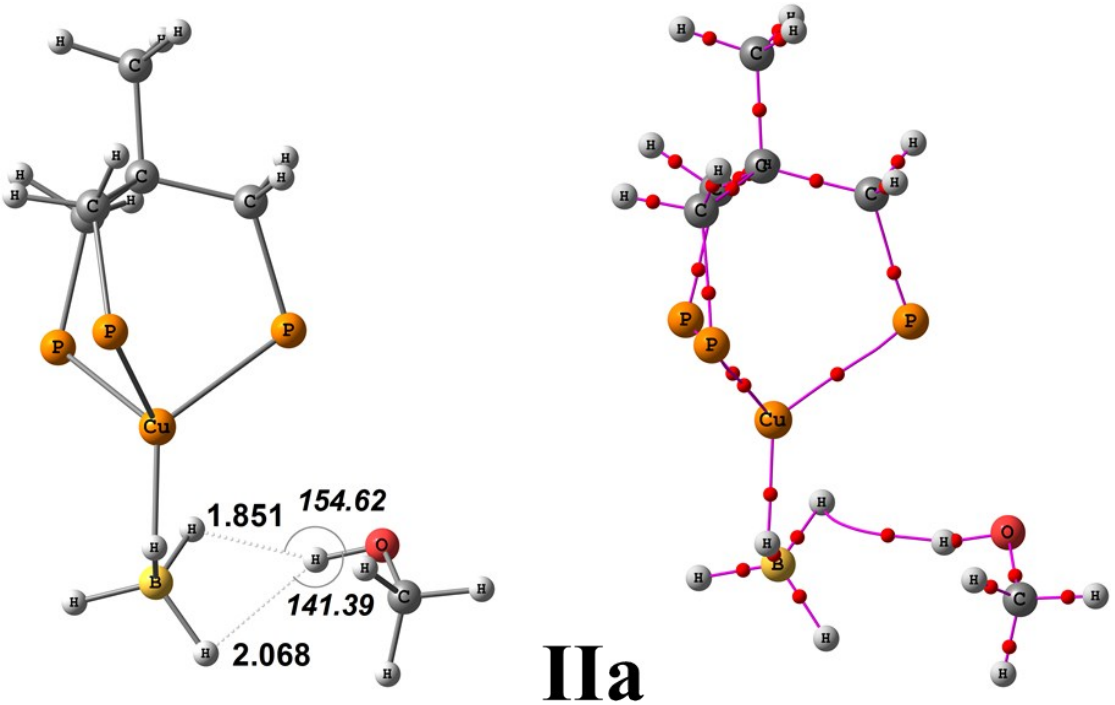
MeOH

	$E_{H\cdots X}$, kcal/mol	$\nabla^2\rho_c$, au	ρ_c, au	ε	*contact*
IIcb	−2.3	0.04	0.01	0.46	**Cu···HO**
IIa	−3.3	0.05	0.02	0.69	**BH^{t}_{1}···HO**
IIab	−2.7	0.04	0.02	0.97	**BH^{t}_{1}···HO**
IIIab	−4.0	0.05	0.02	0.32	**BH^{t}_{1}···HO**

Figure S8. M06-optimized geometries of **2**·MeOH DHB complexes and AIM graphs. Me-groups of phosphine ligands are omitted for clarity.

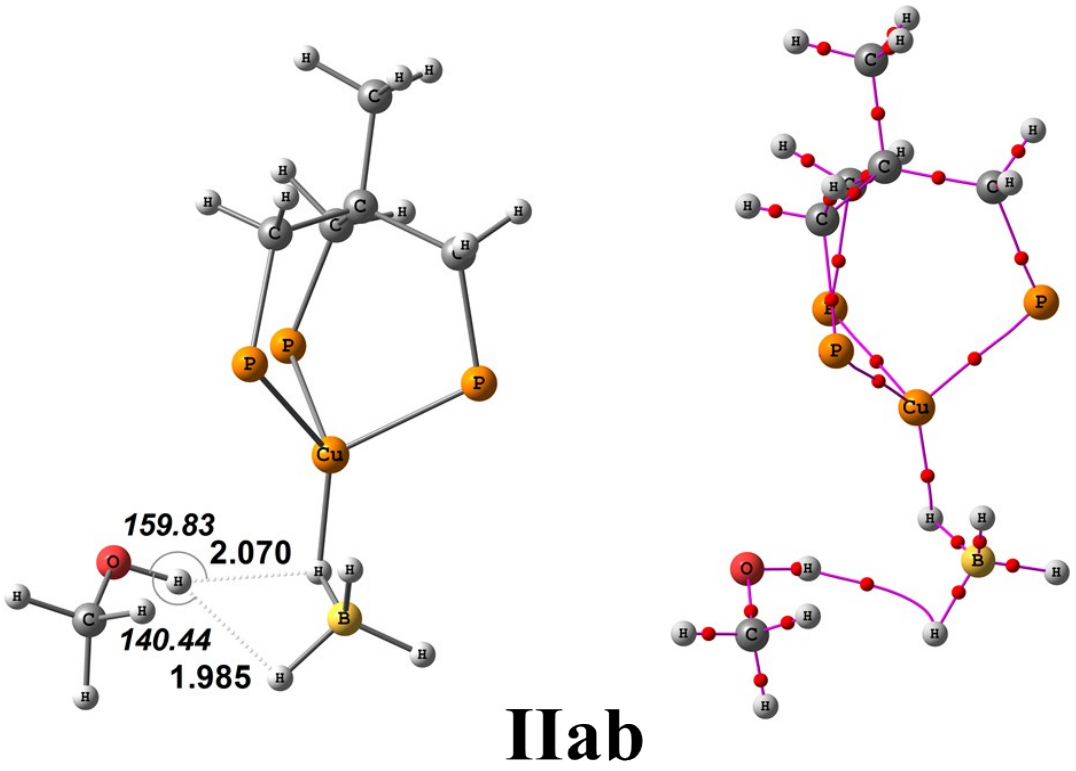


IIcb

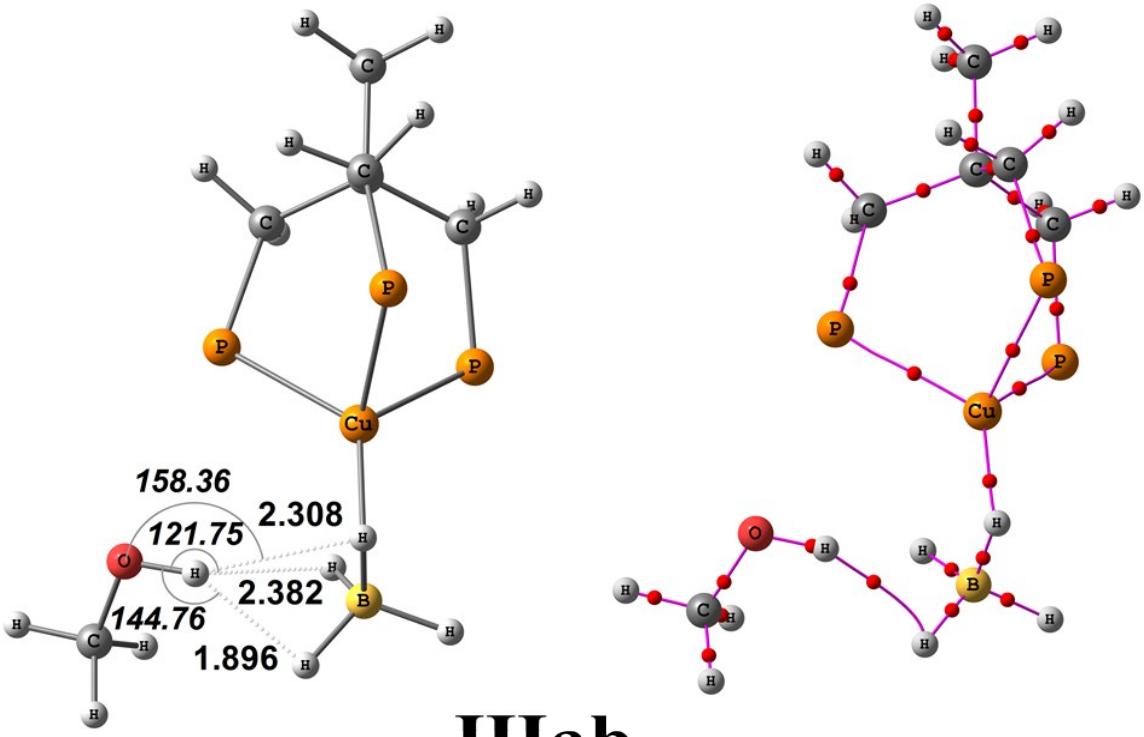


IIa

Figure S9. M06-optimized geometries of **2**·MeOH DHB complexes and AIM graphs. Me-groups of phosphine ligands are omitted for clarity.



IIab



IIIab

Figure S10. M06-optimized geometries of **2**·TFE DHB complexes and AIM graphs. Me-groups of phosphine ligands are omitted for clarity.

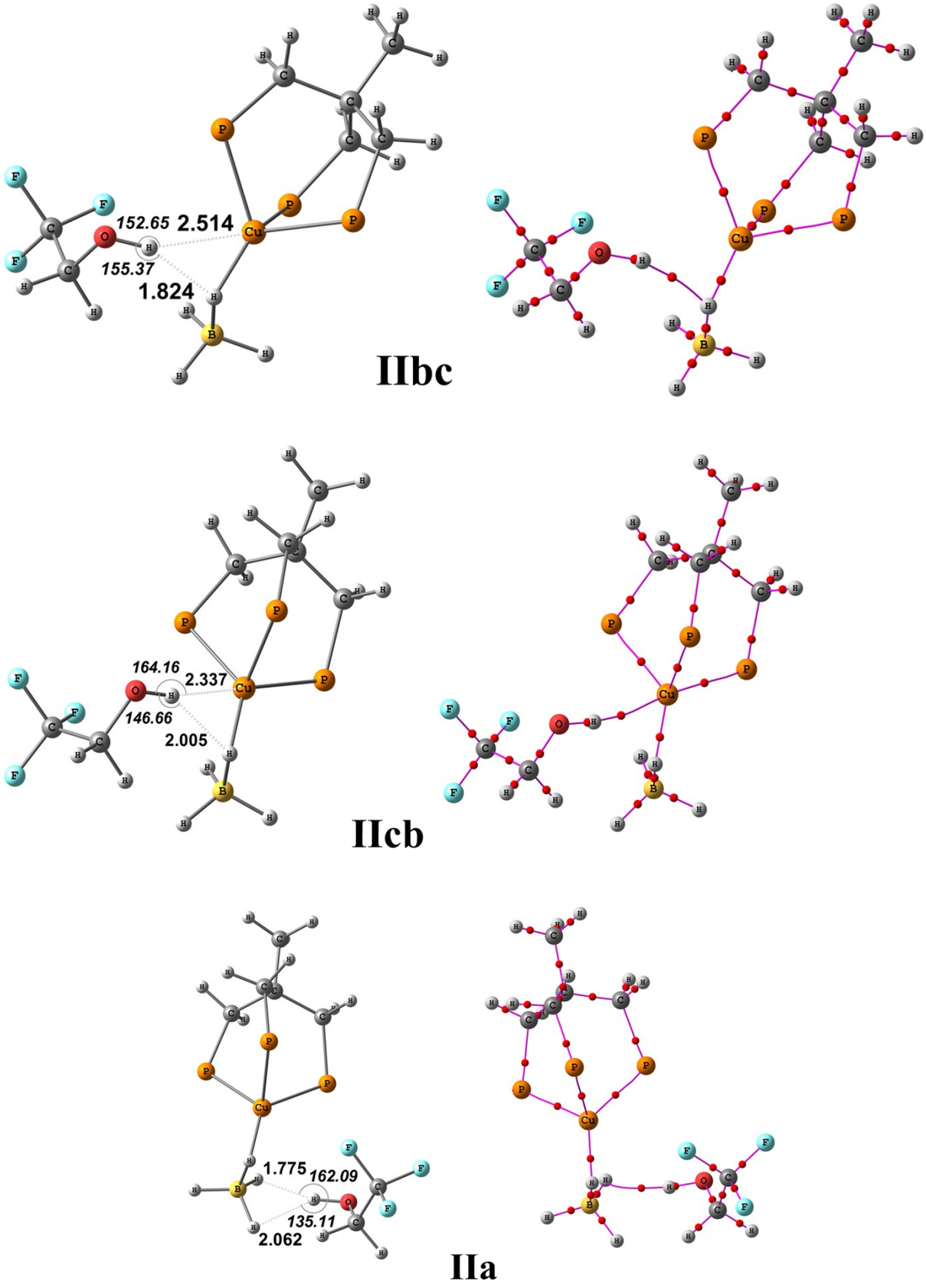
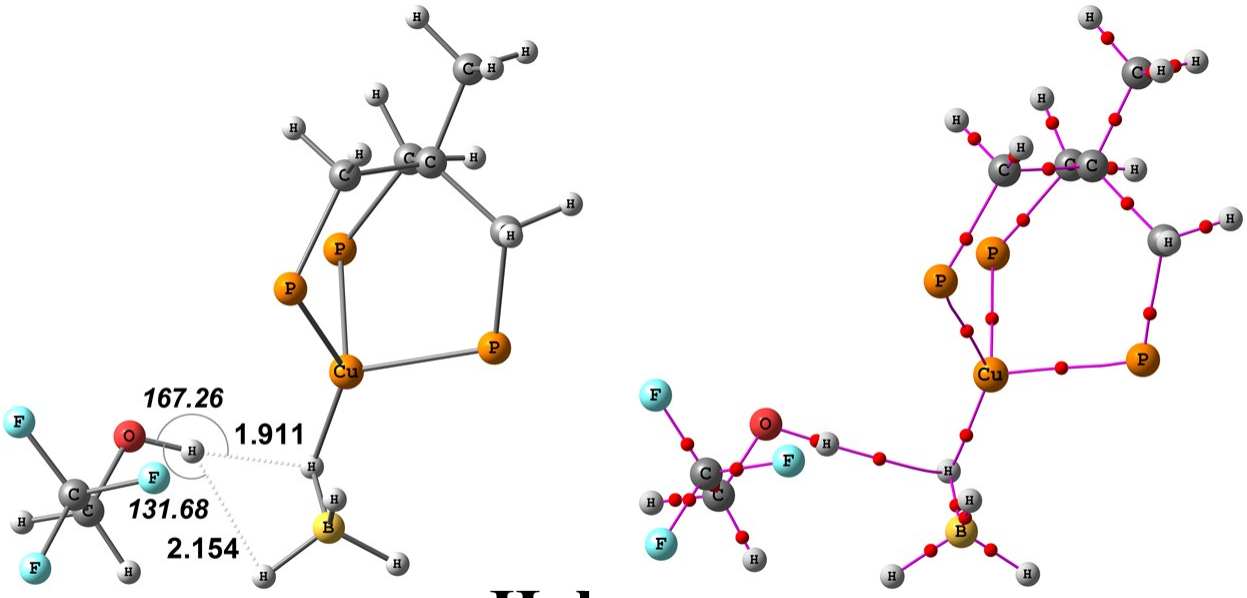
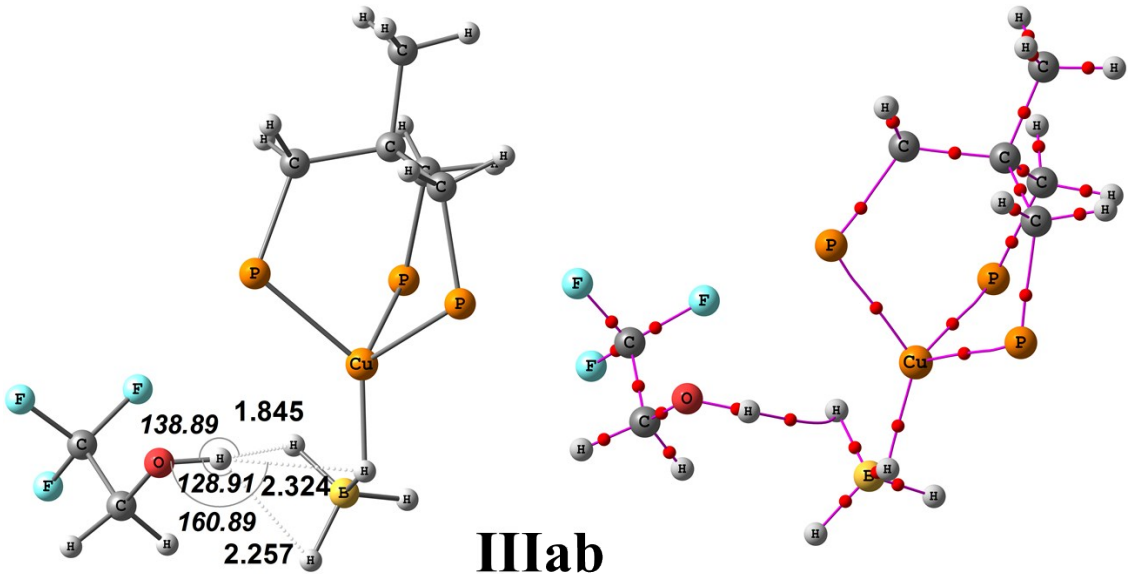


Figure S11. M06-optimized geometries of **2**·TFE DHB complexes and AIM graphs. Me-groups of phosphine ligands are omitted for clarity.

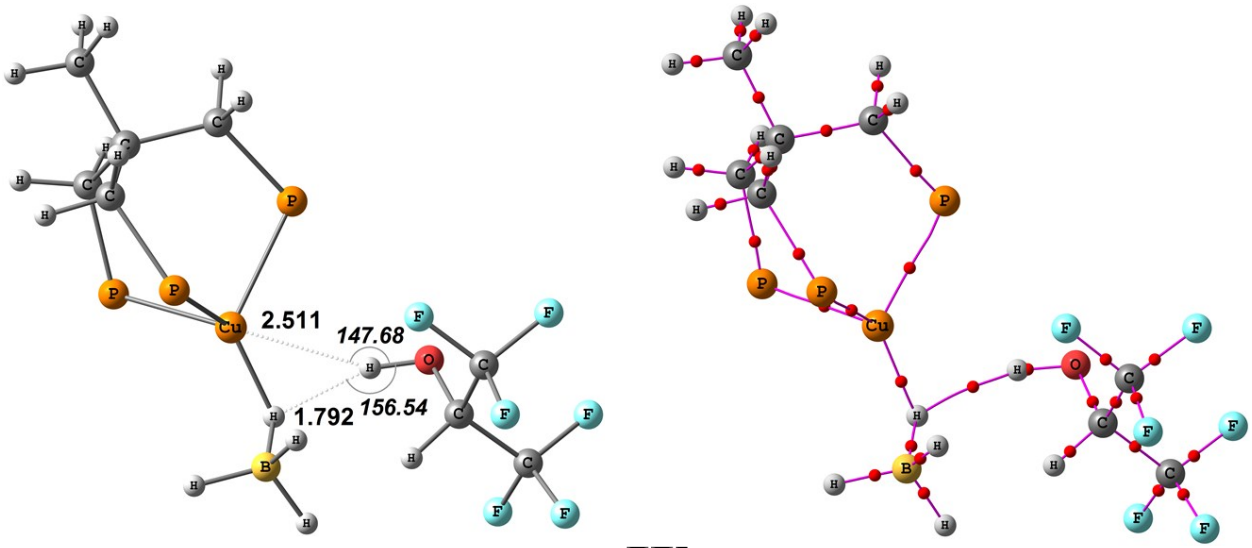


IIab

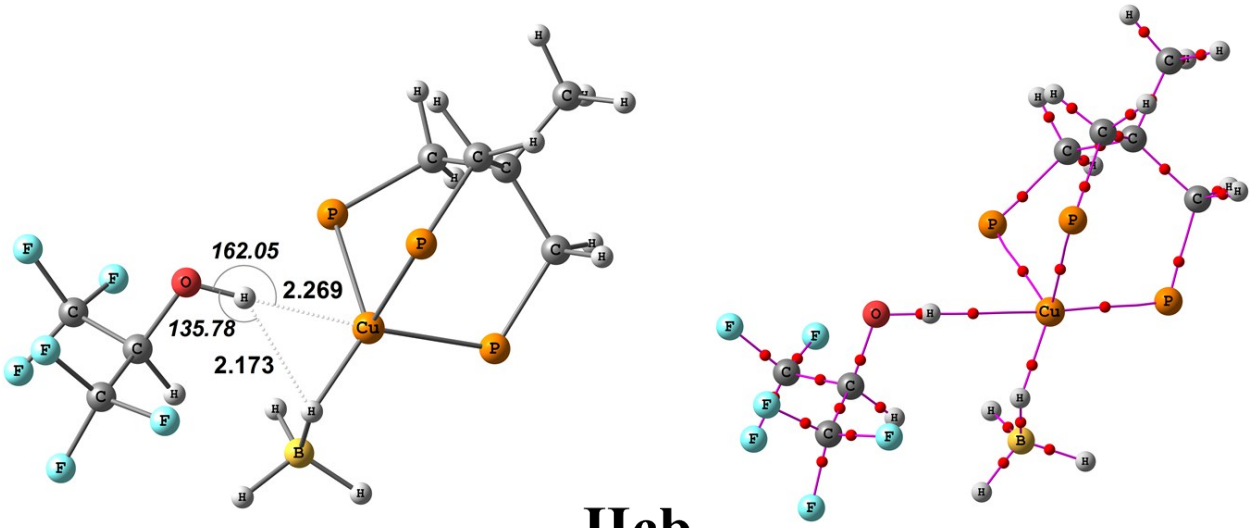


IIIab

Figure S12. M06-optimized geometries of **2**·HFIP DHB complexes and AIM graphs. Me-groups of phosphine ligands are omitted for clarity.

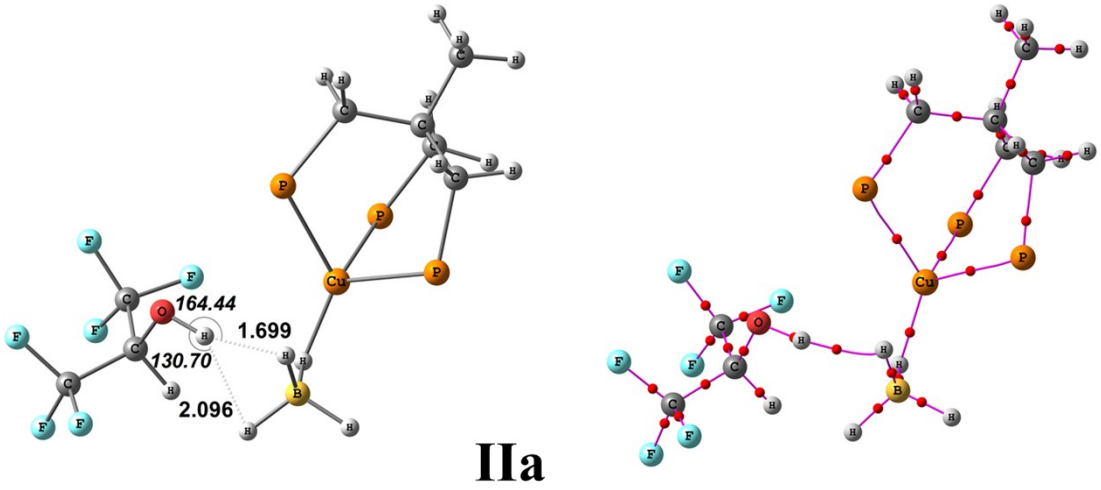


IIbc

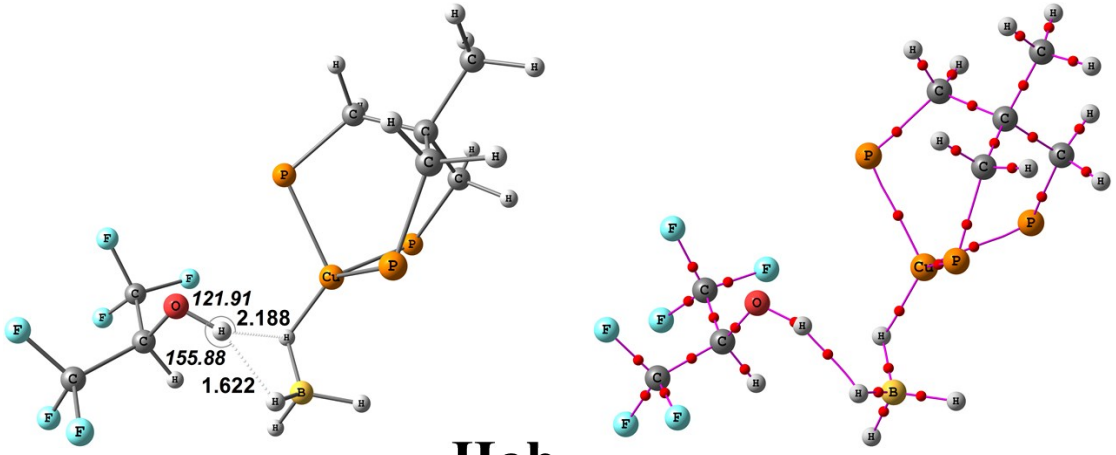


IIcb

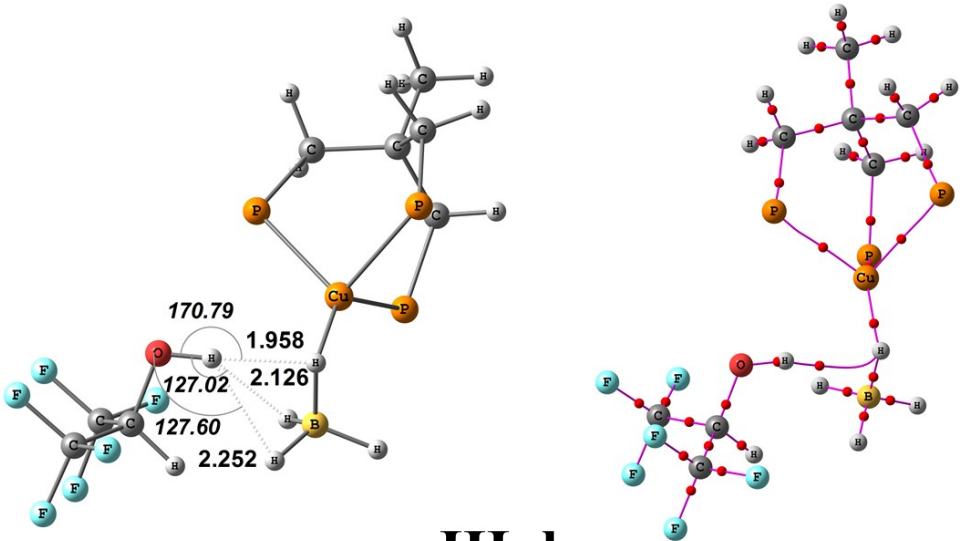
Figure S13. M06-optimized geometries of **2**·HFIP DHB complexes and AIM graphs. Me-groups of phosphine ligands are omitted for clarity.



IIa



IIab



IIIab

Figure S14. Energy profile protonation **2** by CF_3OH. The blue lines denotes to mechanism goes via *BH pathway*, red lines denotes to mechanism goes via *CuH pathway*.

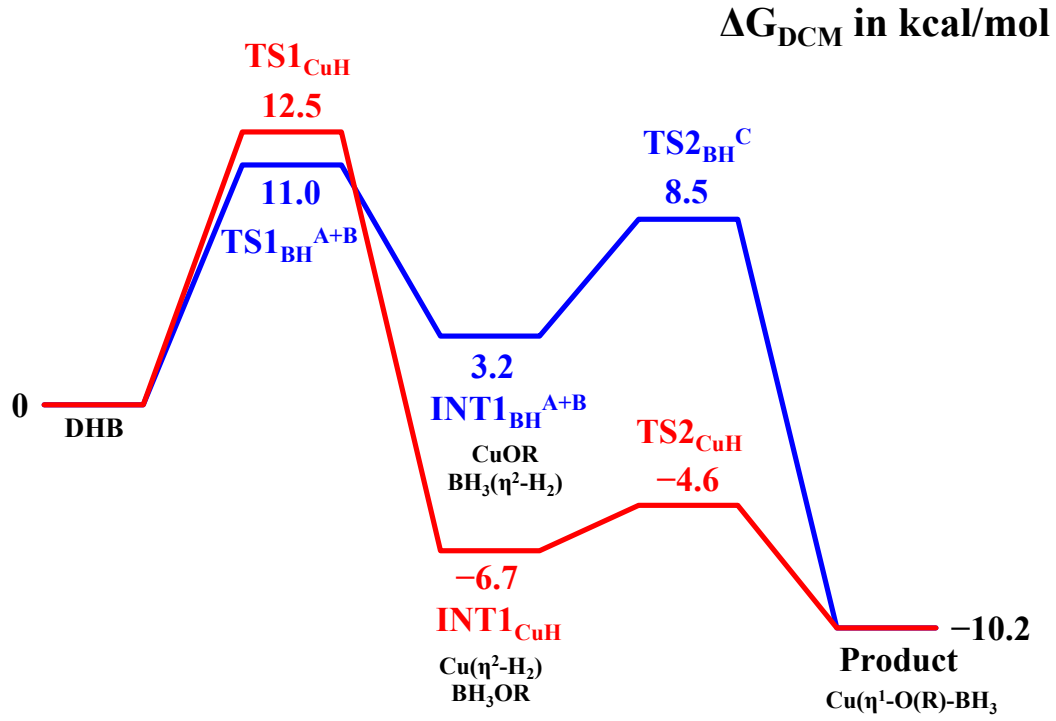


Figure S15 Energy profile protonation **2** by MeOH (dash-and-dot line), TFE (solid line) and HFIP (dashed line). The blue lines denotes to mechanism goes via *BH pathway*, red lines denotes to mechanism goes via *CuH pathway*.

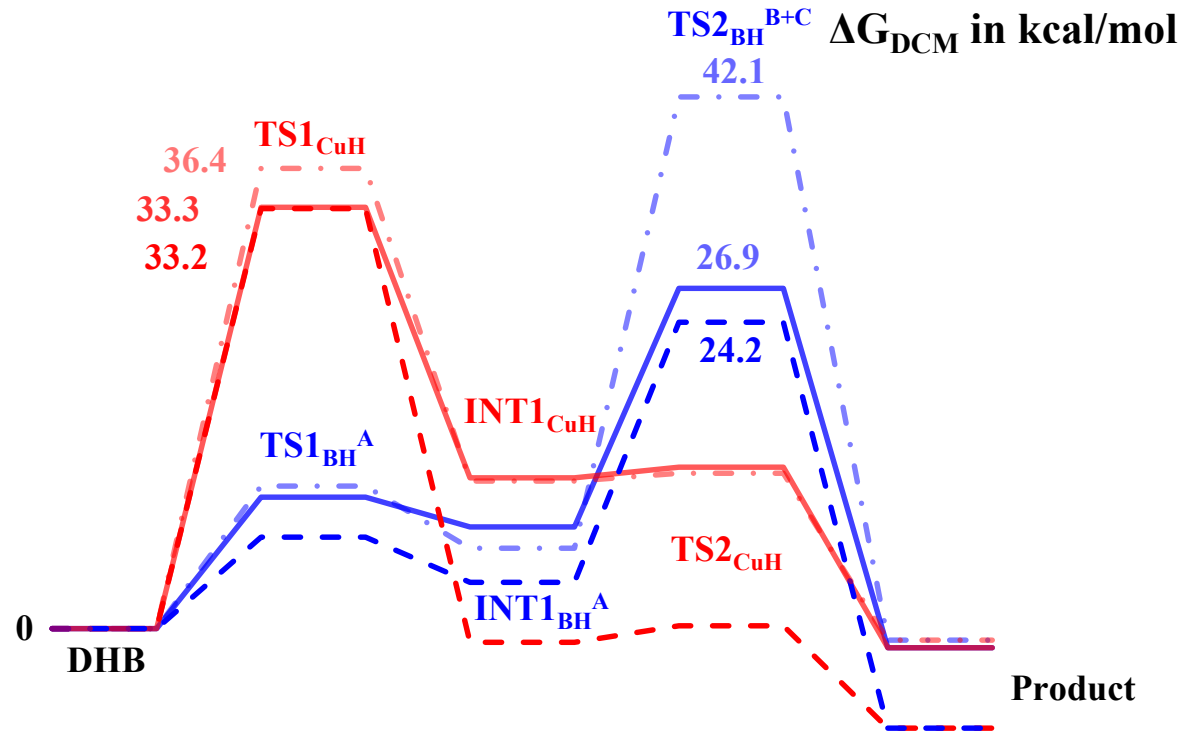
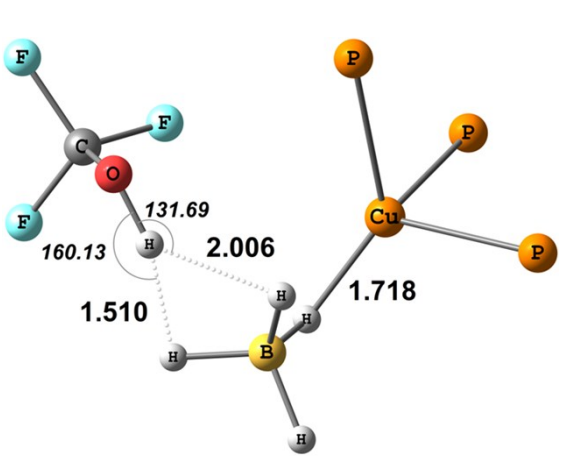
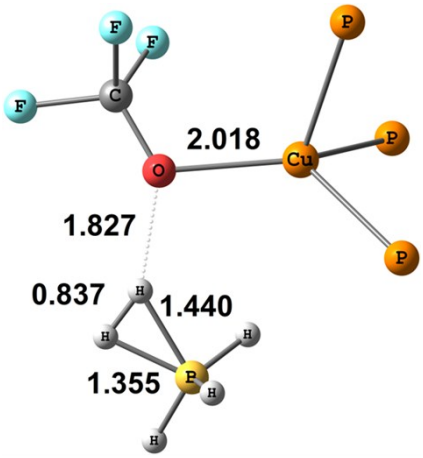


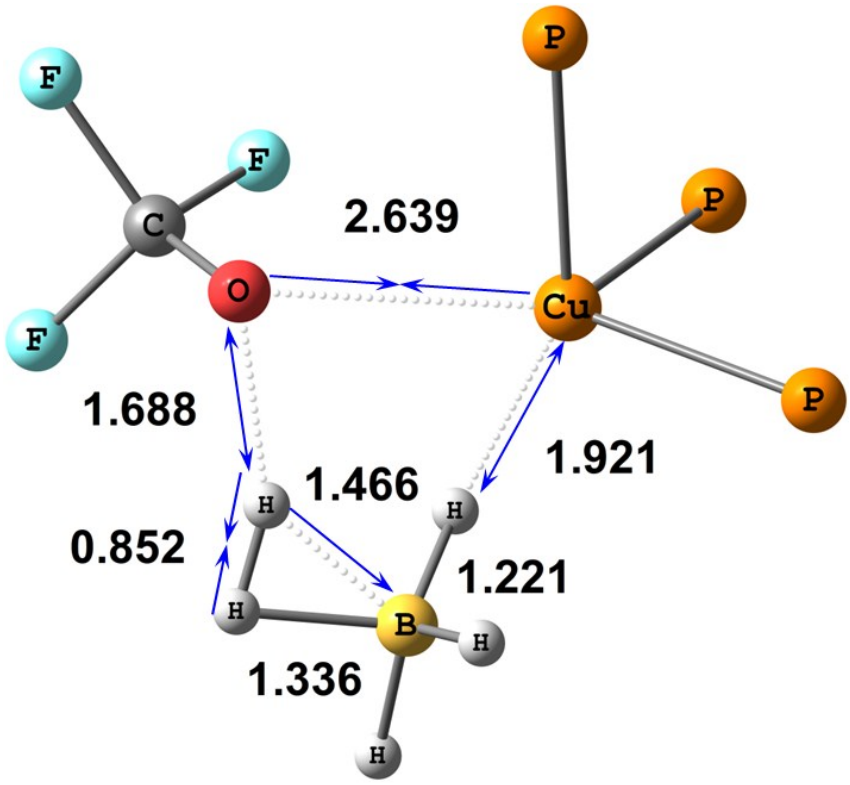
Figure S16. M06-optimized geometries of *BH pathway* **TS1**$_{BH}^{A+B}$ and intermediates for **2**·CF_3OH.



$CF_3OH\_DHB\_IIa$

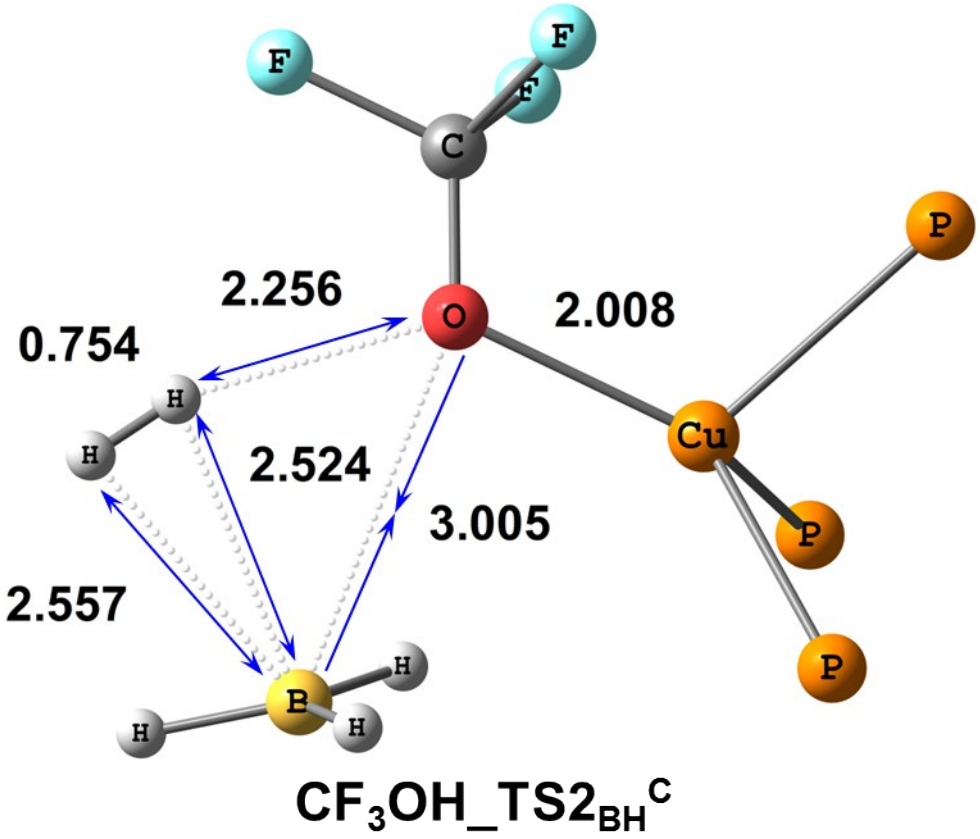


$CF_3OH\_INT^{A+B}$

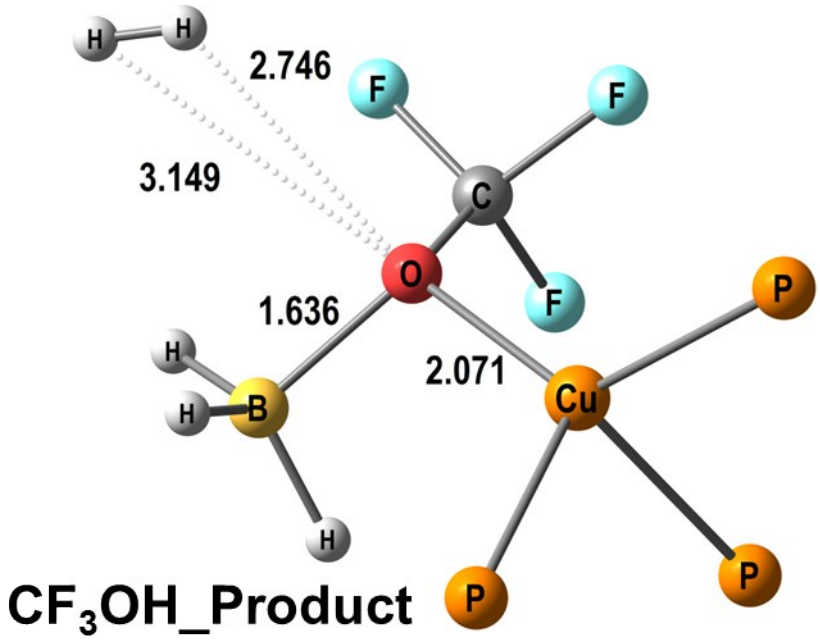


$CF_3OH\_TS1_{BH}^{A+B}$

Figure S17. M06-optimized geometries of *BH pathway* **TS2$_{BH}^{C}$** and product for **2**·CF_3OH.

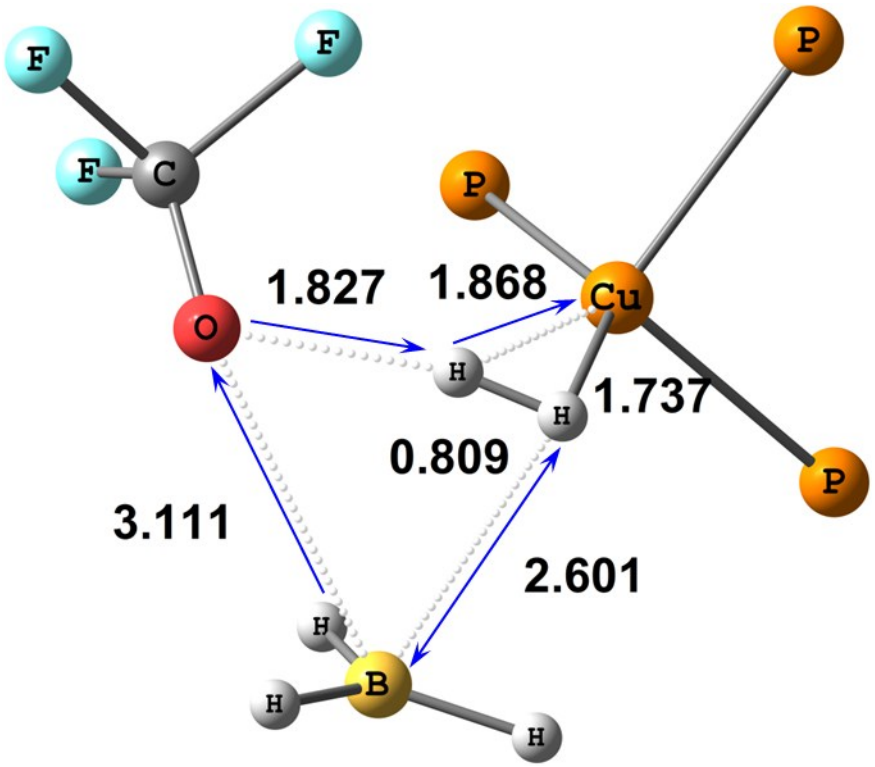


$CF_3OH\_TS2_{BH}^{C}$

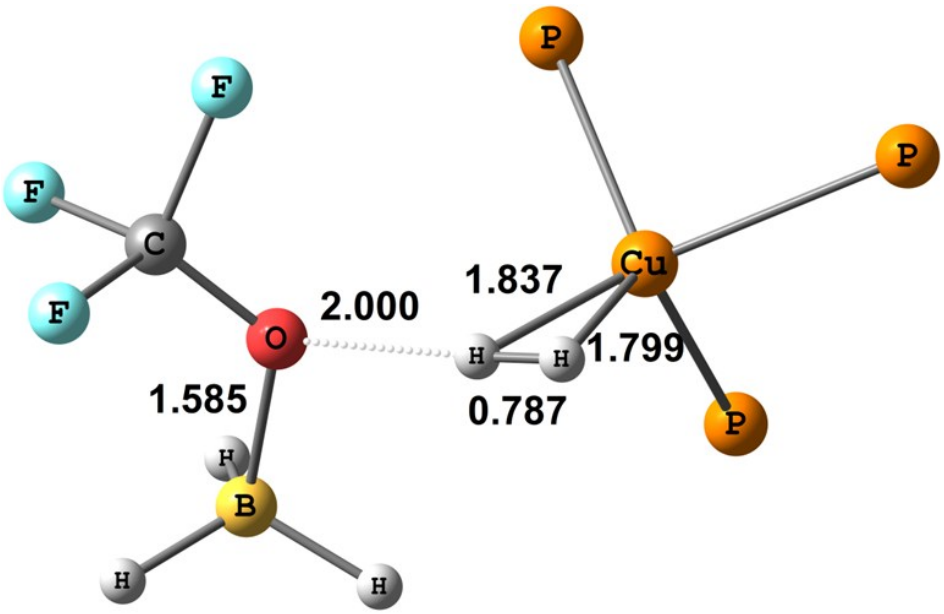


$CF_3OH\_Product$

Figure S18. M06-optimized geometries of *CuH pathway* $\mathbf{TS_{CuH}}$ and intermediate for **2**·CF_3OH.

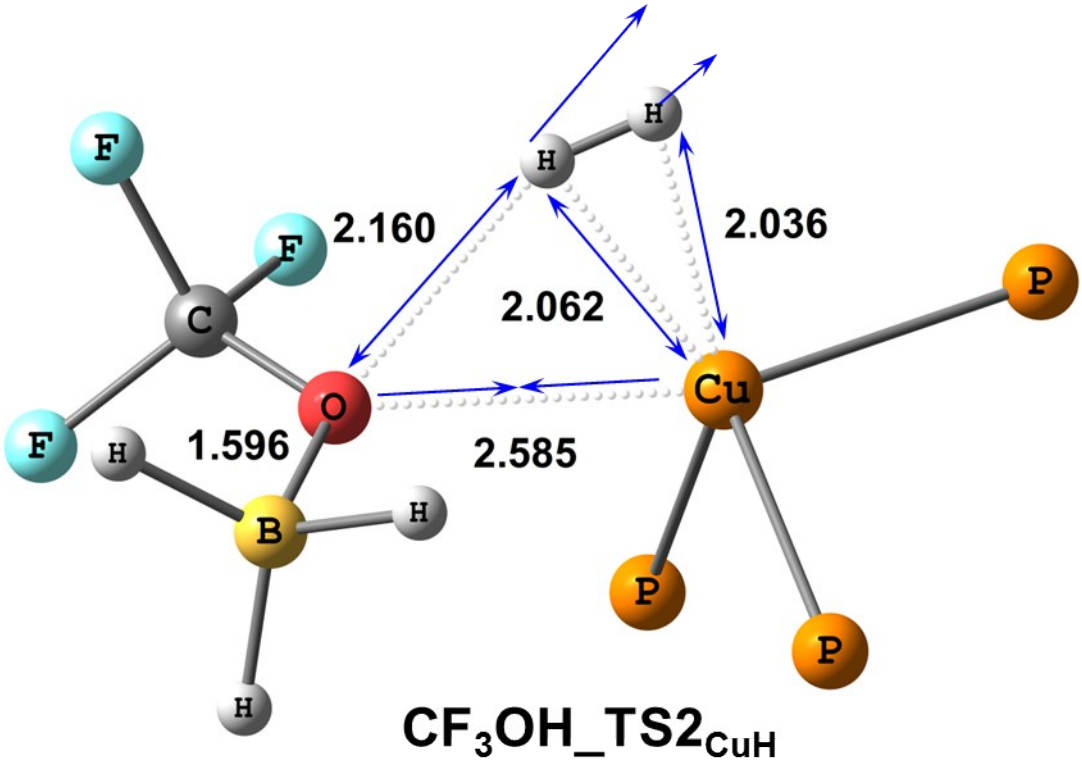


$CF_3OH\_TS1_{CuH}$



CF_3OH_INT1

Figure S19. M06-optimized geometries of *CuH pathway* **TS2$_{CuH}$** and product for **2**·CF_3OH.



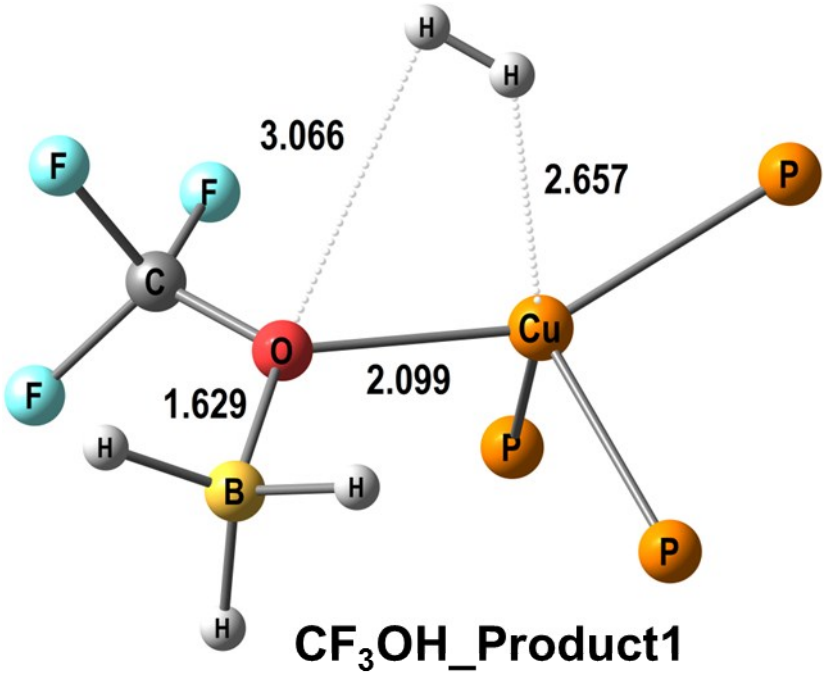
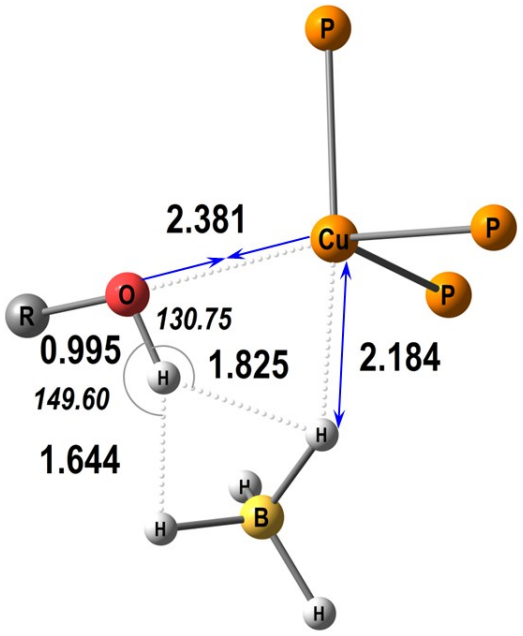
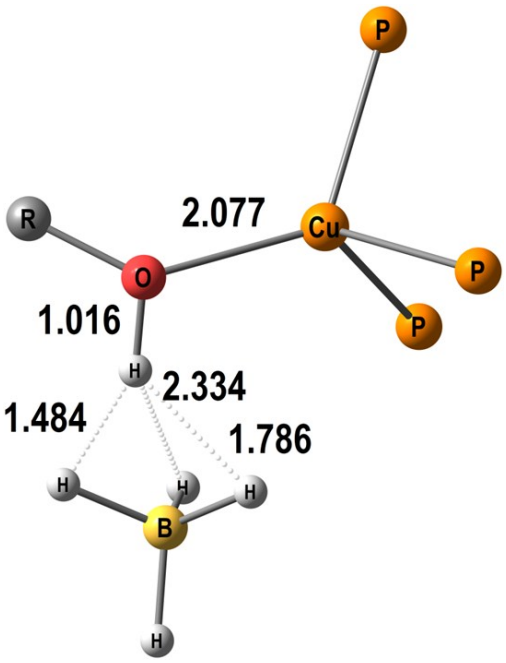


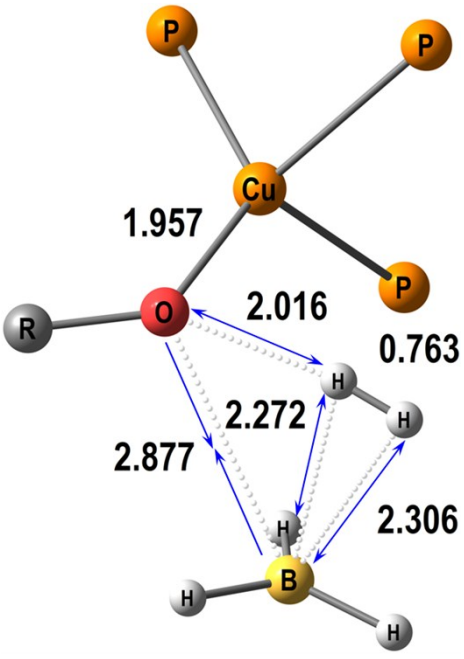
Figure S20. M06-optimized geometries of *BH pathway* TSs and intermediates for **2**·HFIP.



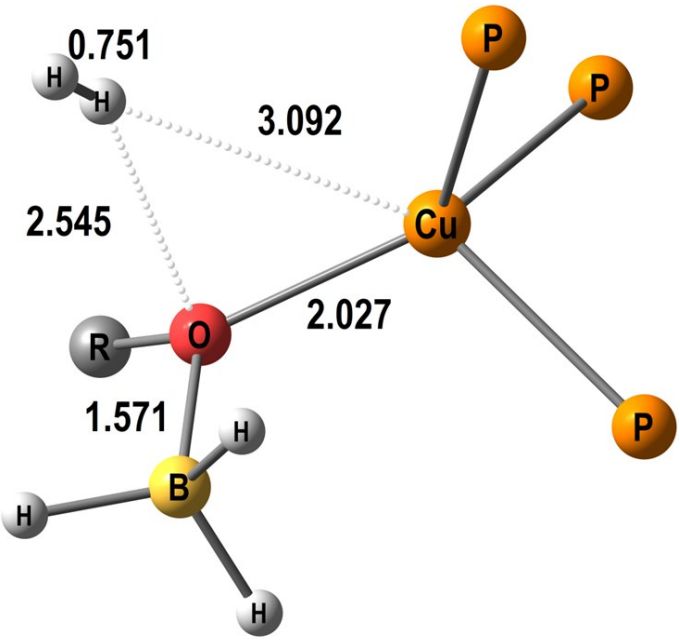
HFIP_TS1$_{BH}^{A}$



HFIP_INT^{A}

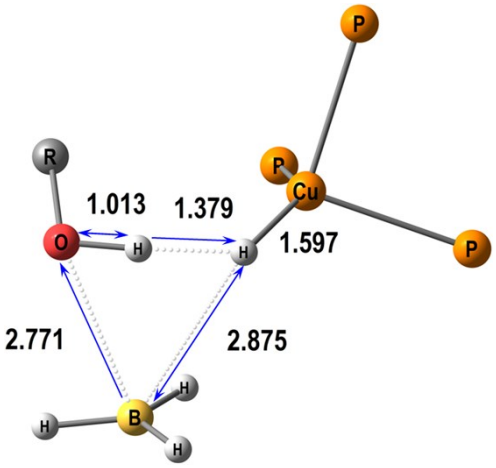


HFIP_TS2$_{BH}^{B+C}$

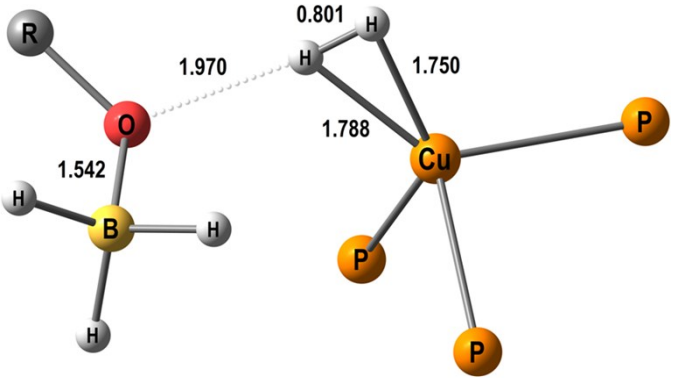


HFIP_Product

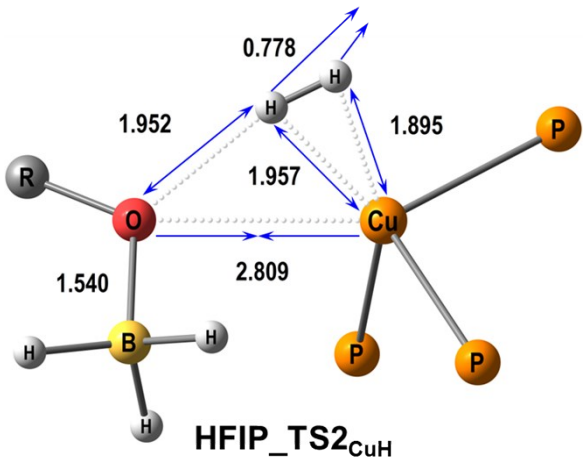
Figure S21. M06-optimized geometries of *CuH pathway* TSs and intermediates for **2**·HFIP.



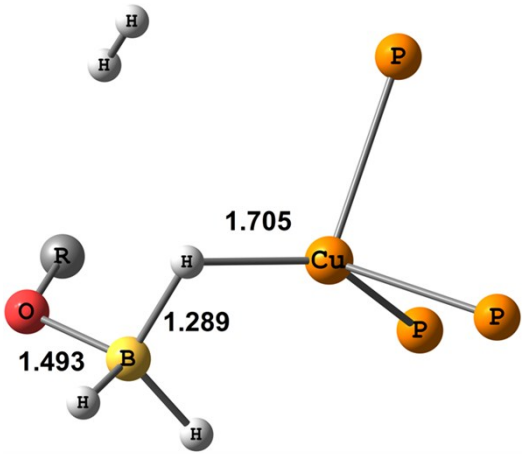
HFIP_TS1$_{CuH}$



HFIP_INT1



HFIP_TS2$_{CuH}$



HFIP_Product1

Figure S22. M06-optimized geometries of *BH pathway* TSs and intermediates for **2**·TFE.

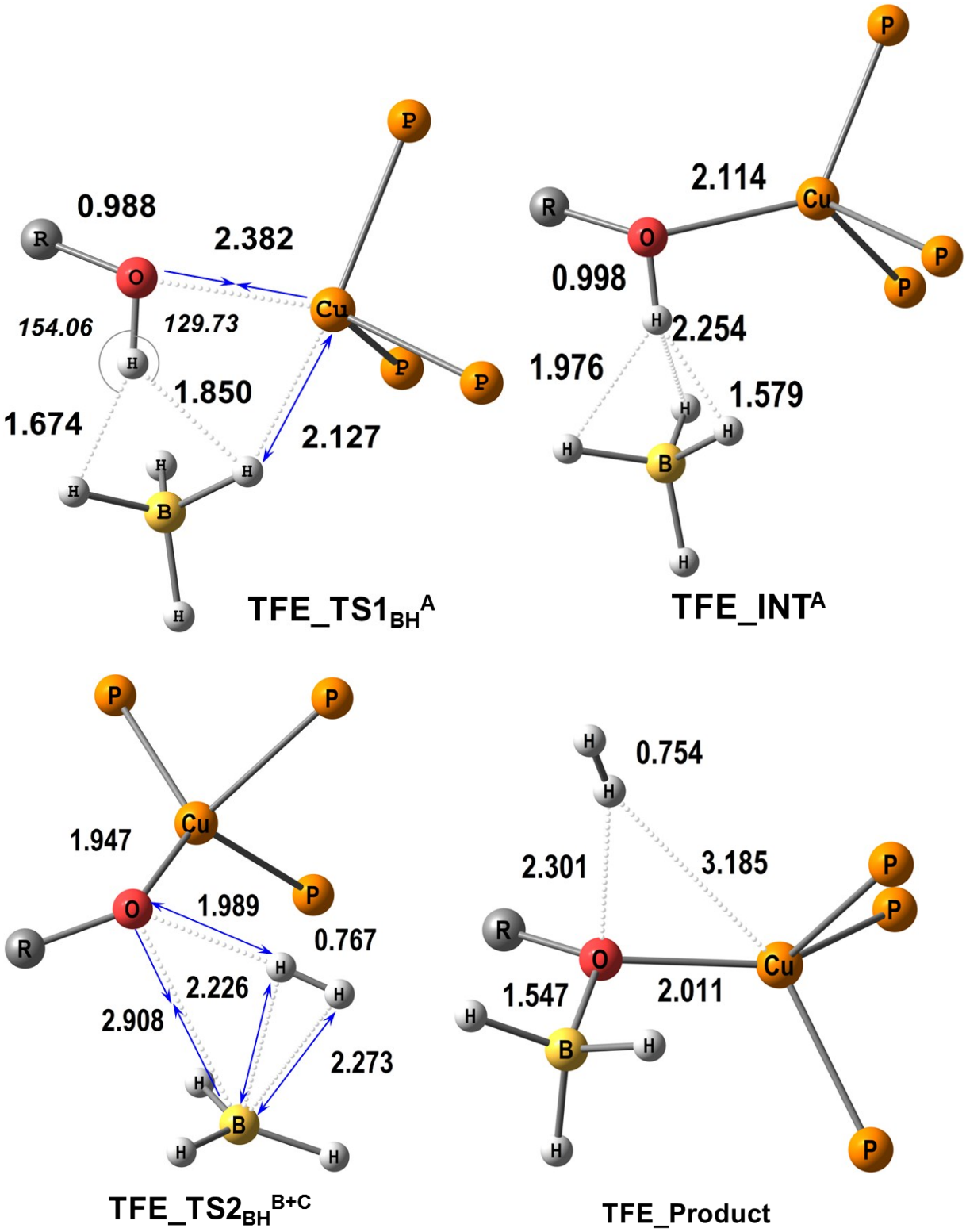


Figure S23. M06-optimized geometries of *CuH pathway* TSs and intermediates for **2**·TFE.

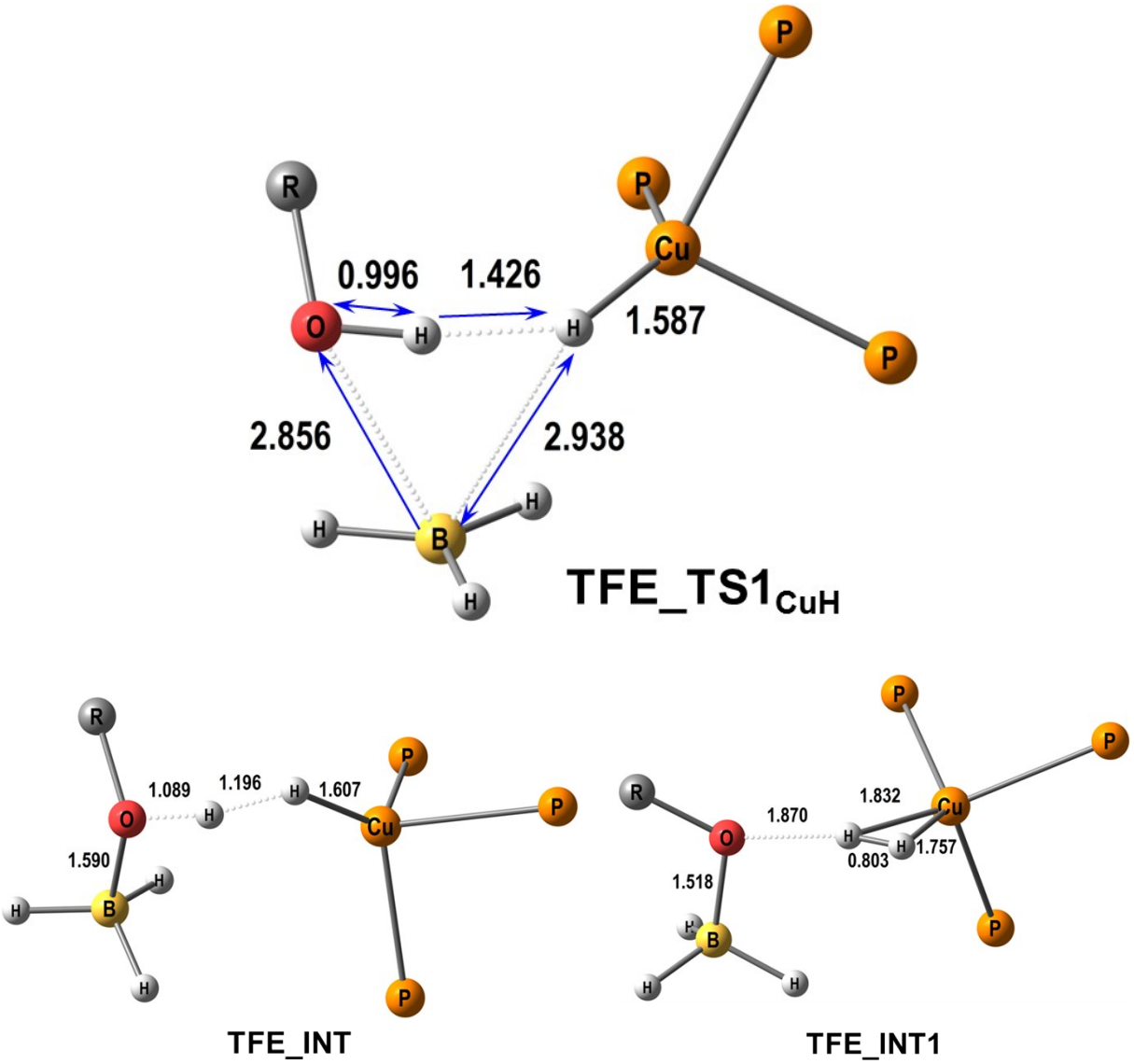
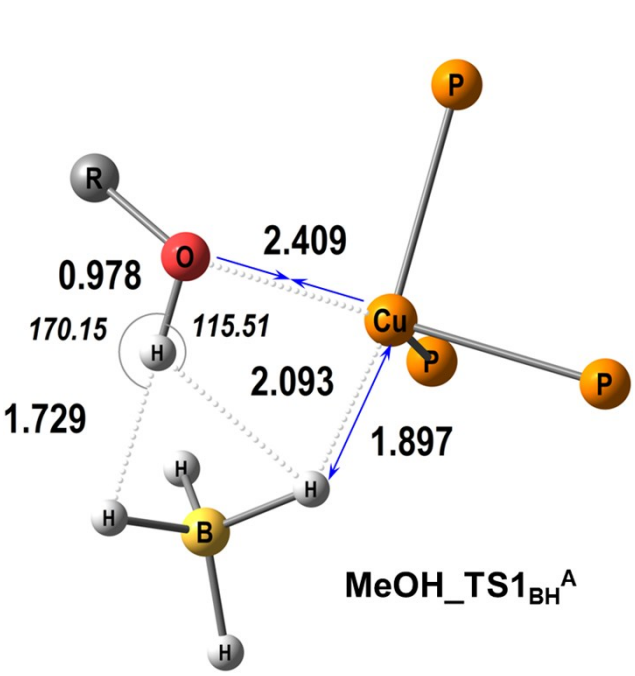
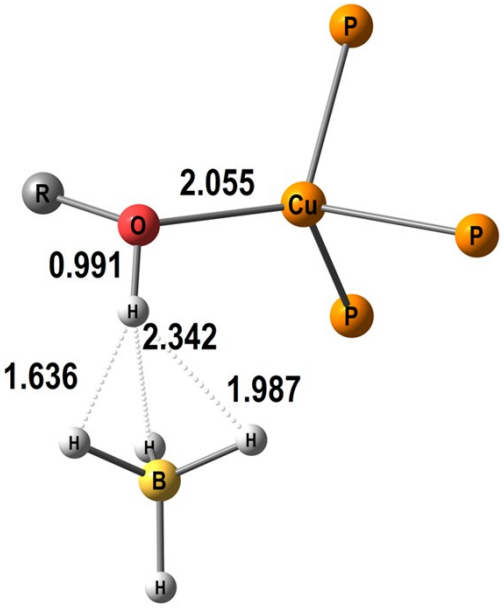


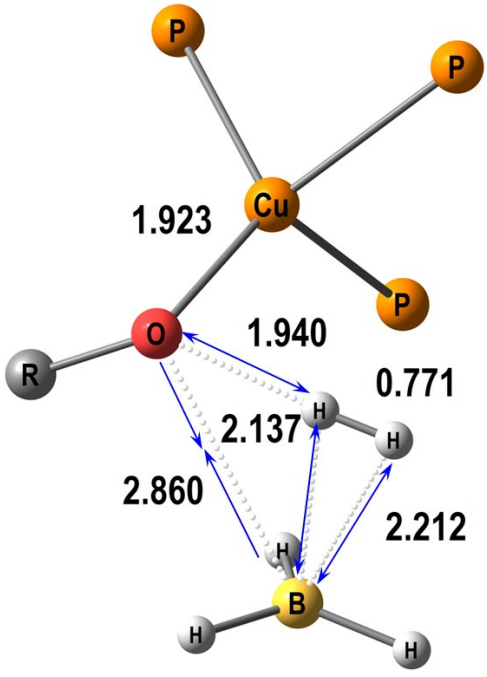
Figure S24. M06-optimized geometries of *BH pathway* TSs and intermediates for **2**·MeOH.



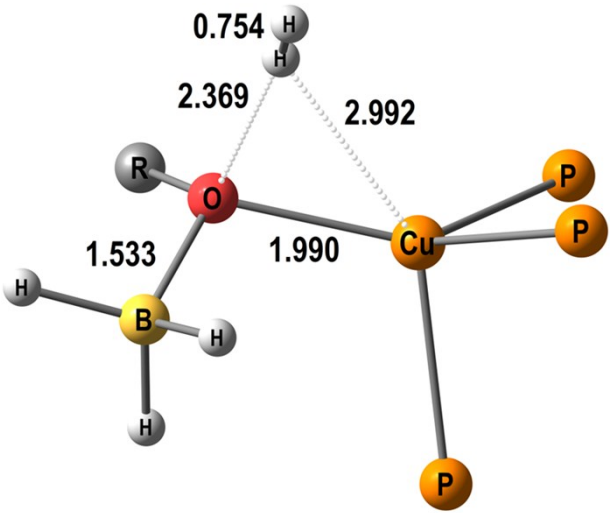
MeOH_TS1$_{BH}^{A}$



MeOH_INT^{A}



MeOH_TS2$_{BH}^{B+C}$



MeOH_Product

Figure S25. M06-optimized geometries of *CuH pathway* TSs and intermediates for **2**·MeOH.

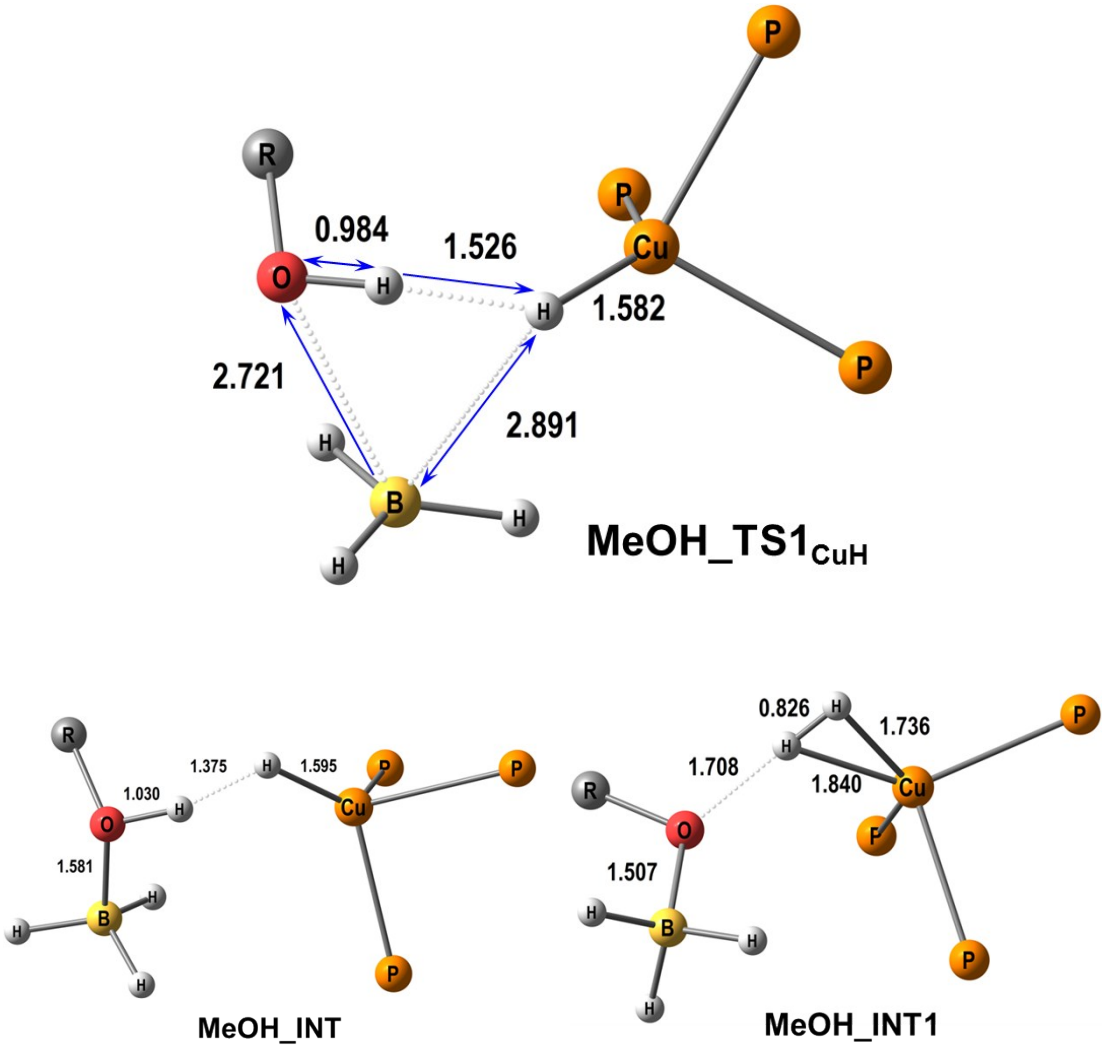


Table S12. M06-optimised geometries (Cartesian coordinates) and electronic energies.

(triphos)Cu(η1-BH4) (1)

E_{el} = -4275.83462808 Ha

E_{ZPVE} = -4275.104995 Ha

H = -4275.060427 Ha

G = -4275.180657 Ha

C	8.081623000000	-3.878814000000	-2.658024000000
C	6.669452000000	-4.476267000000	-2.938158000000
C	8.363071000000	-3.672158000000	-1.143869000000
C	8.374010000000	-2.596724000000	-3.487911000000
H	6.450637000000	-5.216932000000	-2.151655000000
H	6.715372000000	-5.037739000000	-3.883607000000
H	9.276037000000	-3.064331000000	-1.057333000000
H	8.599833000000	-4.648882000000	-0.695810000000
H	8.007577000000	-2.765504000000	-4.511957000000
H	9.466533000000	-2.477311000000	-3.556843000000
C	9.094478000000	-4.938581000000	-3.139850000000
H	10.119811000000	-4.648310000000	-2.873261000000
H	8.883383000000	-5.913682000000	-2.680468000000
H	9.042636000000	-5.053498000000	-4.231467000000
P	7.604391000000	-1.007057000000	-2.896193000000
P	7.043359000000	-2.879790000000	-0.078284000000
P	5.231906000000	-3.297648000000	-2.954047000000
Cu	5.730102000000	-1.547460000000	-1.481422000000
H	5.072681000000	0.109391000000	-1.354675000000
B	3.915798000000	-0.265613000000	-0.986496000000
H	3.914227000000	-1.424796000000	-0.540653000000
H	3.165597000000	-0.190994000000	-1.950624000000
H	3.632950000000	0.490775000000	-0.080187000000
C	5.117339000000	-2.705986000000	-4.691289000000
C	5.580200000000	-3.416445000000	-5.808381000000
C	4.503495000000	-1.458042000000	-4.884643000000
C	5.455722000000	-2.879376000000	-7.089350000000
C	4.364811000000	-0.930493000000	-6.168636000000
C	4.850089000000	-1.634752000000	-7.270165000000
H	6.038761000000	-4.396861000000	-5.690354000000
H	4.149444000000	-0.894830000000	-4.019405000000
H	5.825896000000	-3.434955000000	-7.946993000000
H	3.895202000000	0.039665000000	-6.302722000000
H	4.758981000000	-1.214091000000	-8.267806000000
C	3.769026000000	-4.392044000000	-2.827010000000
C	3.765405000000	-5.757532000000	-3.140610000000
C	2.581701000000	-3.784896000000	-2.383786000000
C	2.596106000000	-6.506895000000	-3.007876000000
C	1.412939000000	-4.535471000000	-2.262114000000
C	1.419457000000	-5.897230000000	-2.569983000000
H	4.672784000000	-6.244833000000	-3.491337000000
H	2.584193000000	-2.726489000000	-2.119118000000
H	2.602795000000	-7.566031000000	-3.251299000000
H	0.499766000000	-4.056637000000	-1.920031000000
H	0.509215000000	-6.482210000000	-2.470286000000
C	7.547475000000	0.024422000000	-4.412277000000
C	8.201041000000	-0.271169000000	-5.615320000000
C	6.775692000000	1.195387000000	-4.325937000000
C	8.085327000000	0.587767000000	-6.709552000000
C	6.671879000000	2.057391000000	-5.414997000000
C	7.325001000000	1.752621000000	-6.611027000000
H	8.803031000000	-1.172051000000	-5.711450000000
H	6.243330000000	1.417237000000	-3.401096000000
H	8.594202000000	0.346773000000	-7.639218000000
H	6.073874000000	2.960663000000	-5.333194000000
H	7.240120000000	2.420605000000	-7.463731000000
C	8.948037000000	-0.160946000000	-1.963517000000
C	8.564438000000	0.591814000000	-0.843473000000
C	10.299390000000	-0.179721000000	-2.340271000000
C	9.513990000000	1.305652000000	-0.110128000000
C	11.249612000000	0.521053000000	-1.598721000000
C	10.856942000000	1.264492000000	-0.482022000000
H	7.517158000000	0.605496000000	-0.541286000000
H	10.613240000000	-0.727597000000	-3.227787000000
H	9.203483000000	1.877674000000	0.759446000000
H	12.294300000000	0.498182000000	-1.897202000000
H	11.598455000000	1.813660000000	0.091764000000
C	8.004134000000	-2.426949000000	1.424994000000
C	7.398649000000	-2.561279000000	2.686312000000
C	9.275283000000	-1.836345000000	1.352324000000
C	8.054318000000	-2.136713000000	3.839782000000
C	9.930318000000	-1.413520000000	2.509153000000
C	9.324781000000	-1.565254000000	3.755748000000
H	6.408261000000	-3.003328000000	2.765447000000
H	9.760914000000	-1.677036000000	0.391790000000
H	7.570553000000	-2.251946000000	4.805716000000
H	10.914214000000	-0.958413000000	2.428647000000
H	9.835821000000	-1.235182000000	4.655773000000
C	6.115096000000	-4.356106000000	0.511036000000
C	6.761489000000	-5.484052000000	1.045234000000
C	4.717455000000	-4.359596000000	0.413983000000
C	6.026790000000	-6.597030000000	1.446088000000
C	3.980980000000	-5.479204000000	0.810185000000
C	4.634434000000	-6.598605000000	1.320394000000
H	7.843639000000	-5.485330000000	1.167828000000
H	4.205804000000	-3.481569000000	0.022712000000
H	6.537180000000	-7.462965000000	1.859087000000
H	2.899009000000	-5.471035000000	0.712183000000
H	4.063080000000	-7.470675000000	1.626141000000

(triphos^{Me})Cu(η1-BH4) (2)

Eel = -3126.53313384 Ha

EZPVE = -3126.130654 Ha

H = -3126.104137 Ha

G = -3126.181887Ha

C	8.050320000000	-3.718372000000	-2.708365000000
C	6.675586000000	-4.297543000000	-3.145505000000
C	8.202211000000	-3.636372000000	-1.166219000000
C	8.367872000000	-2.367675000000	-3.407411000000
H	6.469528000000	-5.187841000000	-2.527763000000
H	6.759133000000	-4.656645000000	-4.185529000000
H	9.171790000000	-3.153664000000	-0.954080000000
H	8.278498000000	-4.661893000000	-0.764747000000
H	8.103399000000	-2.473338000000	-4.473155000000
H	9.459629000000	-2.206819000000	-3.380566000000
C	9.117880000000	-4.720734000000	-3.195676000000
H	10.116635000000	-4.433647000000	-2.839515000000
H	8.899422000000	-5.731149000000	-2.824412000000
H	9.143579000000	-4.758620000000	-4.293209000000
P	7.567766000000	-0.780241000000	-2.802437000000
P	6.910519000000	-2.727498000000	-0.156653000000
P	5.199286000000	-3.160327000000	-3.014689000000
Cu	5.671814000000	-1.394245000000	-1.592354000000
C	7.926579000000	-2.322182000000	1.333815000000
H	8.474165000000	-3.203092000000	1.696390000000
H	8.643446000000	-1.523297000000	1.112325000000
H	7.261617000000	-1.966106000000	2.128821000000
C	7.724639000000	0.223023000000	-4.346121000000
H	7.511509000000	1.272952000000	-4.115441000000
H	8.734387000000	0.149135000000	-4.773155000000
H	6.994394000000	-0.109824000000	-5.092619000000
C	4.900304000000	-2.684767000000	-4.769479000000
H	5.729263000000	-2.079768000000	-5.155208000000
H	4.766277000000	-3.562023000000	-5.416695000000
H	3.993069000000	-2.068777000000	-4.800388000000
C	3.809452000000	-4.338709000000	-2.777158000000
H	3.796036000000	-5.116513000000	-3.551959000000
H	3.861526000000	-4.808494000000	-1.788740000000
H	2.876834000000	-3.763079000000	-2.813015000000
C	8.956075000000	-0.029059000000	-1.840642000000
H	9.139645000000	-0.595698000000	-0.920178000000
H	9.884693000000	0.006989000000	-2.426842000000

H	8.676824000000	0.990704000000	-1.551130000000
C	5.927024000000	-4.116523000000	0.550851000000
H	5.375068000000	-4.642411000000	-0.235907000000
H	6.566072000000	-4.834022000000	1.083370000000
H	5.185528000000	-3.701597000000	1.243639000000
H	4.539837000000	-0.215444000000	-1.203218000000
B	3.451738000000	-0.909415000000	-1.065159000000
H	3.619777000000	-1.963164000000	-0.461212000000
H	2.948346000000	-1.099459000000	-2.161333000000
H	2.814610000000	-0.128333000000	-0.394243000000

MeOH

E_{el} = -115.661275547 Ha
E_{ZPVE} = -115.609525 Ha
H = -115.605229 Ha
G = -115.632309 Ha

C	-0.044757000000	0.668762000000	0.000000000000
H	-1.092210000000	0.977639000000	0.000000000000
H	0.439025000000	1.081880000000	0.894805000000
H	0.439025000000	1.081880000000	-0.894805000000
O	-0.044986000000	-0.761361000000	0.000000000000
H	0.861378000000	-1.072911000000	0.000000000000

TFE

E_{el} = -452.519722579 Ha
E_{ZPVE} = -452.461511 Ha
H = -452.454791 Ha
G = -452.491019 Ha

C	-1.146956000000	0.264025000000	0.008633000000
H	-0.571505000000	0.419334000000	-0.906443000000
H	-0.515904000000	0.527499000000	0.867397000000
C	-2.320573000000	1.199516000000	0.002496000000
O	-1.564343000000	-1.083500000000	0.022530000000
H	-2.089401000000	-1.240336000000	0.813143000000
F	-3.123047000000	1.039751000000	-1.095269000000
F	-3.110081000000	0.988017000000	1.119632000000
F	-1.898089000000	2.505999000000	0.032739000000

HFIP

E_{el} = -789.364392739 Ha
E_{ZPVE} = -789.301654 Ha
H = -789.291555 Ha
G = -789.337006 Ha

O	8.652723000000	0.479256000000	-11.073253000000
C	8.667597000000	-0.848324000000	-10.628145000000
H	9.681763000000	-1.261069000000	-10.521145000000
C	8.011568000000	-0.956953000000	-9.262946000000
C	7.985619000000	-1.663982000000	-11.707697000000
F	8.727874000000	-1.611835000000	-12.856379000000
F	6.727753000000	-1.218908000000	-11.991907000000
F	7.897533000000	-2.979597000000	-11.326288000000
F	6.683075000000	-0.651271000000	-9.280590000000
F	8.165493000000	-2.201185000000	-8.718344000000
F	8.641011000000	-0.056563000000	-8.424190000000
H	9.181315000000	1.026223000000	-10.485224000000

CF_3OH

E_{el} = -413.258291658 Ha
E_{ZPVE} = -413.229453 Ha
H = -413.224003 Ha
G = -413.257055 Ha

C	-0.595572000000	-0.139000000000	-0.209430000000
F	-0.260223000000	0.787716000000	0.757450000000
F	-1.135490000000	-1.221886000000	0.405164000000
F	0.592708000000	-0.521349000000	-0.798491000000
O	-1.474035000000	0.343210000000	-1.094705000000
H	-1.110005000000	1.119378000000	-1.535908000000

1_DHB_IIa _MeOH

E_{el} = -4391.49714159 Ha
E_{ZPVE} = -4390.712481 Ha
H = -4390.664018 Ha
G = -4390.792494 Ha

C	8.366062000000	-4.190847000000	-2.287862000000
C	7.032839000000	-4.909499000000	-2.646899000000
C	8.429446000000	-3.785375000000	-0.794853000000
C	8.721612000000	-3.022678000000	-3.249996000000
H	6.777965000000	-5.573405000000	-1.806061000000
H	7.218915000000	-5.559232000000	-3.515031000000
H	9.331873000000	-3.172486000000	-0.649870000000
H	8.582433000000	-4.692144000000	-0.189820000000
H	8.498264000000	-3.358774000000	-4.274788000000
H	9.811952000000	-2.873720000000	-3.216675000000
C	9.474199000000	-5.248891000000	-2.486871000000
H	10.442059000000	-4.868528000000	-2.133631000000
H	9.240586000000	-6.164745000000	-1.926955000000
H	9.574987000000	-5.510729000000	-3.548906000000
P	7.898839000000	-1.347707000000	-3.061017000000
P	7.010378000000	-2.812307000000	-0.072280000000
P	5.537905000000	-3.852705000000	-2.970209000000
Cu	5.859164000000	-1.748296000000	-2.009635000000
B	4.031094000000	-0.395372000000	-1.808006000000
H	4.329133000000	-0.826275000000	-2.932927000000
H	3.953211000000	0.822466000000	-1.872017000000
H	2.996779000000	-0.915611000000	-1.428215000000
C	5.438912000000	-3.755471000000	-4.808198000000
C	5.799508000000	-4.805750000000	-5.665894000000
C	4.912148000000	-2.579517000000	-5.363233000000
C	5.666173000000	-4.669177000000	-7.047314000000
C	4.769607000000	-2.446502000000	-6.745236000000
C	5.154730000000	-3.487066000000	-7.589268000000
H	6.169693000000	-5.745905000000	-5.260806000000
H	4.626329000000	-1.760616000000	-4.704580000000
H	5.952127000000	-5.488608000000	-7.701243000000
H	4.370803000000	-1.523288000000	-7.156874000000
H	5.051114000000	-3.383824000000	-8.665908000000
C	4.118936000000	-4.957885000000	-2.618602000000
C	4.198957000000	-6.346980000000	-2.460711000000
C	2.868181000000	-4.326369000000	-2.509995000000
C	3.050082000000	-7.090399000000	-2.183940000000
C	1.722116000000	-5.073227000000	-2.246973000000
C	1.812443000000	-6.456077000000	-2.076659000000
H	5.154251000000	-6.859949000000	-2.550350000000
H	2.802026000000	-3.241985000000	-2.608455000000
H	3.123387000000	-8.167132000000	-2.055908000000
H	0.760863000000	-4.573709000000	-2.164342000000
H	0.920198000000	-7.037924000000	-1.862201000000
C	8.298322000000	-0.617191000000	-4.703147000000
C	7.994020000000	-1.307476000000	-5.887438000000
C	8.811223000000	0.685753000000	-4.800206000000
C	8.200308000000	-0.714337000000	-7.132508000000
C	9.023843000000	1.273946000000	-6.046489000000
C	8.718482000000	0.577927000000	-7.216324000000
H	7.570455000000	-2.309159000000	-5.851247000000
H	9.023145000000	1.252614000000	-3.897922000000
H	7.948431000000	-1.266750000000	-8.034226000000
H	9.422350000000	2.283387000000	-6.100282000000
H	8.879323000000	1.040752000000	-8.186101000000
C	9.026817000000	-0.401096000000	-1.962465000000
C	8.445017000000	0.530348000000	-1.089328000000
C	10.425342000000	-0.513696000000	-1.999163000000
C	9.242306000000	1.328943000000	-0.268114000000
C	11.221730000000	0.274397000000	-1.168087000000
C	10.630135000000	1.197842000000	-0.302167000000
H	7.361903000000	0.632772000000	-1.062784000000
H	10.902337000000	-1.200268000000	-2.696404000000
H	8.775474000000	2.046259000000	0.400023000000
H	12.303517000000	0.178167000000	-1.205984000000
H	11.252107000000	1.817258000000	0.338444000000

C	7.779992000000	-2.262002000000	1.510513000000
C	7.096274000000	-2.389493000000	2.730938000000
C	9.024629000000	-1.609975000000	1.507402000000
C	7.650154000000	-1.896856000000	3.912188000000
C	9.577597000000	-1.122543000000	2.690044000000
C	8.894444000000	-1.266697000000	3.897642000000
H	6.126760000000	-2.880677000000	2.760294000000
H	9.564942000000	-1.456035000000	0.575069000000
H	7.106239000000	-2.008324000000	4.846210000000
H	10.542066000000	-0.622013000000	2.660447000000
H	9.324736000000	-0.885001000000	4.819261000000
C	5.841203000000	-4.094584000000	0.534732000000
C	6.238088000000	-5.323344000000	1.086398000000
C	4.473815000000	-3.782439000000	0.489763000000
C	5.288356000000	-6.228762000000	1.555543000000
C	3.523841000000	-4.683892000000	0.973686000000
C	3.928656000000	-5.910925000000	1.495085000000
H	7.294896000000	-5.571755000000	1.169195000000
H	4.153271000000	-2.831109000000	0.064384000000
H	5.607492000000	-7.179507000000	1.974252000000
H	2.468360000000	-4.433252000000	0.914537000000
H	3.188786000000	-6.619919000000	1.856424000000
H	4.924261000000	-0.627789000000	-0.948367000000
H	5.486312000000	1.184025000000	-2.720541000000
O	6.154550000000	1.552167000000	-3.325974000000
C	5.550964000000	1.595050000000	-4.616973000000
H	4.524283000000	1.983299000000	-4.568833000000
H	5.532811000000	0.600546000000	-5.092175000000
H	6.155035000000	2.261853000000	-5.240264000000

1_DHB_IIa_TFE

E_{el} = -4728.36577827 Ha

E_{ZPVE} = -4727.575238 Ha

H = -4727.523769 Ha

G = -4727.660060 Ha

C	8.304708000000	-4.354861000000	-2.363213000000
C	6.892248000000	-4.936044000000	-2.685672000000
C	8.468746000000	-3.988894000000	-0.861451000000
C	8.728188000000	-3.185307000000	-3.294737000000
H	6.569428000000	-5.537958000000	-1.820420000000
H	6.988669000000	-5.642054000000	-3.524077000000
H	9.418849000000	-3.443341000000	-0.755245000000
H	8.565226000000	-4.920700000000	-0.282682000000
H	8.429743000000	-3.439860000000	-4.323117000000
H	9.827573000000	-3.133314000000	-3.304722000000
C	9.304010000000	-5.498792000000	-2.636042000000
H	10.316032000000	-5.215566000000	-2.316659000000
H	9.012913000000	-6.406437000000	-2.090173000000
H	9.337200000000	-5.736977000000	-3.708338000000
P	8.067556000000	-1.464829000000	-2.967888000000
P	7.127525000000	-2.938441000000	-0.109323000000
P	5.507686000000	-3.738263000000	-3.012836000000
Cu	5.993053000000	-1.789992000000	-1.886407000000
B	4.308900000000	-0.270579000000	-1.705609000000
H	4.855694000000	-0.898145000000	-0.762309000000
H	3.151173000000	-0.633831000000	-1.785407000000
H	4.416100000000	0.912053000000	-1.421483000000
C	5.475089000000	-3.498451000000	-4.835469000000
C	6.097140000000	-4.338547000000	-5.769340000000
C	4.753836000000	-2.383380000000	-5.299935000000
C	6.010925000000	-4.065024000000	-7.136342000000
C	4.659874000000	-2.117074000000	-6.665573000000
C	5.293038000000	-2.955827000000	-7.585279000000
H	6.655006000000	-5.214505000000	-5.443771000000
H	4.274751000000	-1.714331000000	-4.582853000000
H	6.500251000000	-4.722993000000	-7.849476000000
H	4.105619000000	-1.247869000000	-7.005693000000
H	5.225781000000	-2.745178000000	-8.648962000000
C	3.996267000000	-4.736533000000	-2.740749000000
C	3.952297000000	-6.132694000000	-2.844278000000
C	2.827005000000	-4.034325000000	-2.407351000000
C	2.762504000000	-6.818949000000	-2.601576000000
C	1.636118000000	-4.722314000000	-2.176890000000
C	1.604812000000	-6.115069000000	-2.266533000000
H	4.844297000000	-6.693132000000	-3.116404000000
H	2.857396000000	-2.947252000000	-2.314462000000
H	2.738231000000	-7.902610000000	-2.677488000000
H	0.736295000000	-4.169772000000	-1.921694000000
H	0.678686000000	-6.651400000000	-2.078931000000
C	8.527625000000	-0.630811000000	-4.541337000000
C	8.130335000000	-1.173806000000	-5.775340000000
C	9.161239000000	0.622183000000	-4.529311000000
C	8.373732000000	-0.488253000000	-6.964294000000
C	9.403582000000	1.305282000000	-5.721464000000
C	9.013039000000	0.752589000000	-6.941862000000
H	7.603584000000	-2.126310000000	-5.817833000000
H	9.453436000000	1.072674000000	-3.584298000000
H	8.053121000000	-0.923981000000	-7.906742000000
H	9.893872000000	2.274283000000	-5.693051000000
H	9.198919000000	1.288078000000	-7.868489000000
C	9.260564000000	-0.734694000000	-1.780589000000
C	8.750923000000	0.148134000000	-0.816397000000
C	10.641485000000	-0.986804000000	-1.808236000000
C	9.600510000000	0.747224000000	0.115118000000
C	11.487893000000	-0.394787000000	-0.872389000000
C	10.965789000000	0.469109000000	0.093550000000
H	7.681916000000	0.361734000000	-0.795935000000
H	11.064289000000	-1.635803000000	-2.573604000000
H	9.189374000000	1.418820000000	0.862903000000
H	12.554586000000	-0.600276000000	-0.900611000000
H	11.625263000000	0.926701000000	0.825810000000
C	7.923288000000	-2.164233000000	1.347741000000
C	7.138956000000	-1.214733000000	2.025972000000
C	9.220375000000	-2.424358000000	1.805845000000
C	7.637765000000	-0.550994000000	3.143354000000
C	9.722746000000	-1.749449000000	2.920320000000
C	8.934601000000	-0.815416000000	3.591266000000
H	6.135557000000	-0.991273000000	1.662694000000
H	9.851417000000	-3.152207000000	1.300929000000
H	7.018816000000	0.177368000000	3.659574000000
H	10.732869000000	-1.956532000000	3.263703000000
H	9.327973000000	-0.294008000000	4.459426000000
C	6.048258000000	-4.189225000000	0.699368000000
C	6.558341000000	-5.202626000000	1.526369000000
C	4.666447000000	-4.122714000000	0.479051000000
C	5.705604000000	-6.149393000000	2.088517000000
C	3.812320000000	-5.080373000000	1.031051000000
C	4.332372000000	-6.096096000000	1.830227000000
H	7.624662000000	-5.240054000000	1.746034000000
H	4.260262000000	-3.319745000000	-0.133853000000
H	6.108426000000	-6.929076000000	2.729391000000
H	2.747617000000	-5.031936000000	0.817645000000
H	3.671195000000	-6.843909000000	2.259119000000
H	4.865368000000	-0.477792000000	-2.798361000000
H	5.466243000000	1.443176000000	-2.709803000000
O	6.058108000000	1.906304000000	-3.339473000000
C	5.838030000000	1.382782000000	-4.620766000000
H	5.847816000000	0.280857000000	-4.642857000000
H	6.636028000000	1.744297000000	-5.278902000000
C	4.529116000000	1.833404000000	-5.202961000000
F	3.445291000000	1.392695000000	-4.473976000000
F	4.424320000000	3.198170000000	-5.301581000000
F	4.383629000000	1.324240000000	-6.485111000000

1_DHB_IIab_TFE

E_{el} = -4728.36188722 Ha

E_{ZPVE} = -4727.571649 Ha

H = -4727.519900 Ha

G = -4727.657274 Ha

C	8.499813000000	-4.261915000000	-2.336915000000
C	7.116975000000	-4.863712000000	-2.716043000000
C	8.580072000000	-3.802136000000	-0.856808000000

C	8.983863000000	-3.163561000000	-3.318403000000
H	6.818869000000	-5.534040000000	-1.894976000000
H	7.253300000000	-5.498619000000	-3.605117000000
H	9.512925000000	-3.230437000000	-0.739878000000
H	8.696135000000	-4.692151000000	-0.221065000000
H	8.803231000000	-3.520327000000	-4.344099000000
H	10.076888000000	-3.072243000000	-3.218444000000
C	9.510860000000	-5.422087000000	-2.474793000000
H	10.502146000000	-5.117541000000	-2.113213000000
H	9.184808000000	-6.291833000000	-1.888527000000
H	9.608433000000	-5.731353000000	-3.524323000000
P	8.237027000000	-1.453809000000	-3.197418000000
P	7.209415000000	-2.755637000000	-0.132078000000
P	5.692826000000	-3.697612000000	-2.994996000000
Cu	6.163948000000	-1.688221000000	-1.953375000000
B	4.400008000000	-0.201011000000	-1.887751000000
H	4.262196000000	-1.264917000000	-1.273675000000
H	3.611474000000	-0.169396000000	-2.812079000000
H	4.241348000000	0.736477000000	-1.113133000000
C	5.553133000000	-3.534094000000	-4.820561000000
C	5.800523000000	-4.580827000000	-5.721003000000
C	5.104204000000	-2.299469000000	-5.314365000000
C	5.624811000000	-4.389630000000	-7.091216000000
C	4.913672000000	-2.114810000000	-6.684712000000
C	5.180775000000	-3.155479000000	-7.573528000000
H	6.112701000000	-5.558008000000	-5.355444000000
H	4.911272000000	-1.481059000000	-4.619930000000
H	5.820709000000	-5.205716000000	-7.781549000000
H	4.567605000000	-1.154020000000	-7.054194000000
H	5.038506000000	-3.010124000000	-8.640982000000
C	4.212766000000	-4.710253000000	-2.623128000000
C	4.214927000000	-6.099224000000	-2.446899000000
C	3.001908000000	-4.005486000000	-2.507899000000
C	3.028606000000	-6.773398000000	-2.153962000000
C	1.817624000000	-4.683983000000	-2.227717000000
C	1.830087000000	-6.068541000000	-2.046508000000
H	5.138548000000	-6.666940000000	-2.535400000000
H	2.997825000000	-2.920137000000	-2.615714000000
H	3.042065000000	-7.850749000000	-2.012318000000
H	0.887882000000	-4.129128000000	-2.139634000000
H	0.907590000000	-6.595824000000	-1.819486000000
C	8.626751000000	-0.794546000000	-4.873429000000
C	8.299905000000	-1.528973000000	-6.025537000000
C	9.147456000000	0.500290000000	-5.032796000000
C	8.506052000000	-0.993612000000	-7.295663000000
C	9.351494000000	1.034127000000	-6.304747000000
C	9.036185000000	0.288327000000	-7.440509000000
H	7.857130000000	-2.519877000000	-5.941325000000
H	9.400452000000	1.094306000000	-4.157945000000
H	8.237738000000	-1.581447000000	-8.169810000000
H	9.759212000000	2.036144000000	-6.406246000000
H	9.195151000000	0.706322000000	-8.430533000000
C	9.423104000000	-0.500964000000	-2.166424000000
C	8.892055000000	0.450335000000	-1.281902000000
C	10.817733000000	-0.621979000000	-2.275834000000
C	9.736697000000	1.264605000000	-0.524525000000
C	11.660427000000	0.181253000000	-1.508957000000
C	11.119775000000	1.127828000000	-0.633976000000
H	7.811228000000	0.546116000000	-1.177390000000
H	11.250198000000	-1.326979000000	-2.984044000000
H	9.309183000000	1.990104000000	0.161065000000
H	12.738248000000	0.078701000000	-1.601994000000
H	11.777868000000	1.756875000000	-0.040786000000
C	8.037533000000	-2.129000000000	1.388394000000
C	7.324795000000	-2.093542000000	2.597430000000
C	9.328316000000	-1.581380000000	1.352681000000
C	7.891998000000	-1.532743000000	3.739422000000
C	9.897210000000	-1.026113000000	2.499117000000
C	9.181655000000	-1.000032000000	3.695296000000
H	6.315180000000	-2.490935000000	2.641240000000
H	9.898059000000	-1.563750000000	0.425950000000
H	7.321743000000	-1.513791000000	4.664352000000
H	10.899451000000	-0.608027000000	2.449097000000
H	9.624185000000	-0.565174000000	4.587447000000
C	6.055957000000	-4.001950000000	0.576086000000
C	6.490808000000	-5.183309000000	1.199174000000
C	4.683144000000	-3.718263000000	0.553709000000
C	5.573083000000	-6.069640000000	1.758559000000
C	3.765519000000	-4.594511000000	1.136438000000
C	4.207444000000	-5.775737000000	1.727461000000
H	7.553327000000	-5.407251000000	1.275036000000
H	4.329052000000	-2.803798000000	0.081902000000
H	5.923749000000	-6.982146000000	2.233378000000
H	2.708350000000	-4.346791000000	1.123002000000
H	3.493569000000	-6.463015000000	2.173008000000
H	5.560907000000	-0.046010000000	-2.356542000000
H	5.037144000000	-0.074585000000	0.177614000000
O	5.401030000000	-0.115103000000	1.086855000000
C	4.447190000000	0.433419000000	1.952533000000
H	3.861163000000	1.236015000000	1.482324000000
H	4.959296000000	0.839666000000	2.832563000000
C	3.480021000000	-0.609965000000	2.437432000000
F	2.773643000000	-1.194243000000	1.407871000000
F	4.101241000000	-1.630242000000	3.124492000000
F	2.560041000000	-0.046896000000	3.297481000000

1_DHB_IIa_HFIP

E_{el} = -5065.21721284 Ha

E_{ZPVE} = -5064.422162 Ha

H = -5064.367494 Ha

G = -5064.510191 Ha

C	8.444023000000	-4.484366000000	-2.395478000000
C	7.054713000000	-5.060246000000	-2.795206000000
C	8.509359000000	-4.044002000000	-0.905589000000
C	8.948565000000	-3.384888000000	-3.365943000000
H	6.726525000000	-5.709568000000	-1.968542000000
H	7.193763000000	-5.711607000000	-3.671746000000
H	9.436937000000	-3.469097000000	-0.763833000000
H	8.612077000000	-4.940960000000	-0.277223000000
H	8.748706000000	-3.726194000000	-4.393366000000
H	10.044061000000	-3.323096000000	-3.278981000000
C	9.439145000000	-5.657366000000	-2.534365000000
H	10.429577000000	-5.371701000000	-2.155558000000
H	9.092713000000	-6.529524000000	-1.963556000000
H	9.546842000000	-5.954818000000	-3.586251000000
P	8.246970000000	-1.659184000000	-3.228254000000
P	7.108329000000	-3.012178000000	-0.241819000000
P	5.647678000000	-3.879939000000	-3.121678000000
Cu	6.194857000000	-1.886054000000	-2.074877000000
B	4.382611000000	-0.460296000000	-1.424284000000
H	4.503550000000	-0.795117000000	-0.244822000000
H	3.637775000000	-1.231548000000	-2.003280000000
H	3.978671000000	0.685753000000	-1.507413000000
C	5.566915000000	-3.706176000000	-4.950477000000
C	5.834718000000	-4.747659000000	-5.850739000000
C	5.131298000000	-2.468690000000	-5.448536000000
C	5.692413000000	-4.547772000000	-7.223617000000
C	4.973244000000	-2.274571000000	-6.821243000000
C	5.260434000000	-3.310654000000	-7.709262000000
H	6.136676000000	-5.727284000000	-5.483441000000
H	4.927707000000	-1.654159000000	-4.753013000000
H	5.904789000000	-5.359533000000	-7.914006000000
H	4.637155000000	-1.311469000000	-7.193887000000
H	5.143444000000	-3.159050000000	-8.778800000000
C	4.158743000000	-4.910201000000	-2.823816000000
C	4.169120000000	-6.299075000000	-2.643785000000
C	2.931810000000	-4.226321000000	-2.788444000000
C	2.976424000000	-6.991285000000	-2.427481000000
C	1.742247000000	-4.920806000000	-2.581237000000
C	1.762867000000	-6.304785000000	-2.396322000000
H	5.102664000000	-6.855964000000	-2.675739000000
H	2.917445000000	-3.142133000000	-2.901908000000

H	2.997387000000	-8.068612000000	-2.286631000000
H	0.800476000000	-4.379833000000	-2.555958000000
H	0.835500000000	-6.845637000000	-2.229174000000
C	8.663527000000	-0.985402000000	-4.891909000000
C	8.336124000000	-1.693957000000	-6.059391000000
C	9.226948000000	0.294401000000	-5.021536000000
C	8.578737000000	-1.145463000000	-7.317704000000
C	9.467405000000	0.841012000000	-6.281553000000
C	9.147902000000	0.122591000000	-7.433538000000
H	7.867514000000	-2.674386000000	-5.997170000000
H	9.483043000000	0.867824000000	-4.134090000000
H	8.309942000000	-1.712568000000	-8.205266000000
H	9.906234000000	1.831699000000	-6.360564000000
H	9.335008000000	0.550776000000	-8.414213000000
C	9.432160000000	-0.741444000000	-2.170416000000
C	8.912324000000	0.302386000000	-1.390059000000
C	10.817954000000	-0.968592000000	-2.166262000000
C	9.757034000000	1.099470000000	-0.615286000000
C	11.659787000000	-0.179879000000	-1.383232000000
C	11.129643000000	0.856031000000	-0.608490000000
H	7.840666000000	0.494918000000	-1.376265000000
H	11.251875000000	-1.745896000000	-2.792606000000
H	9.334248000000	1.894662000000	-0.008760000000
H	12.730665000000	-0.364661000000	-1.386339000000
H	11.788250000000	1.472406000000	-0.002751000000
C	7.793220000000	-2.298576000000	1.299287000000
C	6.955641000000	-2.149038000000	2.416958000000
C	9.069166000000	-1.715945000000	1.326621000000
C	7.384313000000	-1.430940000000	3.530736000000
C	9.496724000000	-1.005792000000	2.447172000000
C	8.655102000000	-0.856132000000	3.548694000000
H	5.956154000000	-2.579385000000	2.410204000000
H	9.725677000000	-1.774708000000	0.459882000000
H	6.714880000000	-1.303992000000	4.376705000000
H	10.484271000000	-0.551778000000	2.445932000000
H	8.981759000000	-0.283589000000	4.411916000000
C	5.909446000000	-4.254310000000	0.384134000000
C	6.294467000000	-5.450002000000	1.011506000000
C	4.542282000000	-3.968728000000	0.249259000000
C	5.334193000000	-6.354994000000	1.459050000000
C	3.581620000000	-4.867555000000	0.716379000000
C	3.975495000000	-6.065905000000	1.307657000000
H	7.347891000000	-5.673788000000	1.170062000000
H	4.231716000000	-3.037953000000	-0.225131000000
H	5.644463000000	-7.280634000000	1.936368000000
H	2.527646000000	-4.632464000000	0.600941000000
H	3.227770000000	-6.773082000000	1.655870000000
H	5.515129000000	-0.324960000000	-2.000794000000
H	5.920218000000	-0.082427000000	0.235733000000
O	6.421331000000	0.604080000000	0.723430000000
C	5.530902000000	1.654712000000	0.942289000000
H	4.625177000000	1.564643000000	0.319931000000
C	6.230503000000	2.930130000000	0.533842000000
F	7.361431000000	3.171425000000	1.279168000000
F	6.619254000000	2.847223000000	-0.781472000000
F	5.418797000000	4.029509000000	0.652522000000
C	5.085553000000	1.622810000000	2.390940000000
F	4.391776000000	0.457176000000	2.621408000000
F	6.127814000000	1.662278000000	3.280130000000
F	4.239841000000	2.663343000000	2.694785000000

2_DHB_IIcb_MeOH

E_{el} = -3242.21290484 Ha

E_{ZPVE} = -3241.755476 Ha

H = -3241.725190 Ha

G = -3241.810880 Ha

C	-2.574499000000	0.582840000000	1.376994000000
C	-3.293449000000	-0.396070000000	0.407001000000
C	-2.093232000000	1.878565000000	0.665769000000
C	-1.435903000000	-0.112524000000	2.177425000000
H	-4.005436000000	0.187622000000	-0.200623000000
H	-3.901358000000	-1.100177000000	1.000766000000
H	-1.497059000000	2.458518000000	1.390462000000
H	-2.978393000000	2.497519000000	0.438999000000
H	-1.791311000000	-1.112625000000	2.477058000000
H	-1.269807000000	0.447051000000	3.113647000000
C	-3.630184000000	1.022297000000	2.412582000000
H	-3.224768000000	1.795515000000	3.079355000000
H	-4.520417000000	1.430648000000	1.915129000000
H	-3.944673000000	0.169950000000	3.030044000000
P	0.224989000000	-0.318981000000	1.338980000000
P	-1.079604000000	1.779853000000	-0.914457000000
P	-2.222814000000	-1.375311000000	-0.766070000000
Cu	-0.173226000000	-0.363591000000	-0.954961000000
C	-0.179499000000	3.385197000000	-0.807534000000
H	-0.854654000000	4.214846000000	-0.556739000000
H	0.618889000000	3.319095000000	-0.059028000000
H	0.300493000000	3.590181000000	-1.771583000000
C	0.913239000000	-1.770537000000	2.235304000000
H	1.975087000000	-1.863079000000	1.976908000000
H	0.813415000000	-1.668608000000	3.324074000000
H	0.420185000000	-2.690850000000	1.902398000000
C	-2.163343000000	-3.038551000000	0.014971000000
H	-1.684160000000	-2.980028000000	0.999227000000
H	-3.164511000000	-3.475138000000	0.128852000000
H	-1.543294000000	-3.685241000000	-0.618133000000
C	-3.389598000000	-1.716665000000	-2.147936000000
H	-4.333054000000	-2.148758000000	-1.788346000000
H	-3.603265000000	-0.801731000000	-2.712003000000
H	-2.905467000000	-2.424662000000	-2.831185000000
C	1.191639000000	1.038320000000	2.128974000000
H	0.748285000000	2.012362000000	1.887611000000
H	1.225393000000	0.923189000000	3.220837000000
H	2.207381000000	1.040633000000	1.716663000000
C	-2.353781000000	2.216026000000	-2.176347000000
H	-3.099154000000	1.415691000000	-2.255744000000
H	-2.864698000000	3.155958000000	-1.927019000000
H	-1.870586000000	2.320472000000	-3.154509000000
H	0.909688000000	-0.732948000000	-2.199526000000
B	1.006757000000	-2.029235000000	-2.112117000000
H	0.141966000000	-2.521740000000	-2.812751000000
H	0.954336000000	-2.449136000000	-0.962782000000
H	2.121573000000	-2.178771000000	-2.562639000000
O	2.650926000000	1.311834000000	-0.845597000000
H	1.839176000000	0.922173000000	-1.202779000000
C	3.648400000000	0.282619000000	-0.875144000000
H	3.782309000000	-0.125376000000	-1.883783000000
H	3.393755000000	-0.552800000000	-0.205214000000
H	4.584272000000	0.738851000000	-0.541264000000

2_DHB_IIa_MeOH

E_{el} = -3242.21774116 Ha

E_{ZPVE} = -3241.760578 Ha

H = -3241.729941 Ha

G = -3241.817537 Ha

C	-5.338196000000	-2.715068000000	-2.987450000000
C	-6.031952000000	-1.428405000000	-2.461259000000
C	-4.524050000000	-3.440896000000	-1.877834000000
C	-4.501594000000	-2.446726000000	-4.268148000000
H	-6.489125000000	-1.666920000000	-1.485863000000
H	-6.869262000000	-1.181259000000	-3.136757000000
H	-3.958375000000	-4.259879000000	-2.352636000000
H	-5.230997000000	-3.920716000000	-1.179337000000
H	-5.124657000000	-1.842852000000	-4.950111000000
H	-4.328102000000	-3.407125000000	-4.783814000000
C	-6.467931000000	-3.681648000000	-3.398982000000
H	-6.056193000000	-4.658172000000	-3.687298000000
H	-7.170274000000	-3.838296000000	-2.568865000000
H	-7.030588000000	-3.282228000000	-4.253638000000
P	-2.846203000000	-1.577951000000	-4.119176000000
P	-3.316361000000	-2.419821000000	-0.884401000000
P	-5.037708000000	0.146587000000	-2.223595000000

Cu	-2.806693000000	-0.509473000000	-2.066091000000
C	-2.069972000000	-3.672306000000	-0.379633000000
H	-2.538729000000	-4.557738000000	0.069995000000
H	-1.458548000000	-3.977590000000	-1.236086000000
H	-1.396098000000	-3.204425000000	0.348011000000
C	-2.686484000000	-0.890372000000	-5.821045000000
H	-1.648690000000	-0.556737000000	-5.938237000000
H	-2.912995000000	-1.649495000000	-6.582168000000
H	-3.349266000000	-0.028839000000	-5.964083000000
C	-5.523378000000	1.113412000000	-3.720999000000
H	-5.089840000000	0.668105000000	-4.623899000000
H	-6.614607000000	1.164453000000	-3.837158000000
H	-5.126613000000	2.131358000000	-3.630098000000
C	-6.120071000000	0.982193000000	-0.981060000000
H	-7.177123000000	0.947476000000	-1.279193000000
H	-6.008672000000	0.506829000000	0.000473000000
H	-5.812899000000	2.029466000000	-0.881963000000
C	-1.666045000000	-2.982931000000	-4.258588000000
H	-1.697638000000	-3.614124000000	-3.362997000000
H	-1.882432000000	-3.600390000000	-5.141163000000
H	-0.657850000000	-2.561333000000	-4.348065000000
C	-4.200449000000	-2.213853000000	0.720611000000
H	-5.095107000000	-1.592812000000	0.596398000000
H	-4.493846000000	-3.180098000000	1.153046000000
H	-3.527917000000	-1.696646000000	1.415919000000
H	-0.564650000000	-1.108156000000	-1.716737000000
B	-0.680346000000	-0.021624000000	-1.154670000000
H	-0.723067000000	-0.177662000000	0.048045000000
H	-1.713878000000	0.657057000000	-1.512549000000
H	0.214037000000	0.726460000000	-1.501144000000
C	0.147721000000	1.169520000000	-4.491909000000
H	0.368567000000	1.306428000000	-5.555526000000
H	0.900907000000	1.707026000000	-3.902213000000
H	-0.839721000000	1.604829000000	-4.272692000000
O	0.174711000000	-0.233188000000	-4.229930000000
H	0.102341000000	-0.345644000000	-3.266414000000

2_DHB_IIab_MeOH

E_{el} = -3242.21312909 Ha

E_{ZPVE} = -3241.756218 Ha

H = -3241.725551 Ha

G = -3241.812891 Ha

C	-1.457920000000	-2.946596000000	-0.776845000000
C	-2.354252000000	-1.913446000000	-1.518565000000
C	-1.014385000000	-2.454029000000	0.626627000000
C	-0.257538000000	-3.422349000000	-1.639190000000
H	-3.092096000000	-1.525315000000	-0.796656000000
H	-2.934178000000	-2.444897000000	-2.292605000000
H	-0.319753000000	-3.205204000000	1.039581000000
H	-1.893263000000	-2.451638000000	1.294646000000
H	-0.640008000000	-3.649391000000	-2.648761000000
H	0.107620000000	-4.381128000000	-1.231346000000
C	-2.339997000000	-4.190895000000	-0.539525000000
H	-1.808594000000	-4.933925000000	0.070520000000
H	-3.265647000000	-3.916951000000	-0.015377000000
H	-2.614036000000	-4.663352000000	-1.492638000000
P	1.242058000000	-2.313706000000	-1.860323000000
P	-0.170331000000	-0.787847000000	0.774472000000
P	-1.527183000000	-0.444201000000	-2.326883000000
Cu	0.534035000000	-0.144749000000	-1.352387000000
C	0.766553000000	-1.038820000000	2.340520000000
H	0.132905000000	-1.493129000000	3.114755000000
H	1.648827000000	-1.664243000000	2.168591000000
H	1.133402000000	-0.067058000000	2.689256000000
C	1.901013000000	-3.035381000000	-3.429316000000
H	2.913134000000	-2.652356000000	-3.602170000000
H	1.939280000000	-4.132582000000	-3.382117000000
H	1.279075000000	-2.734867000000	-4.280770000000
C	-1.569909000000	-0.927038000000	-4.106785000000
H	-0.899356000000	-1.774380000000	-4.292886000000
H	-2.584575000000	-1.197164000000	-4.429818000000
H	-1.214620000000	-0.082066000000	-4.708216000000
C	-2.877755000000	0.804810000000	-2.318623000000
H	-3.817611000000	0.401115000000	-2.718479000000
H	-3.045743000000	1.184337000000	-1.304433000000
H	-2.556625000000	1.655489000000	-2.931770000000
C	2.436626000000	-3.066904000000	-0.673609000000
H	2.108428000000	-2.906726000000	0.359176000000
H	2.556608000000	-4.145125000000	-0.847587000000
H	3.407893000000	-2.571206000000	-0.784257000000
C	-1.535786000000	0.272271000000	1.415998000000
H	-2.325948000000	0.382297000000	0.664348000000
H	-1.971444000000	-0.137438000000	2.337321000000
H	-1.134218000000	1.273086000000	1.615846000000
H	1.651529000000	1.032722000000	-1.896091000000
B	1.087640000000	2.125140000000	-1.519858000000
H	0.156096000000	1.977125000000	-0.733629000000
H	0.714776000000	2.668814000000	-2.536760000000
H	1.991862000000	2.724386000000	-0.967888000000
C	2.907601000000	1.887545000000	1.664778000000
H	3.551101000000	2.713421000000	1.333609000000
H	3.252351000000	1.546795000000	2.646632000000
H	1.880090000000	2.273530000000	1.753810000000
O	2.976914000000	0.769836000000	0.781277000000
H	2.631006000000	1.071844000000	-0.073427000000

2_DHB_IIIab_MeOH

E_{el} = -3242.21628014 Ha

E_{ZPVE} = -3241.759853 Ha

H =-3241.728940 Ha

G = -3241.817104 Ha

C	8.059072000000	-3.717002000000	-2.705023000000
C	6.739039000000	-4.437073000000	-3.098898000000
C	8.254872000000	-3.628977000000	-1.167075000000
C	8.219588000000	-2.334202000000	-3.395753000000
H	6.667341000000	-5.357878000000	-2.495423000000
H	6.816088000000	-4.763461000000	-4.150291000000
H	9.150910000000	-3.012425000000	-0.982510000000
H	8.495418000000	-4.636770000000	-0.785776000000
H	7.951049000000	-2.454507000000	-4.459064000000
H	9.288318000000	-2.059075000000	-3.381436000000
C	9.206988000000	-4.603102000000	-3.234365000000
H	10.181027000000	-4.213350000000	-2.908809000000
H	9.108994000000	-5.632628000000	-2.863705000000
H	9.200680000000	-4.632633000000	-4.332324000000
P	7.244938000000	-0.875485000000	-2.734339000000
P	6.891452000000	-2.938543000000	-0.079512000000
P	5.127884000000	-3.511635000000	-2.889409000000
Cu	5.486109000000	-1.717039000000	-1.488614000000
C	7.913264000000	-2.403121000000	1.363993000000
H	8.622118000000	-3.185968000000	1.667470000000
H	8.469662000000	-1.490956000000	1.119557000000
H	7.252263000000	-2.175445000000	2.207937000000
C	7.109153000000	0.163005000000	-4.246058000000
H	6.783073000000	1.158520000000	-3.924190000000
H	8.071929000000	0.241662000000	-4.768998000000
H	6.353155000000	-0.236870000000	-4.931549000000
C	4.721140000000	-3.009649000000	-4.612722000000
H	5.473561000000	-2.313685000000	-4.999745000000
H	4.655916000000	-3.875913000000	-5.284635000000
H	3.760266000000	-2.481012000000	-4.595857000000
C	3.933983000000	-4.904412000000	-2.704873000000
H	4.056367000000	-5.654240000000	-3.498149000000
H	4.045711000000	-5.391562000000	-1.729995000000
H	2.919876000000	-4.489931000000	-2.755389000000
C	8.525615000000	0.081571000000	-1.822940000000
H	8.857271000000	-0.463162000000	-0.931253000000
H	9.397865000000	0.300457000000	-2.453933000000
H	8.055348000000	1.020545000000	-1.502298000000
C	6.185170000000	-4.489562000000	0.631520000000
H	5.664464000000	-5.062488000000	-0.144101000000
H	6.964794000000	-5.121986000000	1.077941000000

H	5.450076000000	-4.229426000000	1.401821000000
H	4.256741000000	-0.868089000000	-0.689773000000
B	3.491015000000	-0.466997000000	-1.644690000000
H	2.515595000000	-1.187364000000	-1.642070000000
H	4.018705000000	-0.431322000000	-2.750211000000
H	3.232023000000	0.667492000000	-1.281707000000
O	5.706039000000	1.890941000000	-1.754492000000
H	5.088401000000	1.212728000000	-1.436977000000
C	4.935066000000	2.777997000000	-2.567674000000
H	4.172674000000	3.306300000000	-1.980741000000
H	5.626600000000	3.513386000000	-2.990970000000
H	4.431846000000	2.238723000000	-3.383164000000

2_DHB_IIbc_TFE

E_{el} = -3579.08242437 Ha

E_{ZPVE} = -3578.617000 Ha

H = -3578.584501 Ha

G = -3578.675808 Ha

C	8.057990000000	-3.719619000000	-2.712463000000
C	6.688440000000	-4.323289000000	-3.135955000000
C	8.224031000000	-3.637178000000	-1.171672000000
C	8.351578000000	-2.364843000000	-3.413536000000
H	6.503149000000	-5.213484000000	-2.511482000000
H	6.772384000000	-4.688667000000	-4.173644000000
H	9.177893000000	-3.121130000000	-0.967444000000
H	8.337620000000	-4.660017000000	-0.772426000000
H	8.100388000000	-2.480285000000	-4.481389000000
H	9.439137000000	-2.179952000000	-3.376482000000
C	9.136727000000	-4.706055000000	-3.208623000000
H	10.133293000000	-4.403166000000	-2.859676000000
H	8.937151000000	-5.719850000000	-2.835919000000
H	9.155334000000	-4.742854000000	-4.306146000000
P	7.509504000000	-0.793555000000	-2.831248000000
P	6.913181000000	-2.771728000000	-0.155223000000
P	5.181214000000	-3.223021000000	-3.020772000000
Cu	5.662894000000	-1.461810000000	-1.615115000000
C	7.916622000000	-2.325234000000	1.330152000000
H	8.494029000000	-3.186336000000	1.693744000000
H	8.605646000000	-1.503784000000	1.103505000000
H	7.243100000000	-1.988866000000	2.126495000000
C	7.630358000000	0.211327000000	-4.367626000000
H	7.358754000000	1.245875000000	-4.128215000000
H	8.650036000000	0.184028000000	-4.774961000000
H	6.923058000000	-0.146861000000	-5.123234000000
C	4.885178000000	-2.769426000000	-4.779955000000
H	5.688672000000	-2.125261000000	-5.155534000000
H	4.807646000000	-3.659759000000	-5.418452000000
H	3.952080000000	-2.195966000000	-4.838155000000
C	3.821859000000	-4.438345000000	-2.785693000000
H	3.847312000000	-5.231567000000	-3.544515000000
H	3.866032000000	-4.887110000000	-1.787227000000
H	2.871918000000	-3.895106000000	-2.857315000000
C	8.848433000000	0.013647000000	-1.851137000000
H	9.040325000000	-0.537977000000	-0.923304000000
H	9.782990000000	0.083658000000	-2.424452000000
H	8.520410000000	1.025110000000	-1.580804000000
C	5.969129000000	-4.184153000000	0.559866000000
H	5.432807000000	-4.729694000000	-0.224114000000
H	6.626547000000	-4.881783000000	1.096380000000
H	5.217439000000	-3.786999000000	1.252374000000
H	4.643725000000	-0.370288000000	-0.830037000000
B	3.439139000000	-0.802305000000	-1.069046000000
H	3.262896000000	-1.861635000000	-0.496300000000
H	3.197979000000	-0.859199000000	-2.261653000000
H	2.826250000000	0.103383000000	-0.541852000000
O	5.517788000000	1.910617000000	-2.064936000000
H	5.474196000000	1.044744000000	-1.627903000000
C	4.242568000000	2.145360000000	-2.628574000000
H	3.458920000000	1.547890000000	-2.143593000000
H	3.996976000000	3.208149000000	-2.533111000000
C	4.246602000000	1.811497000000	-4.089272000000
F	3.006500000000	2.036618000000	-4.643656000000
F	4.575020000000	0.492598000000	-4.335801000000
F	5.153338000000	2.573670000000	-4.800431000000

2_DHB_IIcb_TFE

E_{el} = -3579.08216634 Ha

E_{ZPVE} = -3578.619268 Ha

H = -3578.585856Ha

G = -3578.679579 Ha

C	8.003991000000	-3.705734000000	-2.567212000000
C	6.701631000000	-4.492861000000	-2.883052000000
C	8.057427000000	-3.199363000000	-1.099444000000
C	8.271275000000	-2.567029000000	-3.593307000000
H	6.523134000000	-5.205481000000	-2.060115000000
H	6.871147000000	-5.103953000000	-3.786049000000
H	8.952663000000	-2.562591000000	-0.999595000000
H	8.224550000000	-4.065298000000	-0.435869000000
H	8.038062000000	-2.953516000000	-4.599705000000
H	9.352087000000	-2.345521000000	-3.595454000000
C	9.163099000000	-4.713064000000	-2.719825000000
H	10.116460000000	-4.262025000000	-2.413081000000
H	8.990034000000	-5.603526000000	-2.100258000000
H	9.259162000000	-5.036995000000	-3.764982000000
P	7.369036000000	-0.935231000000	-3.392639000000
P	6.624566000000	-2.225227000000	-0.376870000000
P	5.141376000000	-3.501359000000	-3.125842000000
Cu	5.427651000000	-1.414098000000	-2.213113000000
C	7.518835000000	-1.308122000000	0.950827000000
H	8.163016000000	-1.979104000000	1.535967000000
H	8.126848000000	-0.505083000000	0.519189000000
H	6.787247000000	-0.840360000000	1.619309000000
C	7.374086000000	-0.328083000000	-5.128382000000
H	7.105917000000	0.733592000000	-5.126236000000
H	8.358555000000	-0.453780000000	-5.598493000000
H	6.614525000000	-0.857035000000	-5.715337000000
C	4.939329000000	-3.488849000000	-4.953798000000
H	5.790403000000	-2.986891000000	-5.428354000000
H	4.850932000000	-4.504525000000	-5.361636000000
H	4.036665000000	-2.913580000000	-5.193627000000
C	3.831534000000	-4.710102000000	-2.671775000000
H	3.947205000000	-5.660402000000	-3.209595000000
H	3.835759000000	-4.902805000000	-1.593110000000
H	2.861834000000	-4.265705000000	-2.926466000000
C	8.695685000000	0.119304000000	-2.668618000000
H	8.937705000000	-0.207436000000	-1.649842000000
H	9.607619000000	0.087900000000	-3.280205000000
H	8.335374000000	1.152202000000	-2.609475000000
C	5.804568000000	-3.516151000000	0.656954000000
H	5.362510000000	-4.292771000000	0.022245000000
H	6.516458000000	-3.985801000000	1.349587000000
H	4.994641000000	-3.055181000000	1.233700000000
H	4.084560000000	-0.461199000000	-1.744127000000
B	3.463383000000	-0.334539000000	-2.876259000000
H	2.577901000000	-1.166323000000	-2.877442000000
H	4.192046000000	-0.441704000000	-3.853889000000
H	3.046355000000	0.802668000000	-2.805415000000
O	5.945863000000	1.425584000000	-0.651395000000
H	5.633939000000	0.578288000000	-1.009662000000
C	5.184350000000	2.449090000000	-1.259055000000
H	4.237334000000	2.073683000000	-1.672123000000
C	5.955676000000	3.083149000000	-2.376646000000
F	7.179702000000	3.571582000000	-1.969062000000
F	6.224760000000	2.196088000000	-3.406968000000
F	5.254348000000	4.134558000000	-2.917597000000
H	4.974911000000	3.229213000000	-0.519657000000

2_DHB_IIa_TFE

E_{el} = -3579.08675370 Ha

E_{ZPVE} = -3578.621429 Ha

H = -3578.588914 Ha

G = -3578.679833 Ha

C	-5.368245000000	-2.740953000000	-2.957552000000
C	-6.013930000000	-1.416847000000	-2.461637000000
C	-4.561680000000	-3.464023000000	-1.841035000000
C	-4.537812000000	-2.541879000000	-4.254393000000
H	-6.474826000000	-1.615092000000	-1.478951000000
H	-6.845791000000	-1.158624000000	-3.139879000000
H	-4.034104000000	-4.314413000000	-2.304965000000
H	-5.271307000000	-3.899941000000	-1.116987000000
H	-5.154011000000	-1.954735000000	-4.956616000000
H	-4.386939000000	-3.525856000000	-4.731374000000
C	-6.534017000000	-3.681360000000	-3.327385000000
H	-6.158634000000	-4.678323000000	-3.594893000000
H	-7.228343000000	-3.792239000000	-2.483464000000
H	-7.096290000000	-3.286517000000	-4.184280000000
P	-2.868633000000	-1.694429000000	-4.162253000000
P	-3.295586000000	-2.469381000000	-0.895099000000
P	-4.965871000000	0.129350000000	-2.271396000000
Cu	-2.765688000000	-0.593825000000	-2.119609000000
C	-2.106137000000	-3.770890000000	-0.369927000000
H	-2.613407000000	-4.619078000000	0.109106000000
H	-1.523703000000	-4.131442000000	-1.225194000000
H	-1.399735000000	-3.320654000000	0.337735000000
C	-2.718940000000	-1.098022000000	-5.897360000000
H	-1.689385000000	-0.753504000000	-6.045849000000
H	-2.948581000000	-1.900826000000	-6.611230000000
H	-3.382141000000	-0.246220000000	-6.084915000000
C	-5.412901000000	1.071238000000	-3.793253000000
H	-5.046130000000	0.553352000000	-4.686685000000
H	-6.499323000000	1.208252000000	-3.879900000000
H	-4.919746000000	2.049303000000	-3.762373000000
C	-6.007018000000	1.039736000000	-1.047245000000
H	-7.067148000000	1.031409000000	-1.335965000000
H	-5.902863000000	0.595409000000	-0.050543000000
H	-5.663567000000	2.078788000000	-0.988734000000
C	-1.707008000000	-3.122848000000	-4.256465000000
H	-1.742070000000	-3.720679000000	-3.338449000000
H	-1.932845000000	-3.769131000000	-5.115648000000
H	-0.688156000000	-2.730975000000	-4.361833000000
C	-4.144943000000	-2.176496000000	0.714300000000
H	-5.000826000000	-1.504106000000	0.585020000000
H	-4.491037000000	-3.114237000000	1.170031000000
H	-3.435047000000	-1.686486000000	1.391946000000
H	-0.471841000000	-1.103460000000	-1.970177000000
B	-0.614032000000	-0.104483000000	-1.265456000000
H	-0.598177000000	-0.424205000000	-0.096584000000
H	-1.674213000000	0.566196000000	-1.507310000000
H	0.252402000000	0.711156000000	-1.523287000000
C	0.064795000000	1.625999000000	-4.261450000000
H	0.904368000000	1.967508000000	-4.879216000000
H	0.206704000000	1.994950000000	-3.236954000000
C	-1.170815000000	2.274187000000	-4.813886000000
O	-0.031623000000	0.223443000000	-4.305918000000
H	-0.092590000000	-0.101881000000	-3.386195000000
F	-1.439857000000	1.882977000000	-6.108938000000
F	-2.310843000000	2.007247000000	-4.079708000000
F	-1.018556000000	3.644630000000	-4.830118000000

2_DHB_IIab_TFE

E_{el} = -3579.08675370 Ha

E_{ZPVE} = -3578.621429 Ha

H = -3578.588914 Ha

G = -3578.679833 Ha

C	-1.496068000000	-2.975655000000	-0.815073000000
C	-2.370137000000	-1.926469000000	-1.561449000000
C	-1.099364000000	-2.521396000000	0.614199000000
C	-0.266523000000	-3.429574000000	-1.647899000000
H	-3.140449000000	-1.566220000000	-0.859316000000
H	-2.912341000000	-2.437795000000	-2.375261000000
H	-0.412842000000	-3.280573000000	1.025953000000
H	-1.998423000000	-2.546307000000	1.254472000000
H	-0.611612000000	-3.622975000000	-2.677631000000
H	0.081551000000	-4.401451000000	-1.256678000000
C	-2.384364000000	-4.226438000000	-0.641600000000
H	-1.874592000000	-4.985231000000	-0.032575000000
H	-3.328812000000	-3.966772000000	-0.144600000000
H	-2.622980000000	-4.673685000000	-1.616286000000
P	1.239353000000	-2.316785000000	-1.777877000000
P	-0.278566000000	-0.854957000000	0.857868000000
P	-1.516535000000	-0.429715000000	-2.278981000000
Cu	0.504934000000	-0.169203000000	-1.224359000000
C	0.595619000000	-1.157938000000	2.450910000000
H	-0.019318000000	-1.760444000000	3.133087000000
H	1.557159000000	-1.653883000000	2.279143000000
H	0.813350000000	-0.193982000000	2.922337000000
C	1.957925000000	-2.982748000000	-3.344322000000
H	2.972627000000	-2.588231000000	-3.469581000000
H	2.002278000000	-4.080597000000	-3.331145000000
H	1.363767000000	-2.658593000000	-4.206825000000
C	-1.469749000000	-0.828316000000	-4.077997000000
H	-0.810346000000	-1.683837000000	-4.267292000000
H	-2.469648000000	-1.053573000000	-4.473061000000
H	-1.057121000000	0.036291000000	-4.611929000000
C	-2.850709000000	0.834400000000	-2.275289000000
H	-3.771702000000	0.467749000000	-2.747552000000
H	-3.069549000000	1.161333000000	-1.252569000000
H	-2.482812000000	1.710901000000	-2.822398000000
C	2.398346000000	-3.095514000000	-0.572547000000
H	2.043311000000	-2.952306000000	0.453964000000
H	2.525299000000	-4.170189000000	-0.761982000000
H	3.371871000000	-2.596720000000	-0.649207000000
C	-1.681382000000	0.170583000000	1.469751000000
H	-2.447593000000	0.285265000000	0.694130000000
H	-2.142213000000	-0.271512000000	2.363468000000
H	-1.300806000000	1.169192000000	1.714689000000
H	1.659750000000	0.989559000000	-1.748539000000
B	1.039423000000	2.090420000000	-1.501425000000
H	0.145055000000	1.991292000000	-0.671362000000
H	0.622159000000	2.487217000000	-2.568521000000
H	1.927557000000	2.795150000000	-1.060793000000
C	3.260379000000	2.091251000000	1.369346000000
H	3.042103000000	2.923448000000	0.687726000000
H	4.302637000000	2.161383000000	1.700756000000
C	2.393562000000	2.256042000000	2.581293000000
O	3.033660000000	0.840553000000	0.764321000000
H	2.485403000000	0.990337000000	-0.025368000000
F	1.045488000000	2.160219000000	2.288515000000
F	2.649077000000	1.302949000000	3.547740000000
F	2.598838000000	3.485917000000	3.163143000000

2_DHB_IIIab_TFE

E_{el} = -3579.08320015 Ha

E_{ZPVE} = -3578.617858 Ha

H = -3578.585138 Ha

G = -3578.677055 Ha

C	8.077978000000	-3.749143000000	-2.690525000000
C	6.721481000000	-4.410568000000	-3.062954000000
C	8.312929000000	-3.690103000000	-1.157606000000
C	8.273604000000	-2.366844000000	-3.367718000000
H	6.616903000000	-5.327055000000	-2.457797000000
H	6.766512000000	-4.739099000000	-4.115443000000
H	9.245664000000	-3.126437000000	-0.985904000000
H	8.503993000000	-4.713910000000	-0.791385000000
H	7.974709000000	-2.465222000000	-4.425037000000
H	9.351977000000	-2.131383000000	-3.378018000000
C	9.177725000000	-4.670992000000	-3.259576000000
H	10.174266000000	-4.325024000000	-2.953370000000
H	9.047185000000	-5.700974000000	-2.900730000000

H	9.143110000000	-4.684565000000	-4.357234000000
P	7.386936000000	-0.857796000000	-2.696109000000
P	7.012461000000	-2.934412000000	-0.040158000000
P	5.164931000000	-3.405841000000	-2.823248000000
Cu	5.626449000000	-1.644963000000	-1.402312000000
C	8.081051000000	-2.477373000000	1.396461000000
H	8.737132000000	-3.309205000000	1.687766000000
H	8.697062000000	-1.603277000000	1.156785000000
H	7.443315000000	-2.214198000000	2.247968000000
C	7.371553000000	0.192358000000	-4.205703000000
H	7.117972000000	1.216301000000	-3.909480000000
H	8.352683000000	0.181644000000	-4.699932000000
H	6.602446000000	-0.139817000000	-4.911590000000
C	4.750307000000	-2.854447000000	-4.528586000000
H	5.503199000000	-2.154870000000	-4.908721000000
H	4.663063000000	-3.701715000000	-5.221878000000
H	3.797203000000	-2.312528000000	-4.487594000000
C	3.898804000000	-4.727110000000	-2.618901000000
H	3.954912000000	-5.473653000000	-3.422532000000
H	4.008798000000	-5.230376000000	-1.652008000000
H	2.909887000000	-4.253839000000	-2.636470000000
C	8.727645000000	0.001912000000	-1.767286000000
H	9.013117000000	-0.560089000000	-0.870805000000
H	9.617103000000	0.154194000000	-2.393640000000
H	8.343861000000	0.978351000000	-1.446837000000
C	6.218761000000	-4.440645000000	0.671911000000
H	5.642383000000	-4.972045000000	-0.093320000000
H	6.964384000000	-5.126601000000	1.096865000000
H	5.519783000000	-4.137398000000	1.459858000000
H	4.465447000000	-0.749490000000	-0.547743000000
B	3.480585000000	-0.637264000000	-1.370587000000
H	2.767832000000	-1.615075000000	-1.299262000000
H	3.832197000000	-0.439236000000	-2.528808000000
H	2.952992000000	0.358738000000	-0.918184000000
O	5.276195000000	1.794838000000	-2.268263000000
H	4.950600000000	0.915773000000	-2.003541000000
C	4.202132000000	2.450795000000	-2.897946000000
H	3.233278000000	2.022655000000	-2.609704000000
H	4.215173000000	3.513004000000	-2.629875000000
C	4.323737000000	2.367125000000	-4.391205000000
F	5.513164000000	2.898173000000	-4.847736000000
F	4.266869000000	1.071685000000	-4.868789000000
F	3.305943000000	3.068776000000	-4.997718000000

2_DHB_IIbc_TFE

E_{el} = -3915.93476870 Ha

E_{ZPVE} = -3915.463857 Ha

H = -3915.428427 Ha

G = -3915.526756 Ha

C	8.060045000000	-3.724779000000	-2.712588000000
C	6.683809000000	-4.309929000000	-3.140494000000
C	8.226980000000	-3.650860000000	-1.171188000000
C	8.370823000000	-2.371139000000	-3.408840000000
H	6.489767000000	-5.204172000000	-2.524580000000
H	6.763757000000	-4.666432000000	-4.181486000000
H	9.185838000000	-3.145165000000	-0.964445000000
H	8.330737000000	-4.676479000000	-0.776637000000
H	8.114719000000	-2.478824000000	-4.476403000000
H	9.460694000000	-2.200653000000	-3.373735000000
C	9.126589000000	-4.722352000000	-3.212970000000
H	10.126697000000	-4.433837000000	-2.862279000000
H	8.914321000000	-5.735343000000	-2.845332000000
H	9.145335000000	-4.754192000000	-4.310600000000
P	7.549859000000	-0.793282000000	-2.819120000000
P	6.924745000000	-2.779084000000	-0.150033000000
P	5.186757000000	-3.197747000000	-3.015175000000
Cu	5.698185000000	-1.450223000000	-1.609226000000
C	7.927755000000	-2.345910000000	1.338503000000
H	8.498460000000	-3.212601000000	1.699100000000
H	8.622905000000	-1.528085000000	1.117786000000
H	7.254996000000	-2.008920000000	2.135209000000
C	7.682884000000	0.220654000000	-4.348480000000
H	7.397748000000	1.251690000000	-4.109069000000
H	8.708334000000	0.204868000000	-4.741205000000
H	6.990965000000	-0.141031000000	-5.116463000000
C	4.876852000000	-2.732101000000	-4.768243000000
H	5.667327000000	-2.072604000000	-5.144545000000
H	4.802723000000	-3.616521000000	-5.415022000000
H	3.936620000000	-2.169104000000	-4.812126000000
C	3.815832000000	-4.397708000000	-2.771428000000
H	3.825638000000	-5.189370000000	-3.532051000000
H	3.862437000000	-4.849075000000	-1.774259000000
H	2.871838000000	-3.843044000000	-2.834693000000
C	8.890646000000	-0.003936000000	-1.828570000000
H	9.071959000000	-0.560494000000	-0.901588000000
H	9.829318000000	0.061309000000	-2.395443000000
H	8.569396000000	1.009242000000	-1.555876000000
C	5.965677000000	-4.186192000000	0.555169000000
H	5.440409000000	-4.734448000000	-0.234512000000
H	6.613730000000	-4.883510000000	1.103232000000
H	5.205202000000	-3.785455000000	1.235889000000
H	4.693323000000	-0.353705000000	-0.809609000000
B	3.477256000000	-0.722598000000	-1.087291000000
H	3.231970000000	-1.765568000000	-0.516153000000
H	3.268623000000	-0.775871000000	-2.287162000000
H	2.893120000000	0.219001000000	-0.588883000000
O	5.467391000000	1.870595000000	-2.154387000000
H	5.444133000000	1.047570000000	-1.636410000000
C	4.169719000000	2.068432000000	-2.654017000000
H	3.443625000000	1.375862000000	-2.197808000000
C	3.746132000000	3.472501000000	-2.289847000000
C	4.166415000000	1.789156000000	-4.140369000000
F	2.902731000000	1.814190000000	-4.673156000000
F	4.678135000000	0.531253000000	-4.377531000000
F	4.937701000000	2.675915000000	-4.852588000000
F	4.634887000000	4.426062000000	-2.716159000000
F	2.518739000000	3.785411000000	-2.823132000000
F	3.644089000000	3.581265000000	-0.926329000000

2_DHB_IIcb_TFE

E_{el} = -3915.93530995 Ha

E_{ZPVE} = -3915.466672 Ha

H = -3915.430347 Ha

G = -3915.530911 Ha

C	7.987947000000	-3.736608000000	-2.557874000000
C	6.672593000000	-4.498899000000	-2.881746000000
C	8.058330000000	-3.261709000000	-1.079295000000
C	8.260412000000	-2.579264000000	-3.562084000000
H	6.479148000000	-5.216838000000	-2.066876000000
H	6.831147000000	-5.102741000000	-3.791269000000
H	8.960012000000	-2.635287000000	-0.972443000000
H	8.222544000000	-4.143173000000	-0.436231000000
H	8.010404000000	-2.938939000000	-4.574212000000
H	9.343873000000	-2.372851000000	-3.572045000000
C	9.133107000000	-4.754391000000	-2.740235000000
H	10.094237000000	-4.322669000000	-2.430170000000
H	8.952517000000	-5.656065000000	-2.139386000000
H	9.218098000000	-5.056595000000	-3.792751000000
P	7.386379000000	-0.940735000000	-3.305905000000
P	6.636751000000	-2.295383000000	-0.327030000000
P	5.134858000000	-3.471060000000	-3.112604000000
Cu	5.451319000000	-1.437898000000	-2.106458000000
C	7.539944000000	-1.337354000000	0.962186000000
H	8.202992000000	-1.983455000000	1.553317000000
H	8.130303000000	-0.537096000000	0.500355000000
H	6.812453000000	-0.862431000000	1.630786000000
C	7.314905000000	-0.289719000000	-5.021977000000
H	7.072991000000	0.777814000000	-4.975228000000
H	8.268534000000	-0.421559000000	-5.549965000000
H	6.509472000000	-0.782158000000	-5.578646000000
C	4.916179000000	-3.442619000000	-4.937544000000
H	5.779069000000	-2.967941000000	-5.418940000000

H	4.790354000000	-4.453008000000	-5.348485000000
H	4.029546000000	-2.838347000000	-5.165891000000
C	3.799181000000	-4.638819000000	-2.635146000000
H	3.877169000000	-5.592984000000	-3.172529000000
H	3.822768000000	-4.828178000000	-1.555793000000
H	2.836358000000	-4.169449000000	-2.870422000000
C	8.755482000000	0.083077000000	-2.614827000000
H	9.053308000000	-0.288200000000	-1.625908000000
H	9.631987000000	0.068787000000	-3.276557000000
H	8.409876000000	1.116040000000	-2.491600000000
C	5.844572000000	-3.578537000000	0.734131000000
H	5.401700000000	-4.367571000000	0.115064000000
H	6.570780000000	-4.032761000000	1.421901000000
H	5.038785000000	-3.118195000000	1.316881000000
H	4.109511000000	-0.482068000000	-1.737200000000
B	3.533733000000	-0.278411000000	-2.886613000000
H	2.878462000000	-1.251474000000	-3.197851000000
H	4.316956000000	0.063441000000	-3.760103000000
H	2.829035000000	0.657104000000	-2.563710000000
O	6.181107000000	1.474372000000	-0.973799000000
H	5.918508000000	0.547202000000	-1.112691000000
C	5.181406000000	2.278642000000	-1.547739000000
H	4.486082000000	1.701789000000	-2.180530000000
C	5.869548000000	3.277235000000	-2.443850000000
F	6.857603000000	3.984509000000	-1.809557000000
F	6.468318000000	2.604085000000	-3.492358000000
F	4.993418000000	4.178191000000	-2.988112000000
C	4.347732000000	2.897307000000	-0.447025000000
F	3.263229000000	3.573713000000	-0.945635000000
F	3.871237000000	1.904811000000	0.374482000000
F	5.062518000000	3.775253000000	0.330619000000

2_DHB_IIa_TFE

E_{el} = -3915.93882008 Ha

E_{ZPVE} = -3915.469570 Ha

H = -3915.433355 Ha

G = -3915.534687 Ha

C	-7.636044000000	0.593303000000	-6.188984000000
C	-7.992755000000	2.074842000000	-6.495391000000
C	-7.436866000000	0.336078000000	-4.668903000000
C	-6.443718000000	0.080711000000	-7.039258000000
H	-8.744411000000	2.395816000000	-5.754166000000
H	-8.495707000000	2.118382000000	-7.476936000000
H	-7.047358000000	-0.688198000000	-4.544471000000
H	-8.424253000000	0.350892000000	-4.176298000000
H	-6.628714000000	0.374921000000	-8.086519000000
H	-6.451504000000	-1.022813000000	-7.027191000000
C	-8.861870000000	-0.243617000000	-6.611916000000
H	-8.729150000000	-1.296415000000	-6.328381000000
H	-9.774511000000	0.128654000000	-6.127047000000
H	-9.009128000000	-0.198268000000	-7.699400000000
P	-4.709717000000	0.644740000000	-6.615198000000
P	-6.302141000000	1.486986000000	-3.734185000000
P	-6.653073000000	3.391869000000	-6.513690000000
Cu	-4.912558000000	2.518190000000	-5.257885000000
C	-5.747530000000	0.421060000000	-2.341817000000
H	-6.594381000000	-0.075692000000	-1.849743000000
H	-5.034408000000	-0.334488000000	-2.690055000000
H	-5.223035000000	1.051813000000	-1.614733000000
C	-3.878319000000	0.417696000000	-8.241847000000
H	-2.798506000000	0.514543000000	-8.081638000000
H	-4.103059000000	-0.569738000000	-8.666503000000
H	-4.174765000000	1.196091000000	-8.953774000000
C	-6.366447000000	3.597943000000	-8.323701000000
H	-5.851073000000	2.722644000000	-8.734257000000
H	-7.310526000000	3.746699000000	-8.865426000000
H	-5.716808000000	4.465207000000	-8.486829000000
C	-7.710069000000	4.875936000000	-6.214762000000
H	-8.598556000000	4.870307000000	-6.861027000000
H	-8.028473000000	4.912949000000	-5.166463000000
H	-7.127494000000	5.780965000000	-6.420559000000
C	-4.019865000000	-0.823735000000	-5.740825000000
H	-4.487345000000	-0.952895000000	-4.758055000000
H	-4.156054000000	-1.741695000000	-6.328225000000
H	-2.947077000000	-0.659128000000	-5.580979000000
C	-7.496404000000	2.564029000000	-2.832857000000
H	-8.067501000000	3.183150000000	-3.535006000000
H	-8.197158000000	1.974356000000	-2.226300000000
H	-6.929300000000	3.236017000000	-2.177187000000
H	-2.996490000000	1.794302000000	-4.008329000000
B	-3.061890000000	3.012772000000	-3.839854000000
H	-3.534886000000	3.248850000000	-2.751213000000
H	-3.719262000000	3.630302000000	-4.745828000000
H	-1.953951000000	3.504769000000	-3.959052000000
O	-1.623710000000	1.910257000000	-6.281028000000
H	-2.006713000000	1.963022000000	-5.378288000000
H	-1.355452000000	3.912388000000	-5.819087000000
C	-1.097165000000	3.166690000000	-6.587361000000
C	-1.705152000000	3.639382000000	-7.890306000000
C	0.415958000000	3.070159000000	-6.613561000000
F	1.006075000000	4.301444000000	-6.765050000000
F	0.861777000000	2.551098000000	-5.425709000000
F	0.874946000000	2.262820000000	-7.624186000000
F	-1.156113000000	4.822033000000	-8.318806000000
F	-3.056457000000	3.860090000000	-7.726291000000
F	-1.569221000000	2.728656000000	-8.907514000000

2_DHB_IIab_TFE

E_{el} = -3915.93777867 Ha

E_{ZPVE} = -3915.468574 Ha

H = -3915.432437 Ha

G = -3915.532248 Ha

C	-7.646739000000	0.413715000000	-6.067117000000
C	-8.355810000000	1.794961000000	-6.161799000000
C	-6.955349000000	0.199450000000	-4.690386000000
C	-6.691953000000	0.158082000000	-7.266008000000
H	-8.869180000000	1.980989000000	-5.203037000000
H	-9.148853000000	1.731342000000	-6.926611000000
H	-6.377384000000	-0.738325000000	-4.741365000000
H	-7.735234000000	0.037387000000	-3.926622000000
H	-7.217381000000	0.468514000000	-8.185176000000
H	-6.531357000000	-0.929644000000	-7.361211000000
C	-8.759024000000	-0.651676000000	-6.162114000000
H	-8.348879000000	-1.657136000000	-5.997371000000
H	-9.537008000000	-0.472030000000	-5.407608000000
H	-9.232794000000	-0.633637000000	-7.152976000000
P	-4.999745000000	0.968639000000	-7.299415000000
P	-5.810783000000	1.541822000000	-4.082910000000
P	-7.331455000000	3.313079000000	-6.548786000000
Cu	-5.178571000000	2.816144000000	-5.897621000000
C	-4.700679000000	0.626229000000	-2.937001000000
H	-5.267204000000	0.027948000000	-2.211148000000
H	-4.018995000000	-0.028518000000	-3.491500000000
H	-4.087774000000	1.359018000000	-2.397320000000
C	-4.640906000000	0.907146000000	-9.106426000000
H	-3.570655000000	1.101093000000	-9.243882000000
H	-4.883568000000	-0.076286000000	-9.531396000000
H	-5.197285000000	1.683607000000	-9.643602000000
C	-7.667865000000	3.524929000000	-8.350455000000
H	-7.206347000000	2.710530000000	-8.921310000000
H	-8.745903000000	3.541622000000	-8.560371000000
H	-7.222910000000	4.466368000000	-8.692468000000
C	-8.420982000000	4.635120000000	-5.871681000000
H	-9.465955000000	4.496726000000	-6.180638000000
H	-8.363844000000	4.652079000000	-4.777293000000
H	-8.066303000000	5.606563000000	-6.234401000000
C	-3.919053000000	-0.419243000000	-6.754158000000
H	-4.069526000000	-0.638529000000	-5.691508000000
H	-4.113503000000	-1.327086000000	-7.341056000000
H	-2.873477000000	-0.115344000000	-6.874509000000
C	-6.853422000000	2.439329000000	-2.860409000000
H	-7.692609000000	2.933447000000	-3.364300000000

H	-7.245983000000	1.767948000000	-2.084988000000
H	-6.239433000000	3.219179000000	-2.393793000000
H	-3.164401000000	3.547327000000	-4.045101000000
B	-3.765842000000	4.376098000000	-4.727878000000
H	-4.797879000000	4.705639000000	-4.176811000000
H	-3.938995000000	3.964929000000	-5.926433000000
H	-3.050004000000	5.330782000000	-4.942023000000
O	-2.045626000000	1.883455000000	-5.617841000000
H	-2.685863000000	2.387751000000	-5.073372000000
H	-1.441431000000	3.856361000000	-5.865411000000
C	-1.152810000000	2.825885000000	-6.132507000000
C	-1.189688000000	2.724098000000	-7.644257000000
C	0.218141000000	2.573836000000	-5.536728000000
F	1.112730000000	3.563364000000	-5.864530000000
F	0.130535000000	2.546836000000	-4.169231000000
F	0.751959000000	1.376696000000	-5.948213000000
F	-0.202060000000	3.460573000000	-8.244340000000
F	-2.395924000000	3.190202000000	-8.118968000000
F	-1.072687000000	1.427937000000	-8.092265000000

2_DHB_IIIab_TFE

E_{el} = -3915.93547337 Ha

E_{ZPVE} = -3915.465312 Ha

H = -3915.429451 Ha

G = -3915.528853 Ha

C	8.068988000000	-3.761682000000	-2.670365000000
C	6.700496000000	-4.392662000000	-3.055913000000
C	8.272627000000	-3.664377000000	-1.135048000000
C	8.324222000000	-2.406682000000	-3.384530000000
H	6.553868000000	-5.287977000000	-2.428234000000
H	6.760907000000	-4.753442000000	-4.096888000000
H	9.216451000000	-3.120672000000	-0.959281000000
H	8.427627000000	-4.681572000000	-0.735334000000
H	8.048344000000	-2.528211000000	-4.445611000000
H	9.409140000000	-2.204094000000	-3.374203000000
C	9.151101000000	-4.734191000000	-3.186530000000
H	10.150969000000	-4.412079000000	-2.865633000000
H	8.978208000000	-5.748405000000	-2.801830000000
H	9.142254000000	-4.778693000000	-4.283811000000
P	7.465901000000	-0.855577000000	-2.779397000000
P	6.968971000000	-2.841388000000	-0.071526000000
P	5.170319000000	-3.334312000000	-2.886390000000
Cu	5.665542000000	-1.553425000000	-1.505989000000
C	8.010220000000	-2.371765000000	1.379958000000
H	8.630797000000	-3.214565000000	1.714032000000
H	8.660326000000	-1.524616000000	1.134465000000
H	7.356878000000	-2.064602000000	2.204426000000
C	7.518182000000	0.158382000000	-4.313013000000
H	7.223299000000	1.182849000000	-4.057329000000
H	8.527494000000	0.160975000000	-4.746423000000
H	6.803620000000	-0.211751000000	-5.055898000000
C	4.815449000000	-2.830720000000	-4.619886000000
H	5.593380000000	-2.159143000000	-4.999942000000
H	4.731902000000	-3.698909000000	-5.287278000000
H	3.871585000000	-2.271502000000	-4.627904000000
C	3.850313000000	-4.596717000000	-2.661802000000
H	3.876285000000	-5.361402000000	-3.449510000000
H	3.934886000000	-5.083621000000	-1.684003000000
H	2.883619000000	-4.079647000000	-2.692138000000
C	8.799435000000	-0.005042000000	-1.832670000000
H	9.028192000000	-0.538735000000	-0.903381000000
H	9.718402000000	0.090814000000	-2.426684000000
H	8.440484000000	0.997053000000	-1.566563000000
C	6.109812000000	-4.298994000000	0.664213000000
H	5.536631000000	-4.837730000000	-0.098042000000
H	6.822345000000	-4.992410000000	1.131305000000
H	5.400478000000	-3.948807000000	1.422902000000
H	4.595579000000	-0.512262000000	-0.708026000000
B	3.502669000000	-0.539028000000	-1.396331000000
H	2.833653000000	-1.480249000000	-1.035578000000
H	3.687817000000	-0.543992000000	-2.604848000000
H	3.028016000000	0.524409000000	-1.043564000000
O	5.336548000000	1.740415000000	-2.420919000000
H	5.053037000000	0.942864000000	-1.936206000000
C	4.195813000000	2.304552000000	-3.001102000000
H	3.286680000000	1.742401000000	-2.737081000000
C	4.335826000000	2.246055000000	-4.506485000000
F	5.431884000000	2.937467000000	-4.963209000000
F	4.483219000000	0.937238000000	-4.913434000000
F	3.232303000000	2.741930000000	-5.152160000000
C	4.036710000000	3.705835000000	-2.449382000000
F	2.945482000000	4.347788000000	-2.983152000000
F	3.853388000000	3.643721000000	-1.091757000000
F	5.134399000000	4.495139000000	-2.684440000000

MFE

E_{el} = -254.118597632 Ha

E_{ZPVE} = -254.045005 Ha

H = -254.039117 Ha

G = −254.072429Ha

C	-1.183559000000	0.274786000000	0.000161000000
H	-0.648571000000	0.418851000000	-0.942368000000
H	-0.475929000000	0.459145000000	0.819244000000
C	-2.338716000000	1.248185000000	0.086821000000
O	-1.664759000000	-1.072044000000	-0.003026000000
H	-1.864729000000	-1.339967000000	0.896335000000
F	-1.798762000000	2.565570000000	0.062797000000
H	-3.016992000000	1.130073000000	-0.763518000000
H	-2.900980000000	1.125877000000	1.020204000000

2_DHB_IIa_MFE

E_{el} = -3380.68110591 Ha

E_{ZPVE} = -3380.201581 Ha

H = -3380.169405 Ha

G = -3380.261361 Ha

C	-5.366234000000	-2.756461000000	-2.988068000000
C	-6.077356000000	-1.470857000000	-2.482004000000
C	-4.528545000000	-3.450864000000	-1.876472000000
C	-4.545449000000	-2.499663000000	-4.280329000000
H	-6.532159000000	-1.699805000000	-1.503234000000
H	-6.917384000000	-1.246641000000	-3.162092000000
H	-3.954914000000	-4.267027000000	-2.346788000000
H	-5.218216000000	-3.931488000000	-1.161549000000
H	-5.187177000000	-1.927418000000	-4.972116000000
H	-4.351788000000	-3.467634000000	-4.774155000000
C	-6.483485000000	-3.749083000000	-3.370994000000
H	-6.058275000000	-4.723332000000	-3.647106000000
H	-7.173564000000	-3.903429000000	-2.530364000000
H	-7.063065000000	-3.374725000000	-4.225659000000
P	-2.913734000000	-1.584169000000	-4.171306000000
P	-3.323173000000	-2.399195000000	-0.916742000000
P	-5.107410000000	0.122681000000	-2.267390000000
Cu	-2.866041000000	-0.491108000000	-2.121673000000
C	-2.055498000000	-3.627112000000	-0.403659000000
H	-2.507261000000	-4.503949000000	0.078958000000
H	-1.459017000000	-3.952376000000	-1.263415000000
H	-1.371679000000	-3.134795000000	0.298047000000
C	-2.796392000000	-0.952209000000	-5.899262000000
H	-1.773625000000	-0.584501000000	-6.043257000000
H	-3.002575000000	-1.748514000000	-6.627466000000
H	-3.493929000000	-0.123240000000	-6.069305000000
C	-5.599139000000	1.066279000000	-3.776474000000
H	-5.159955000000	0.614917000000	-4.673595000000
H	-6.690408000000	1.107281000000	-3.895859000000
H	-5.210891000000	2.088810000000	-3.696946000000
C	-6.197740000000	0.960459000000	-1.034352000000
H	-7.254313000000	0.909735000000	-1.331549000000
H	-6.080731000000	0.499153000000	-0.046785000000
H	-5.902947000000	2.012469000000	-0.949067000000
C	-1.688861000000	-2.952493000000	-4.290920000000
H	-1.683290000000	-3.558987000000	-3.378075000000
H	-1.897888000000	-3.601149000000	-5.152516000000
H	-0.696081000000	-2.501718000000	-4.409639000000

C	-4.187556000000	-2.167583000000	0.694536000000
H	-5.087989000000	-1.555241000000	0.569811000000
H	-4.468004000000	-3.127128000000	1.149725000000
H	-3.510176000000	-1.631630000000	1.370707000000
H	-0.603281000000	-0.991733000000	-1.851962000000
B	-0.742253000000	0.067174000000	-1.242571000000
H	-0.726831000000	-0.144063000000	-0.048442000000
H	-1.821445000000	0.702798000000	-1.521474000000
H	0.105466000000	0.866273000000	-1.591146000000
C	0.361498000000	1.272187000000	-4.549738000000
H	0.728646000000	1.368254000000	-5.577383000000
H	1.145194000000	1.634091000000	-3.870366000000
C	-0.888488000000	2.107869000000	-4.371882000000
O	0.075858000000	-0.107990000000	-4.325242000000
H	-0.003293000000	-0.239760000000	-3.362884000000
H	-1.688040000000	1.772428000000	-5.044856000000
H	-1.240488000000	2.079111000000	-3.335451000000
F	-0.566974000000	3.459358000000	-4.704866000000

2_DHB_IIab_MFE

E_{el} = -3380.68183808 Ha

E_{ZPVE} = -3380.202196 Ha

H = -3380.170210 Ha

G = -3380.260835 Ha

C	-1.568342000000	-2.897031000000	-0.731207000000
C	-2.216056000000	-1.638873000000	-1.375715000000
C	-0.920623000000	-2.589468000000	0.644315000000
C	-0.585269000000	-3.620689000000	-1.693911000000
H	-2.783721000000	-1.110521000000	-0.591531000000
H	-2.954426000000	-1.962589000000	-2.128663000000
H	-0.406267000000	-3.504841000000	0.983308000000
H	-1.725124000000	-2.405655000000	1.377646000000
H	-1.054585000000	-3.658767000000	-2.691790000000
H	-0.482607000000	-4.669587000000	-1.366408000000
C	-2.718837000000	-3.889115000000	-0.461518000000
H	-2.357627000000	-4.766300000000	0.092162000000
H	-3.511841000000	-3.413190000000	0.131006000000
H	-3.160394000000	-4.237726000000	-1.405091000000
P	1.152826000000	-2.954126000000	-1.935614000000
P	0.309808000000	-1.185375000000	0.820541000000
P	-1.049348000000	-0.415119000000	-2.160260000000
Cu	1.076355000000	-0.714708000000	-1.312887000000
C	1.182053000000	-1.747478000000	2.343749000000
H	0.466718000000	-2.064590000000	3.115053000000
H	1.860996000000	-2.578843000000	2.120588000000
H	1.769557000000	-0.905428000000	2.725372000000
C	1.522801000000	-3.694473000000	-3.585841000000
H	2.593079000000	-3.588766000000	-3.795968000000
H	1.256352000000	-4.759980000000	-3.616368000000
H	0.974644000000	-3.164256000000	-4.373119000000
C	-1.244898000000	-0.783389000000	-3.954601000000
H	-0.936177000000	-1.812514000000	-4.172824000000
H	-2.283784000000	-0.648867000000	-4.284834000000
H	-0.593710000000	-0.104163000000	-4.517990000000
C	-1.982533000000	1.164103000000	-2.065638000000
H	-2.986908000000	1.072316000000	-2.499396000000
H	-2.064701000000	1.508051000000	-1.028391000000
H	-1.410286000000	1.920997000000	-2.615863000000
C	2.136824000000	-4.103720000000	-0.877166000000
H	1.959183000000	-3.898673000000	0.184821000000
H	1.895277000000	-5.155130000000	-1.084569000000
H	3.203149000000	-3.938943000000	-1.071558000000
C	-0.721804000000	0.155236000000	1.543874000000
H	-1.375651000000	0.602048000000	0.786757000000
H	-1.329557000000	-0.209960000000	2.382801000000
H	-0.037227000000	0.928861000000	1.910360000000
H	2.365622000000	0.274932000000	-1.771082000000
B	1.827428000000	1.410038000000	-2.055667000000
H	1.073296000000	1.810791000000	-1.179755000000
H	1.278501000000	1.383682000000	-3.140369000000
H	2.848002000000	2.073763000000	-2.105321000000
C	2.146707000000	3.212574000000	1.046950000000
H	1.092286000000	3.015371000000	0.797117000000
H	2.175743000000	3.902319000000	1.897018000000
C	2.824244000000	1.911341000000	1.414364000000
O	2.837283000000	3.832634000000	-0.026185000000
H	2.681314000000	3.298451000000	-0.824266000000
H	2.780335000000	1.187215000000	0.591524000000
H	3.858362000000	2.068239000000	1.733764000000
F	2.105056000000	1.339189000000	2.535497000000

PFTB

E_{el} = -1126.20193811 Ha

E_{ZPVE} = -1126.134899 Ha

H = -1126.121788 Ha

G = -1126.172933 Ha

O	8.726618000000	0.398936000000	-11.148414000000
C	8.709865000000	-0.893132000000	-10.637577000000
C	7.952355000000	-0.917718000000	-9.287433000000
C	7.976570000000	-1.752119000000	-11.685618000000
F	8.386915000000	-1.454614000000	-12.947019000000
F	6.627689000000	-1.545855000000	-11.628843000000
F	8.218880000000	-3.079665000000	-11.448955000000
F	6.832964000000	-0.143555000000	-9.341579000000
F	7.590302000000	-2.177346000000	-8.914474000000
F	8.759849000000	-0.387170000000	-8.307957000000
H	9.230150000000	0.979933000000	-10.565212000000
C	10.161916000000	-1.394484000000	-10.447243000000
F	10.921414000000	-0.372468000000	-9.926620000000
F	10.237614000000	-2.458328000000	-9.599702000000
F	10.725060000000	-1.746517000000	-11.637484000000

2_DHB_IIa_PFTB

E_{el} = -4252.77304799 Ha

E_{ZPVE} = -4252.299437 Ha

H = -4252.260447 Ha

G = -4252.365780 Ha

C	-7.721084000000	0.595269000000	-6.142464000000
C	-8.074327000000	2.089058000000	-6.390389000000
C	-7.490244000000	0.282479000000	-4.636421000000
C	-6.551093000000	0.108077000000	-7.036496000000
H	-8.808341000000	2.389750000000	-5.623296000000
H	-8.596888000000	2.168884000000	-7.359380000000
H	-7.098948000000	-0.745431000000	-4.556434000000
H	-8.467415000000	0.279845000000	-4.123962000000
H	-6.757373000000	0.441934000000	-8.067824000000
H	-6.563964000000	-0.995342000000	-7.065302000000
C	-8.960057000000	-0.220722000000	-6.567977000000
H	-8.825945000000	-1.283472000000	-6.324841000000
H	-9.860364000000	0.137428000000	-6.050532000000
H	-9.130358000000	-0.136348000000	-7.649794000000
P	-4.803899000000	0.646743000000	-6.631699000000
P	-6.338206000000	1.406730000000	-3.691231000000
P	-6.725288000000	3.398082000000	-6.388588000000
Cu	-4.958210000000	2.461457000000	-5.202991000000
C	-5.730894000000	0.312096000000	-2.345704000000
H	-6.553148000000	-0.196597000000	-1.825583000000
H	-5.032369000000	-0.433051000000	-2.742409000000
H	-5.171662000000	0.930305000000	-1.633225000000
C	-4.025129000000	0.469082000000	-8.290381000000
H	-2.939613000000	0.414116000000	-8.154024000000
H	-4.369216000000	-0.445817000000	-8.791877000000
H	-4.235932000000	1.336963000000	-8.924489000000
C	-6.477135000000	3.679223000000	-8.194948000000
H	-5.978695000000	2.818512000000	-8.654778000000
H	-7.429109000000	3.860790000000	-8.712449000000
H	-5.822607000000	4.548188000000	-8.330834000000
C	-7.764383000000	4.875354000000	-6.002768000000
H	-8.671137000000	4.903802000000	-6.622767000000
H	-8.052531000000	4.871209000000	-4.945059000000
H	-7.180092000000	5.783988000000	-6.186750000000
C	-4.100708000000	-0.856617000000	-5.833513000000

H	-4.569683000000	-1.041853000000	-4.861031000000
H	-4.223714000000	-1.744037000000	-6.468767000000
H	-3.031863000000	-0.683432000000	-5.658119000000
C	-7.525744000000	2.448048000000	-2.739058000000
H	-8.115355000000	3.076449000000	-3.417501000000
H	-8.210888000000	1.835521000000	-2.137293000000
H	-6.957430000000	3.110435000000	-2.075404000000
H	-3.089265000000	1.668773000000	-4.159340000000
B	-3.027903000000	2.872817000000	-3.945260000000
H	-3.251205000000	3.109307000000	-2.779682000000
H	-3.792673000000	3.594941000000	-4.665318000000
H	-1.923487000000	3.292106000000	-4.259189000000
O	-1.613843000000	2.130489000000	-6.498775000000
H	-1.824296000000	2.452960000000	-5.578397000000
C	-0.859343000000	3.036759000000	-7.212562000000
C	-0.864611000000	2.523176000000	-8.670960000000
C	0.592222000000	3.068289000000	-6.671627000000
F	1.286611000000	4.158483000000	-7.122631000000
F	0.595821000000	3.095519000000	-5.306609000000
F	1.273296000000	1.944578000000	-7.058661000000
F	0.157897000000	3.060357000000	-9.402945000000
F	-2.041804000000	2.846947000000	-9.299309000000
F	-0.745438000000	1.163152000000	-8.725269000000
C	-1.469329000000	4.464731000000	-7.164694000000
F	-1.038408000000	5.235847000000	-8.214388000000
F	-2.834894000000	4.414017000000	-7.218986000000
F	-1.121170000000	5.109272000000	-6.009988000000

2_DHB_IIab_PFTB

E_{el} = -4252.77130060 Ha

E_{ZPVE} = -4252.298416 Ha

H = -4252.259089 Ha

G = -4252.365921 Ha

C	-7.440078000000	0.354296000000	-6.154268000000
C	-8.393195000000	1.576460000000	-6.277147000000
C	-6.786894000000	0.263860000000	-4.744047000000
C	-6.403488000000	0.312804000000	-7.315146000000
H	-8.981149000000	1.650030000000	-5.346897000000
H	-9.120919000000	1.371801000000	-7.080735000000
H	-6.042921000000	-0.549477000000	-4.757385000000
H	-7.561787000000	-0.043660000000	-4.022140000000
H	-6.929128000000	0.594628000000	-8.243440000000
H	-6.071806000000	-0.729865000000	-7.458092000000
C	-8.319935000000	-0.903085000000	-6.307198000000
H	-7.732631000000	-1.812992000000	-6.123851000000
H	-9.154293000000	-0.885123000000	-5.592759000000
H	-8.738619000000	-0.965017000000	-7.320884000000
P	-4.862760000000	1.372403000000	-7.199436000000
P	-5.957070000000	1.806343000000	-4.089251000000
P	-7.656391000000	3.268231000000	-6.611863000000
Cu	-5.489792000000	3.179007000000	-5.872383000000
C	-4.587900000000	1.149131000000	-3.055115000000
H	-4.913818000000	0.333088000000	-2.397114000000
H	-3.759882000000	0.807987000000	-3.687275000000
H	-4.205793000000	1.976290000000	-2.444081000000
C	-4.398132000000	1.496048000000	-8.976480000000
H	-3.378539000000	1.894605000000	-9.042919000000
H	-4.431708000000	0.518381000000	-9.476301000000
H	-5.066386000000	2.193390000000	-9.494920000000
C	-8.100185000000	3.503117000000	-8.387386000000
H	-7.540821000000	2.796863000000	-9.013227000000
H	-9.175144000000	3.354180000000	-8.557801000000
H	-7.826719000000	4.517418000000	-8.699313000000
C	-8.919263000000	4.344117000000	-5.813646000000
H	-9.939821000000	4.067342000000	-6.110617000000
H	-8.826112000000	4.276134000000	-4.723080000000
H	-8.733599000000	5.386615000000	-6.095298000000
C	-3.645119000000	0.106091000000	-6.640771000000
H	-3.941323000000	-0.307281000000	-5.670044000000
H	-3.580661000000	-0.716588000000	-7.365714000000
H	-2.661255000000	0.572091000000	-6.532153000000
C	-7.116569000000	2.356910000000	-2.768006000000
H	-8.092858000000	2.622239000000	-3.191323000000
H	-7.261157000000	1.583092000000	-2.002067000000
H	-6.696701000000	3.255902000000	-2.300238000000
H	-3.387530000000	4.003283000000	-4.287320000000
B	-4.192961000000	4.816999000000	-4.740951000000
H	-5.149455000000	4.877551000000	-3.991381000000
H	-4.497757000000	4.552622000000	-5.955697000000
H	-3.665849000000	5.892264000000	-4.894708000000
O	-2.173256000000	3.003256000000	-6.220033000000
H	-2.713632000000	3.486084000000	-5.532957000000
C	-0.826316000000	3.292029000000	-6.148015000000
C	-0.227427000000	2.749887000000	-7.466960000000
C	-0.196521000000	2.561115000000	-4.937710000000
F	1.061198000000	3.012605000000	-4.653420000000
F	-0.968922000000	2.716055000000	-3.818897000000
F	-0.121419000000	1.211887000000	-5.178952000000
F	1.127423000000	2.580674000000	-7.380381000000
F	-0.484908000000	3.600853000000	-8.505985000000
F	-0.773469000000	1.540213000000	-7.802369000000
C	-0.564098000000	4.819535000000	-6.043649000000
F	0.717242000000	5.132006000000	-6.424575000000
F	-1.424691000000	5.514310000000	-6.838586000000
F	-0.731515000000	5.255667000000	-4.758487000000

PhOH

E_{el} = -307.224082523 Ha

E_{ZPVE} = -307.118474 Ha

H = -307.112005 Ha

G = -307.147494 Ha

O	-0.899284000000	2.094704000000	-5.468994000000
H	-1.501205000000	2.477958000000	-4.825974000000
C	-1.008991000000	2.766409000000	-6.665481000000
C	-0.199609000000	2.328584000000	-7.714190000000
C	-1.883425000000	3.839108000000	-6.844533000000
C	-0.270084000000	2.971058000000	-8.946516000000
C	-1.945356000000	4.475262000000	-8.084193000000
C	-1.141440000000	4.046074000000	-9.139531000000
H	0.470697000000	1.491959000000	-7.543771000000
H	-2.511158000000	4.173497000000	-6.020105000000
H	0.360085000000	2.630106000000	-9.763138000000
H	-2.627407000000	5.309643000000	-8.221921000000
H	-1.192921000000	4.543062000000	-10.103421000000

2_DHB_IIa_PhOH

E_{el} = -3433.78549522 Ha

E_{ZPVE} = -3433.273920 Ha

H = -3433.241234 Ha

G = -3433.333083 Ha

C	-7.400679000000	0.782653000000	-6.369516000000
C	-7.799472000000	2.271888000000	-6.560445000000
C	-7.319309000000	0.371177000000	-4.872886000000
C	-6.122359000000	0.409467000000	-7.163566000000
H	-8.645759000000	2.479037000000	-5.883558000000
H	-8.192123000000	2.399341000000	-7.584288000000
H	-6.919410000000	-0.655873000000	-4.827179000000
H	-8.342549000000	0.323081000000	-4.462845000000
H	-6.258681000000	0.773659000000	-8.196277000000
H	-6.060555000000	-0.690418000000	-7.235028000000
C	-8.547307000000	-0.052030000000	-6.980080000000
H	-8.385187000000	-1.123414000000	-6.800235000000
H	-9.511971000000	0.226653000000	-6.534549000000
H	-8.612412000000	0.106326000000	-8.065014000000
P	-4.446620000000	1.033440000000	-6.599958000000
P	-6.276611000000	1.427042000000	-3.743120000000
P	-6.544266000000	3.641697000000	-6.282724000000
Cu	-4.823446000000	2.687410000000	-5.012969000000
C	-5.767064000000	0.232958000000	-2.442407000000
H	-6.625172000000	-0.299099000000	-2.011032000000
H	-5.053813000000	-0.495037000000	-2.844885000000
H	-5.249299000000	0.792764000000	-1.654256000000

C	-3.580635000000	1.016656000000	-8.228279000000
H	-2.504143000000	1.159871000000	-8.072351000000
H	-3.747325000000	0.062056000000	-8.746316000000
H	-3.927637000000	1.837528000000	-8.866890000000
C	-6.079070000000	4.085789000000	-8.013251000000
H	-5.463156000000	3.298911000000	-8.463014000000
H	-6.961735000000	4.258530000000	-8.644302000000
H	-5.472976000000	4.999706000000	-7.989456000000
C	-7.722205000000	5.026912000000	-5.946181000000
H	-8.523423000000	5.058935000000	-6.697485000000
H	-8.169581000000	4.916776000000	-4.951373000000
H	-7.178162000000	5.977949000000	-5.966337000000
C	-3.686894000000	-0.464456000000	-5.849175000000
H	-4.200864000000	-0.737644000000	-4.921156000000
H	-3.708646000000	-1.318018000000	-6.539928000000
H	-2.646244000000	-0.224404000000	-5.595652000000
C	-7.539852000000	2.387398000000	-2.805866000000
H	-8.048725000000	3.101037000000	-3.464435000000
H	-8.288764000000	1.735761000000	-2.335574000000
H	-7.022598000000	2.962810000000	-2.028087000000
H	-3.104971000000	1.967326000000	-3.749696000000
B	-3.147054000000	3.155657000000	-3.445888000000
H	-3.578051000000	3.287692000000	-2.320449000000
H	-3.862202000000	3.873489000000	-4.226383000000
H	-2.044904000000	3.659978000000	-3.582620000000
O	-0.947054000000	2.044422000000	-5.506837000000
H	-1.481001000000	2.461564000000	-4.800538000000
C	-1.007890000000	2.761024000000	-6.664595000000
C	-0.184285000000	2.341272000000	-7.716108000000
C	-1.876751000000	3.845743000000	-6.848990000000
C	-0.242591000000	2.988937000000	-8.947888000000
C	-1.923561000000	4.485132000000	-8.088464000000
C	-1.116530000000	4.060910000000	-9.145904000000
H	0.491625000000	1.508730000000	-7.542430000000
H	-2.509055000000	4.173778000000	-6.026323000000
H	0.401427000000	2.656111000000	-9.757811000000
H	-2.599176000000	5.327020000000	-8.223717000000
H	-1.158349000000	4.565376000000	-10.106944000000

2_DHB_IIab_PhOH

E_{el} = -3433.78439251 Ha

E_{ZPVE} = -3433.274455 Ha

H = -3433.241096 Ha

G =-3433.336387 Ha

C	-7.206891000000	0.472225000000	-6.274719000000
C	-8.091710000000	1.751855000000	-6.281963000000
C	-6.553209000000	0.214022000000	-4.887845000000
C	-6.170612000000	0.472129000000	-7.435171000000
H	-8.668661000000	1.776512000000	-5.342191000000
H	-8.833751000000	1.660429000000	-7.093387000000
H	-5.850582000000	-0.629305000000	-4.993701000000
H	-7.334635000000	-0.123159000000	-4.185672000000
H	-6.684474000000	0.834888000000	-8.342099000000
H	-5.880591000000	-0.571418000000	-7.647625000000
C	-8.156639000000	-0.714461000000	-6.536932000000
H	-7.622466000000	-1.669287000000	-6.440154000000
H	-8.987587000000	-0.713483000000	-5.818356000000
H	-8.579809000000	-0.659338000000	-7.549236000000
P	-4.583272000000	1.460375000000	-7.275092000000
P	-5.627391000000	1.631080000000	-4.095288000000
P	-7.250923000000	3.413849000000	-6.472910000000
Cu	-5.082493000000	3.137728000000	-5.751219000000
C	-4.427840000000	0.752569000000	-3.014834000000
H	-4.913500000000	-0.035056000000	-2.423183000000
H	-3.611078000000	0.328168000000	-3.607899000000
H	-3.977144000000	1.487842000000	-2.336753000000
C	-4.143494000000	1.625501000000	-9.059041000000
H	-3.109786000000	1.985031000000	-9.131206000000
H	-4.222943000000	0.664353000000	-9.585665000000
H	-4.791375000000	2.361049000000	-9.549433000000
C	-7.655924000000	3.817108000000	-8.228503000000
H	-7.142266000000	3.126414000000	-8.907662000000
H	-8.736812000000	3.758994000000	-8.415881000000
H	-7.308447000000	4.831488000000	-8.455126000000
C	-8.446740000000	4.518867000000	-5.615217000000
H	-9.481431000000	4.329763000000	-5.931190000000
H	-8.364560000000	4.391805000000	-4.529819000000
H	-8.184925000000	5.559482000000	-5.839299000000
C	-3.384688000000	0.141736000000	-6.806144000000
H	-3.551924000000	-0.191672000000	-5.775786000000
H	-3.458898000000	-0.720488000000	-7.483147000000
H	-2.367627000000	0.552548000000	-6.854860000000
C	-6.820963000000	2.215792000000	-2.819811000000
H	-7.758563000000	2.542643000000	-3.285148000000
H	-7.047100000000	1.428931000000	-2.087576000000
H	-6.379665000000	3.078865000000	-2.306318000000
H	-3.474354000000	4.209160000000	-3.614363000000
B	-4.136323000000	4.861967000000	-4.415192000000
H	-5.302026000000	4.917350000000	-4.058967000000
H	-3.974989000000	4.401985000000	-5.602427000000
H	-3.666627000000	5.969660000000	-4.554530000000
O	-1.887895000000	2.309365000000	-4.512754000000
H	-2.470123000000	3.075667000000	-4.334355000000
C	-1.060444000000	2.565787000000	-5.568882000000
C	-1.100795000000	3.767131000000	-6.287720000000
C	-0.159940000000	1.559648000000	-5.937320000000
C	-0.246082000000	3.944325000000	-7.375776000000
C	0.686240000000	1.749994000000	-7.027531000000
C	0.645970000000	2.940352000000	-7.757194000000
H	-1.794154000000	4.550469000000	-5.989248000000
H	-0.137392000000	0.643774000000	-5.352090000000
H	-0.279337000000	4.880616000000	-7.926791000000
H	1.384554000000	0.964730000000	-7.305507000000
H	1.308687000000	3.087319000000	-8.604952000000

PNA

E_{el} = -491.689803360 Ha

E_{ZPVE} = -491.569635 Ha

H = -491.560474 Ha

G = -491.602846 Ha

C	-3.641966000000	-1.106517000000	-1.055824000000
C	-4.906568000000	-1.725353000000	-1.110694000000
C	-5.993047000000	-1.156471000000	-0.470912000000
C	-5.823618000000	0.037845000000	0.230419000000
C	-4.581239000000	0.669898000000	0.297892000000
C	-3.495912000000	0.099027000000	-0.341871000000
N	-2.567932000000	-1.652622000000	-1.731981000000
N	-6.958896000000	0.633687000000	0.904425000000
O	-6.782049000000	1.713253000000	1.523312000000
O	-8.066334000000	0.043064000000	0.838842000000
H	-5.023665000000	-2.653170000000	-1.665039000000
H	-6.973847000000	-1.617689000000	-0.500312000000
H	-4.489799000000	1.596910000000	0.852616000000
H	-2.522568000000	0.581566000000	-0.301899000000
H	-1.645422000000	-1.353473000000	-1.455734000000
H	-2.627766000000	-2.626243000000	-1.987500000000

2_DHB_IIa_PNA

E_{el} = -3618.25265279 Ha

E_{ZPVE} = -3617.727253 Ha

H = -3617.691471 Ha

G = -3617.790581 Ha

C	-7.315076000000	0.982555000000	-6.586887000000
C	-7.682059000000	2.490128000000	-6.670557000000
C	-7.280091000000	0.459142000000	-5.124952000000
C	-6.022630000000	0.645961000000	-7.374967000000
H	-8.524333000000	2.668969000000	-5.980809000000
H	-8.070630000000	2.697686000000	-7.682538000000
H	-6.911619000000	-0.580442000000	-5.146348000000
H	-8.313328000000	0.412912000000	-4.740539000000
H	-6.117158000000	1.105052000000	-8.373953000000
H	-5.983812000000	-0.444423000000	-7.543262000000

C	-8.459753000000	0.221185000000	-7.289372000000
H	-8.323311000000	-0.864086000000	-7.189511000000
H	-9.430594000000	0.485145000000	-6.848432000000
H	-8.492217000000	0.465020000000	-8.359700000000
P	-4.349414000000	1.176289000000	-6.717290000000
P	-6.230542000000	1.400818000000	-3.906017000000
P	-6.394118000000	3.807734000000	-6.309057000000
Cu	-4.739124000000	2.742164000000	-5.043979000000
C	-5.779537000000	0.096208000000	-2.692215000000
H	-6.661925000000	-0.447763000000	-2.330169000000
H	-5.071922000000	-0.614587000000	-3.134100000000
H	-5.273555000000	0.579205000000	-1.848029000000
C	-3.413540000000	1.187481000000	-8.307784000000
H	-2.340239000000	1.261008000000	-8.091356000000
H	-3.601005000000	0.265672000000	-8.875696000000
H	-3.688397000000	2.050039000000	-8.927617000000
C	-5.935804000000	4.349278000000	-8.012272000000
H	-5.329576000000	3.593475000000	-8.524345000000
H	-6.825950000000	4.560421000000	-8.620376000000
H	-5.329462000000	5.261711000000	-7.955717000000
C	-7.521776000000	5.198333000000	-5.855815000000
H	-8.332643000000	5.312260000000	-6.588344000000
H	-7.955807000000	5.032136000000	-4.863143000000
H	-6.946056000000	6.130053000000	-5.818097000000
C	-3.674429000000	-0.389057000000	-6.015889000000
H	-4.238310000000	-0.695314000000	-5.128023000000
H	-3.688084000000	-1.203688000000	-6.752329000000
H	-2.640302000000	-0.201286000000	-5.698691000000
C	-7.474391000000	2.333440000000	-2.918539000000
H	-7.958828000000	3.099442000000	-3.535362000000
H	-8.243621000000	1.675019000000	-2.493078000000
H	-6.944558000000	2.844995000000	-2.105292000000
H	-2.915238000000	1.910217000000	-3.785174000000
B	-3.184030000000	2.989846000000	-3.267024000000
H	-3.817475000000	2.843489000000	-2.240762000000
H	-3.829439000000	3.787405000000	-4.035094000000
H	-2.164584000000	3.633551000000	-3.079294000000
N	-0.134773000000	2.710646000000	-4.849399000000
H	-0.832486000000	2.819034000000	-4.113384000000
C	-0.496533000000	3.049948000000	-6.120049000000
C	0.253717000000	2.629748000000	-7.244414000000
C	-1.634776000000	3.867079000000	-6.326388000000
C	-0.141437000000	2.976651000000	-8.523533000000
C	-2.040828000000	4.189453000000	-7.603090000000
C	-1.304437000000	3.733249000000	-8.703152000000
H	1.145096000000	2.025350000000	-7.093728000000
H	-2.198542000000	4.208274000000	-5.462783000000
H	0.414278000000	2.649661000000	-9.395882000000
H	-2.934279000000	4.782567000000	-7.768497000000
N	-1.794566000000	3.976383000000	-10.030606000000
O	-1.056173000000	3.697284000000	-11.011131000000
O	-2.966352000000	4.436743000000	-10.160146000000
H	0.555696000000	1.989080000000	-4.719045000000

2_DHB_IIab_PNA

E_{el} = -3618.25158396 Ha

E_{ZPVE} = -3617.725502 Ha

H = -3617.689913 Ha

G = -3617.789215 Ha

C	-6.889480000000	0.507621000000	-6.614453000000
C	-7.805182000000	1.760883000000	-6.507615000000
C	-6.291435000000	0.097070000000	-5.238443000000
C	-5.806280000000	0.670896000000	-7.715982000000
H	-8.405542000000	1.673183000000	-5.586310000000
H	-8.525201000000	1.739564000000	-7.342912000000
H	-5.556354000000	-0.706764000000	-5.409099000000
H	-7.093091000000	-0.345683000000	-4.623601000000
H	-6.286530000000	1.131648000000	-8.595872000000
H	-5.481547000000	-0.332557000000	-8.040964000000
C	-7.796157000000	-0.658308000000	-7.060360000000
H	-7.242855000000	-1.607151000000	-7.052927000000
H	-8.658327000000	-0.759465000000	-6.387105000000
H	-8.174529000000	-0.490799000000	-8.077943000000
P	-4.238933000000	1.650819000000	-7.371031000000
P	-5.465372000000	1.453078000000	-4.257235000000
P	-6.998313000000	3.451088000000	-6.503732000000
Cu	-4.853769000000	3.134524000000	-5.688220000000
C	-4.201633000000	0.548301000000	-3.273729000000
H	-4.611460000000	-0.340626000000	-2.776740000000
H	-3.359970000000	0.257606000000	-3.914013000000
H	-3.816847000000	1.241366000000	-2.514713000000
C	-3.753304000000	2.043214000000	-9.104764000000
H	-2.699624000000	2.351340000000	-9.147565000000
H	-3.879105000000	1.167389000000	-9.755905000000
H	-4.363874000000	2.868832000000	-9.489475000000
C	-7.373393000000	4.020797000000	-8.219630000000
H	-6.828718000000	3.413359000000	-8.952592000000
H	-8.448211000000	3.957134000000	-8.437632000000
H	-7.047269000000	5.060694000000	-8.335051000000
C	-8.239284000000	4.430269000000	-5.563502000000
H	-9.260276000000	4.257596000000	-5.929256000000
H	-8.180766000000	4.181436000000	-4.497646000000
H	-7.995391000000	5.494566000000	-5.659038000000
C	-3.077222000000	0.258932000000	-7.016556000000
H	-3.437718000000	-0.327705000000	-6.162822000000
H	-2.982843000000	-0.405178000000	-7.886664000000
H	-2.085277000000	0.648485000000	-6.762427000000
C	-6.711291000000	1.811258000000	-2.951852000000
H	-7.647116000000	2.156979000000	-3.407201000000
H	-6.921574000000	0.926982000000	-2.335662000000
H	-6.325919000000	2.619621000000	-2.318897000000
H	-4.066923000000	3.904707000000	-3.146499000000
B	-4.307047000000	4.766557000000	-3.977836000000
H	-5.472950000000	5.105047000000	-3.954339000000
H	-3.912563000000	4.421599000000	-5.153147000000
H	-3.575804000000	5.732062000000	-3.811175000000
N	-1.195650000000	4.052372000000	-3.467461000000
H	-2.014295000000	4.662943000000	-3.456377000000
C	-0.867959000000	3.504695000000	-4.676631000000
C	-1.186691000000	4.191674000000	-5.872617000000
C	-0.175973000000	2.273412000000	-4.760906000000
C	-0.881803000000	3.640849000000	-7.099633000000
C	0.141962000000	1.727507000000	-5.988998000000
C	-0.233786000000	2.399436000000	-7.158325000000
H	-1.703319000000	5.144465000000	-5.806814000000
H	0.098267000000	1.755821000000	-3.844549000000
H	-1.139333000000	4.149876000000	-8.022310000000
H	0.655142000000	0.775241000000	-6.071027000000
N	-0.004352000000	1.777107000000	-8.431196000000
O	0.529831000000	0.635963000000	-8.459301000000
O	-0.375422000000	2.385569000000	-9.475847000000
H	-1.157895000000	3.433021000000	-2.671093000000

PNAP

E_{el} = -851.730304551 Ha

E_{ZPVE} = -851.531197 Ha

H = -851.515811 Ha

G = -851.575211 Ha

C	-3.650924000000	-1.093472000000	-0.917166000000
C	-4.944821000000	-1.313880000000	-1.412309000000
C	-6.035885000000	-0.834588000000	-0.712892000000
C	-5.844828000000	-0.130467000000	0.489423000000
C	-4.550068000000	0.084533000000	0.975056000000
C	-3.450049000000	-0.393583000000	0.276722000000
H	-5.057310000000	-1.860756000000	-2.342874000000
H	-7.049172000000	-0.987989000000	-1.069363000000
H	-4.438784000000	0.631020000000	1.906529000000
H	-2.442066000000	-0.229290000000	0.651066000000
O	-2.618569000000	-1.594450000000	-1.657008000000
H	-1.777909000000	-1.390908000000	-1.236702000000
N	-6.886287000000	0.394508000000	1.277737000000
N	-8.069412000000	0.209531000000	0.834935000000

C	-9.102762000000	0.743012000000	1.649918000000
C	-10.401103000000	0.568977000000	1.157018000000
C	-8.885662000000	1.402567000000	2.869363000000
C	-11.489541000000	1.051096000000	1.870557000000
C	-9.965752000000	1.885387000000	3.590269000000
C	-11.251825000000	1.702536000000	3.078222000000
H	-10.523296000000	0.052814000000	0.210554000000
H	-7.868381000000	1.521059000000	3.225500000000
H	-12.506688000000	0.934498000000	1.515473000000
H	-9.839875000000	2.398178000000	4.537098000000
N	-12.390970000000	2.213026000000	3.838958000000
O	-12.161139000000	2.783118000000	4.931688000000
O	-13.538714000000	2.055519000000	3.360011000000

2_DHB_IIa_PNAP

E_{el} = -3978.29577032 Ha

E_{ZPVE} = -3977.690514 Ha

H = -3977.649013 Ha

G = -3977.762514 Ha

C	-7.002472000000	1.289952000000	-6.940368000000
C	-7.061565000000	2.821451000000	-7.194835000000
C	-7.364506000000	0.914422000000	-5.476389000000
C	-5.659619000000	0.667997000000	-7.404523000000
H	-7.984154000000	3.204755000000	-6.726706000000
H	-7.179735000000	2.990228000000	-8.279132000000
H	-7.193618000000	-0.167874000000	-5.351782000000
H	-8.446175000000	1.074434000000	-5.329392000000
H	-5.453746000000	1.048216000000	-8.419821000000
H	-5.794166000000	-0.422560000000	-7.510418000000
C	-8.097845000000	0.662385000000	-7.829164000000
H	-8.188071000000	-0.414408000000	-7.632361000000
H	-9.073247000000	1.128099000000	-7.633782000000
H	-7.862008000000	0.796544000000	-8.893484000000
P	-4.096873000000	0.942197000000	-6.406783000000
P	-6.445921000000	1.792573000000	-4.108808000000
P	-5.661039000000	3.928321000000	-6.619075000000
Cu	-4.524953000000	2.730457000000	-4.977353000000
C	-6.480897000000	0.558183000000	-2.747855000000
H	-7.496985000000	0.191414000000	-2.551423000000
H	-5.826796000000	-0.290476000000	-2.977966000000
H	-6.084976000000	1.037414000000	-1.844435000000
C	-2.854796000000	0.667032000000	-7.743174000000
H	-1.861560000000	0.538525000000	-7.295922000000
H	-3.100205000000	-0.231518000000	-8.326080000000
H	-2.803973000000	1.529458000000	-8.418086000000
C	-4.754246000000	4.235725000000	-8.197010000000
H	-4.210595000000	3.338732000000	-8.514034000000
H	-5.433171000000	4.546963000000	-9.002692000000
H	-4.013753000000	5.027811000000	-8.032522000000
C	-6.583983000000	5.523598000000	-6.502075000000
H	-7.182118000000	5.706381000000	-7.405319000000
H	-7.246438000000	5.518725000000	-5.628641000000
H	-5.870475000000	6.345734000000	-6.376376000000
C	-3.916981000000	-0.655810000000	-5.508414000000
H	-4.715202000000	-0.777076000000	-4.767236000000
H	-3.935976000000	-1.509500000000	-6.199138000000
H	-2.961937000000	-0.646652000000	-4.967861000000
C	-7.703298000000	2.983545000000	-3.482242000000
H	-7.917278000000	3.749698000000	-4.236321000000
H	-8.640072000000	2.482065000000	-3.204655000000
H	-7.289183000000	3.489084000000	-2.601260000000
H	-3.307085000000	1.740881000000	-3.351257000000
B	-3.211582000000	2.924213000000	-3.040269000000
H	-3.855186000000	3.148978000000	-2.039837000000
H	-3.597394000000	3.741366000000	-3.943855000000
H	-2.037429000000	3.232145000000	-2.908582000000
O	-0.796197000000	1.427395000000	-4.450051000000
H	-1.440245000000	1.940575000000	-3.911537000000
C	-0.460766000000	2.076702000000	-5.581386000000
C	0.522997000000	1.473718000000	-6.391304000000
C	-1.064632000000	3.281670000000	-5.983744000000
C	0.888394000000	2.053801000000	-7.589596000000
C	-0.692057000000	3.855950000000	-7.189214000000
C	0.277083000000	3.252971000000	-8.005591000000
H	0.978931000000	0.552805000000	-6.040134000000
H	-1.814807000000	3.742658000000	-5.346115000000
H	1.645281000000	1.609161000000	-8.227807000000
H	-1.135856000000	4.786917000000	-7.532207000000
N	0.574755000000	3.921999000000	-9.200225000000
N	1.468862000000	3.382541000000	-9.941808000000
C	1.755072000000	4.088581000000	-11.137465000000
C	2.728653000000	3.503842000000	-11.957317000000
C	1.139688000000	5.292745000000	-11.516775000000
C	3.093503000000	4.107702000000	-13.151665000000
C	1.496661000000	5.903151000000	-12.707634000000
C	2.469263000000	5.300904000000	-13.508998000000
H	3.181470000000	2.575111000000	-11.626134000000
H	0.392537000000	5.724772000000	-10.860300000000
H	3.843546000000	3.680249000000	-13.806668000000
H	1.045081000000	6.833437000000	-13.033534000000
N	2.844488000000	5.944915000000	-14.763286000000
O	3.721366000000	5.394759000000	-15.471927000000
O	2.269899000000	7.016983000000	-15.071427000000

2_DHB_IIab_PNAP

E_{el} = -3978.29205631 Ha

E_{ZPVE} = -3977.687130 Ha

H = -3977.645353 Ha

G = -3977.760388 Ha

C	-6.835496000000	0.304319000000	-5.633557000000
C	-7.878862000000	1.431594000000	-5.385856000000
C	-5.555998000000	0.484599000000	-4.772014000000
C	-6.512640000000	0.110905000000	-7.141066000000
H	-7.911763000000	1.631789000000	-4.301615000000
H	-8.878318000000	1.048315000000	-5.654074000000
H	-4.820213000000	-0.271264000000	-5.093947000000
H	-5.798326000000	0.251767000000	-3.721068000000
H	-7.469158000000	0.114597000000	-7.691049000000
H	-6.086534000000	-0.897742000000	-7.279637000000
C	-7.495815000000	-1.007593000000	-5.159570000000
H	-6.780653000000	-1.840216000000	-5.200465000000
H	-7.849366000000	-0.911789000000	-4.124039000000
H	-8.356583000000	-1.264365000000	-5.792085000000
P	-5.375824000000	1.313114000000	-8.029020000000
P	-4.719243000000	2.150772000000	-4.835280000000
P	-7.663045000000	3.077163000000	-6.256334000000
Cu	-5.422953000000	3.256984000000	-6.747646000000
C	-2.986445000000	1.729305000000	-4.383670000000
H	-2.945225000000	1.089586000000	-3.492184000000
H	-2.475988000000	1.236470000000	-5.219314000000
H	-2.448905000000	2.664247000000	-4.180052000000
C	-5.960505000000	1.031465000000	-9.757638000000
H	-5.255430000000	1.495499000000	-10.456400000000
H	-6.033545000000	-0.040578000000	-9.986390000000
H	-6.940908000000	1.497953000000	-9.909777000000
C	-8.907868000000	2.916389000000	-7.609297000000
H	-8.590406000000	2.148429000000	-8.324493000000
H	-9.897795000000	2.647526000000	-7.216149000000
H	-8.983786000000	3.867555000000	-8.148302000000
C	-8.576988000000	4.197709000000	-5.117858000000
H	-9.548042000000	3.777763000000	-4.823333000000
H	-7.978191000000	4.398565000000	-4.222057000000
H	-8.738293000000	5.157069000000	-5.622855000000
C	-3.799039000000	0.358803000000	-8.093052000000
H	-3.343457000000	0.299442000000	-7.098422000000
H	-3.958644000000	-0.654751000000	-8.485313000000
H	-3.090339000000	0.897010000000	-8.732760000000
C	-5.268736000000	2.940451000000	-3.266307000000
H	-6.358352000000	3.062177000000	-3.258754000000
H	-4.969924000000	2.353859000000	-2.387333000000
H	-4.819394000000	3.939747000000	-3.211900000000
H	-3.312426000000	4.826029000000	-5.736719000000

B	-4.278498000000	5.291765000000	-6.331236000000
H	-5.219644000000	5.405001000000	-5.565353000000
H	-4.551188000000	4.583434000000	-7.372609000000
H	-4.001722000000	6.343898000000	-6.860274000000
O	-2.183474000000	3.017351000000	-7.302662000000
H	-2.758795000000	3.756837000000	-7.010532000000
C	-0.879793000000	3.298382000000	-7.074495000000
C	-0.437571000000	4.565612000000	-6.662631000000
C	0.039255000000	2.251882000000	-7.276344000000
C	0.918836000000	4.771567000000	-6.459760000000
C	1.388178000000	2.467199000000	-7.077005000000
C	1.840798000000	3.735068000000	-6.665303000000
H	-1.160146000000	5.364277000000	-6.515170000000
H	-0.344035000000	1.285662000000	-7.595120000000
H	1.302539000000	5.737188000000	-6.144146000000
H	2.119884000000	1.680320000000	-7.229296000000
N	3.186408000000	4.059048000000	-6.437805000000
N	4.034424000000	3.121935000000	-6.638308000000
C	5.385231000000	3.482871000000	-6.398412000000
C	5.802133000000	4.750093000000	-5.960748000000
C	6.323842000000	2.469260000000	-6.628126000000
C	7.149394000000	4.996813000000	-5.753662000000
C	7.675359000000	2.706579000000	-6.424547000000
C	8.067214000000	3.970479000000	-5.988319000000
H	5.052139000000	5.515228000000	-5.793009000000
H	5.958637000000	1.505325000000	-6.966874000000
H	7.509488000000	5.961746000000	-5.415300000000
H	8.425858000000	1.943080000000	-6.592947000000
N	9.485852000000	4.231170000000	-5.767620000000
O	10.299551000000	3.302304000000	-5.989679000000
O	9.821914000000	5.371188000000	-5.365996000000

PNP

E_{el} = -851.730304551 Ha

E_{ZPVE} = -851.531197 Ha

H = -851.515811 Ha

G = -851.575211 Ha

C	-3.635346000000	-1.143974000000	-0.913887000000
C	-4.888440000000	-1.759023000000	-1.020257000000
C	-5.995166000000	-1.164075000000	-0.438357000000
C	-5.835814000000	0.042709000000	0.243716000000
C	-4.595020000000	0.665359000000	0.355912000000
C	-3.487451000000	0.067299000000	-0.227289000000
N	-6.996827000000	0.670689000000	0.856082000000
O	-6.830592000000	1.759427000000	1.457785000000
O	-8.105041000000	0.092250000000	0.751551000000
H	-4.966822000000	-2.696779000000	-1.559281000000
H	-6.980293000000	-1.612101000000	-0.500696000000
H	-4.518163000000	1.603211000000	0.894123000000
H	-2.509213000000	0.536089000000	-0.151456000000
O	-2.587136000000	-1.781840000000	-1.507451000000
H	-1.774320000000	-1.283751000000	-1.379635000000

2_DHB_IIa_PNP

E_{el} = -3638.12388673 Ha

E_{ZPVE} = -3637.609660 Ha

H = -3637.574663 Ha

G = -3637.672270 Ha

C	-7.311086000000	0.888277000000	-6.490925000000
C	-7.687248000000	2.389865000000	-6.623989000000
C	-7.286354000000	0.409381000000	-5.012897000000
C	-6.009128000000	0.538297000000	-7.258044000000
H	-8.544651000000	2.580183000000	-5.956325000000
H	-8.056376000000	2.567007000000	-7.648930000000
H	-6.902111000000	-0.624369000000	-4.997673000000
H	-8.324323000000	0.357798000000	-4.642373000000
H	-6.087257000000	0.986108000000	-8.263502000000
H	-5.971520000000	-0.553931000000	-7.413161000000
C	-8.444151000000	0.098623000000	-7.180876000000
H	-8.303642000000	-0.982127000000	-7.044939000000
H	-9.421288000000	0.371594000000	-6.759923000000
H	-8.465701000000	0.307644000000	-8.258856000000
P	-4.347151000000	1.064163000000	-6.572536000000
P	-6.276378000000	1.403352000000	-3.799619000000
P	-6.415151000000	3.722922000000	-6.266839000000
Cu	-4.763509000000	2.688635000000	-4.972514000000
C	-5.820899000000	0.144017000000	-2.541257000000
H	-6.696529000000	-0.409328000000	-2.177314000000
H	-5.089620000000	-0.562524000000	-2.950190000000
H	-5.339769000000	0.659521000000	-1.701428000000
C	-3.374231000000	1.067072000000	-8.140265000000
H	-2.304295000000	1.126985000000	-7.904863000000
H	-3.560298000000	0.151731000000	-8.718790000000
H	-3.623912000000	1.937271000000	-8.758483000000
C	-5.920197000000	4.233920000000	-7.968852000000
H	-5.293497000000	3.466844000000	-8.437368000000
H	-6.793140000000	4.422958000000	-8.608311000000
H	-5.324639000000	5.152609000000	-7.907581000000
C	-7.559550000000	5.116237000000	-5.867031000000
H	-8.354253000000	5.208849000000	-6.619882000000
H	-8.015310000000	4.967620000000	-4.881185000000
H	-6.990927000000	6.052469000000	-5.835416000000
C	-3.705359000000	-0.497163000000	-5.836151000000
H	-4.299330000000	-0.788601000000	-4.962466000000
H	-3.712304000000	-1.318317000000	-6.565396000000
H	-2.677054000000	-0.323037000000	-5.494218000000
C	-7.563452000000	2.333135000000	-2.865239000000
H	-8.044057000000	3.078346000000	-3.509783000000
H	-8.332578000000	1.667373000000	-2.451197000000
H	-7.071122000000	2.869745000000	-2.044903000000
H	-3.074642000000	1.901409000000	-3.689308000000
B	-3.126274000000	3.073828000000	-3.331050000000
H	-3.576698000000	3.153067000000	-2.210580000000
H	-3.822401000000	3.827608000000	-4.091284000000
H	-2.021562000000	3.588630000000	-3.414553000000
O	-0.852649000000	2.120401000000	-5.295539000000
H	-1.442939000000	2.483460000000	-4.595802000000
C	-0.895191000000	2.854406000000	-6.422033000000
C	-0.031846000000	2.470779000000	-7.464027000000
C	-1.775379000000	3.939100000000	-6.600004000000
C	-0.060804000000	3.139398000000	-8.675304000000
C	-1.804199000000	4.607200000000	-7.814164000000
C	-0.957040000000	4.197644000000	-8.845851000000
H	0.649366000000	1.643938000000	-7.290925000000
H	-2.430123000000	4.237332000000	-5.785214000000
H	0.591829000000	2.860493000000	-9.494936000000
H	-2.474938000000	5.443258000000	-7.980666000000
N	-1.011459000000	4.882812000000	-10.120436000000
O	-0.225456000000	4.514839000000	-11.029615000000
O	-1.850051000000	5.809787000000	-10.263659000000

2_DHB_IIab_PNP

E_{el} = -3638.12174864 Ha

E_{ZPVE} = -3637.608742 Ha

H = -3637.573054 Ha

G = -3637.674121 Ha

C	-7.124459000000	0.470520000000	-6.332024000000
C	-8.000490000000	1.753617000000	-6.407915000000
C	-6.560932000000	0.217564000000	-4.905378000000
C	-6.022100000000	0.448709000000	-7.426995000000
H	-8.656733000000	1.772286000000	-5.521828000000
H	-8.671210000000	1.664194000000	-7.279265000000
H	-5.871369000000	-0.641548000000	-4.958277000000
H	-7.391228000000	-0.096538000000	-4.250234000000
H	-6.482096000000	0.784021000000	-8.372280000000
H	-5.716422000000	-0.598209000000	-7.595963000000
C	-8.065768000000	-0.712770000000	-6.640964000000
H	-7.545160000000	-1.670272000000	-6.505244000000
H	-8.938208000000	-0.700986000000	-5.973598000000
H	-8.427680000000	-0.663817000000	-7.676909000000
P	-4.450738000000	1.446843000000	-7.198336000000
P	-5.657792000000	1.622256000000	-4.067531000000

P	-7.149673000000	3.418315000000	-6.524701000000
Cu	-5.021271000000	3.122738000000	-5.696286000000
C	-4.497963000000	0.734010000000	-2.950374000000
H	-4.998498000000	-0.074766000000	-2.401522000000
H	-3.644532000000	0.336499000000	-3.510072000000
H	-4.096057000000	1.459868000000	-2.232667000000
C	-3.928041000000	1.621107000000	-8.958326000000
H	-2.901980000000	2.007571000000	-8.984503000000
H	-3.957947000000	0.658049000000	-9.486190000000
H	-4.569843000000	2.338506000000	-9.482132000000
C	-7.471280000000	3.865869000000	-8.286283000000
H	-6.922133000000	3.200957000000	-8.962922000000
H	-8.541892000000	3.807749000000	-8.525276000000
H	-7.121385000000	4.888791000000	-8.466336000000
C	-8.377680000000	4.514294000000	-5.702004000000
H	-9.395605000000	4.342174000000	-6.076244000000
H	-8.354989000000	4.364172000000	-4.616856000000
H	-8.096134000000	5.557001000000	-5.889604000000
C	-3.265969000000	0.134347000000	-6.674969000000
H	-3.479861000000	-0.199876000000	-5.653696000000
H	-3.303125000000	-0.728512000000	-7.353777000000
H	-2.249691000000	0.548963000000	-6.679778000000
C	-6.884998000000	2.206389000000	-2.825337000000
H	-7.800041000000	2.564806000000	-3.310715000000
H	-7.151210000000	1.409277000000	-2.118249000000
H	-6.443786000000	3.048532000000	-2.278100000000
H	-3.547691000000	4.208083000000	-3.451503000000
B	-4.148657000000	4.855661000000	-4.305462000000
H	-5.330925000000	4.920740000000	-4.021483000000
H	-3.915207000000	4.379574000000	-5.472263000000
H	-3.655819000000	5.955291000000	-4.423584000000
O	-1.937570000000	2.410309000000	-4.307270000000
H	-2.565178000000	3.151983000000	-4.144175000000
C	-1.055228000000	2.708931000000	-5.282949000000
C	-1.043622000000	3.947658000000	-5.949486000000
C	-0.130548000000	1.709744000000	-5.634549000000
C	-0.130562000000	4.168055000000	-6.969581000000
C	0.780729000000	1.931054000000	-6.652676000000
C	0.766830000000	3.158017000000	-7.319663000000
H	-1.748727000000	4.722603000000	-5.660755000000
H	-0.148237000000	0.772910000000	-5.085534000000
H	-0.100053000000	5.112535000000	-7.501268000000
H	1.503859000000	1.177467000000	-6.943905000000
N	1.710349000000	3.386091000000	-8.396376000000
O	2.503363000000	2.458163000000	-8.698291000000
O	1.689466000000	4.497368000000	-8.982426000000

2_DHB_IIa_CF_3OH

E_{el} = -3539.82931227 Ha

E_{ZPVE} = -3539.393733 Ha

H = -3539.362576 Ha

G = -3539.451425 Ha

C	2.440876000000	0.947436000000	1.326430000000
C	2.202093000000	1.989069000000	0.195835000000
C	3.066842000000	-0.374326000000	0.797586000000
C	1.172335000000	0.696876000000	2.184566000000
H	3.099663000000	1.997828000000	-0.446183000000
H	2.148714000000	2.992406000000	0.653080000000
H	3.072476000000	-1.101492000000	1.626860000000
H	4.124770000000	-0.187057000000	0.546458000000
H	0.755102000000	1.679063000000	2.464136000000
H	1.478065000000	0.216948000000	3.130247000000
C	3.489350000000	1.570947000000	2.272046000000
H	3.789620000000	0.853350000000	3.047578000000
H	4.388187000000	1.867547000000	1.714461000000
H	3.085335000000	2.462864000000	2.769575000000
P	-0.235260000000	-0.306999000000	1.462098000000
P	2.261383000000	-1.198429000000	-0.674369000000
P	0.721424000000	1.829283000000	-0.944251000000
Cu	0.104845000000	-0.407120000000	-0.841659000000
C	2.670823000000	-2.970074000000	-0.394600000000
H	3.738796000000	-3.115946000000	-0.184973000000
H	2.078241000000	-3.375877000000	0.433096000000
H	2.396858000000	-3.532599000000	-1.295130000000
C	-1.636974000000	0.343487000000	2.467006000000
H	-2.495662000000	-0.327341000000	2.345266000000
H	-1.367021000000	0.393150000000	3.530653000000
H	-1.941913000000	1.338368000000	2.124025000000
C	-0.441816000000	3.061133000000	-0.214186000000
H	-0.746487000000	2.758126000000	0.793542000000
H	0.013911000000	4.059280000000	-0.159973000000
H	-1.347036000000	3.105792000000	-0.830036000000
C	1.340527000000	2.827122000000	-2.369233000000
H	1.779631000000	3.776647000000	-2.033348000000
H	2.091370000000	2.264846000000	-2.935837000000
H	0.504572000000	3.042994000000	-3.044215000000
C	-0.026060000000	-1.934955000000	2.299916000000
H	0.879115000000	-2.442903000000	1.948885000000
H	0.024789000000	-1.823765000000	3.391446000000
H	-0.884224000000	-2.567811000000	2.040994000000
C	3.460775000000	-0.820066000000	-2.023250000000
H	3.486387000000	0.255876000000	-2.231085000000
H	4.474853000000	-1.155821000000	-1.766996000000
H	3.134628000000	-1.330229000000	-2.937094000000
H	-0.804177000000	-2.482332000000	-0.788288000000
B	-1.114638000000	-2.110661000000	-1.913001000000
H	-0.560949000000	-2.785747000000	-2.747643000000
H	-0.865891000000	-0.892455000000	-2.173862000000
H	-2.669336000000	-1.756458000000	-0.651172000000
C	-3.835248000000	-0.296366000000	-0.218980000000
F	-3.007167000000	0.798743000000	-0.482346000000
O	-3.185596000000	-1.382276000000	0.125816000000
H	-2.330306000000	-2.172391000000	-2.062316000000
F	-4.618322000000	-0.441570000000	-1.348318000000
F	-4.662100000000	0.099978000000	0.806849000000

2_$TS1_{BH}^{A+B}$_CF_3OH

E_{el} = -3539.80574348 Ha

E_{ZPVE} = -3539.374781 Ha

H = -3539.343375 Ha

G = -3539.432634 Ha

C	2.464979000000	0.916314000000	1.366899000000
C	2.209654000000	1.936647000000	0.221246000000
C	2.992272000000	-0.449098000000	0.842093000000
C	1.245626000000	0.756441000000	2.317632000000
H	3.083337000000	1.905516000000	-0.451947000000
H	2.200203000000	2.950848000000	0.656786000000
H	3.029390000000	-1.144386000000	1.697605000000
H	4.036352000000	-0.319205000000	0.508467000000
H	0.893887000000	1.766898000000	2.585985000000
H	1.592262000000	0.294073000000	3.257631000000
C	3.603939000000	1.512613000000	2.221970000000
H	3.917376000000	0.803652000000	3.000117000000
H	4.479088000000	1.747957000000	1.601068000000
H	3.275496000000	2.437185000000	2.715257000000
P	-0.242990000000	-0.198238000000	1.700105000000
P	2.067760000000	-1.320175000000	-0.530127000000
P	0.688070000000	1.799242000000	-0.865307000000
Cu	-0.035134000000	-0.369858000000	-0.603971000000
C	2.565096000000	-3.068159000000	-0.225171000000
H	3.652179000000	-3.162866000000	-0.099578000000
H	2.065082000000	-3.462847000000	0.666243000000
H	2.250190000000	-3.677053000000	-1.081042000000
C	-1.600767000000	0.561381000000	2.677353000000
H	-2.530636000000	0.023468000000	2.458192000000
H	-1.390304000000	0.519145000000	3.754261000000
H	-1.757768000000	1.604145000000	2.380038000000

C	-0.403748000000	3.099825000000	-0.157192000000
H	-0.692112000000	2.838884000000	0.866462000000
H	0.093870000000	4.078922000000	-0.152546000000
H	-1.325215000000	3.154226000000	-0.746876000000
C	1.300411000000	2.697582000000	-2.357120000000
H	1.777016000000	3.648565000000	-2.082697000000
H	2.019365000000	2.083181000000	-2.910997000000
H	0.453694000000	2.905066000000	-3.021102000000
C	-0.081674000000	-1.806180000000	2.580593000000
H	0.811169000000	-2.345445000000	2.242404000000
H	-0.026531000000	-1.672852000000	3.669427000000
H	-0.960535000000	-2.412425000000	2.330694000000
C	3.117060000000	-0.968101000000	-2.004285000000
H	3.081050000000	0.098559000000	-2.254315000000
H	4.162872000000	-1.264337000000	-1.845827000000
H	2.710456000000	-1.524307000000	-2.858590000000
H	-0.185663000000	-2.746568000000	-2.197353000000
B	-0.917569000000	-1.923599000000	-2.664367000000
H	-1.093950000000	-1.976493000000	-3.848446000000
H	-0.780804000000	-0.756630000000	-2.331351000000
H	-2.030364000000	-1.979636000000	-1.712004000000
C	-3.239301000000	-0.545637000000	-0.250330000000
F	-2.687011000000	0.791338000000	-0.400943000000
O	-2.397056000000	-1.456949000000	-0.149620000000
H	-2.168055000000	-2.349738000000	-2.466799000000
F	-4.108311000000	-0.630519000000	-1.372785000000
F	-4.117714000000	-0.377921000000	0.846702000000

2_INT$_{BH}^{A+B}$_CF$_3$OH

E_{el} = -3539.82010082 Ha

E_{ZPVE} = -3539.388906 Ha

H = -3539.356629 Ha

G = -3539.447730 Ha

C	2.421624000000	0.903121000000	1.278875000000
C	2.109185000000	1.888595000000	0.118109000000
C	2.829169000000	-0.512822000000	0.778761000000
C	1.287798000000	0.848732000000	2.340796000000
H	2.923434000000	1.801955000000	-0.621126000000
H	2.161580000000	2.919081000000	0.510037000000
H	2.884869000000	-1.172358000000	1.661444000000
H	3.854530000000	-0.460420000000	0.374208000000
H	0.993225000000	1.885825000000	2.573117000000
H	1.702670000000	0.432253000000	3.274717000000
C	3.660569000000	1.473844000000	2.002745000000
H	4.008888000000	0.783042000000	2.782595000000
H	4.485649000000	1.634817000000	1.295755000000
H	3.425564000000	2.435484000000	2.478628000000
P	-0.269873000000	-0.093471000000	1.919930000000
P	1.777663000000	-1.393749000000	-0.498783000000
P	0.497483000000	1.720738000000	-0.825411000000
Cu	-0.249063000000	-0.388527000000	-0.360243000000
C	2.220819000000	-3.146245000000	-0.139459000000
H	3.308356000000	-3.281059000000	-0.063445000000
H	1.750104000000	-3.478669000000	0.792781000000
H	1.838563000000	-3.775846000000	-0.951792000000
C	-1.532222000000	0.782388000000	2.929533000000
H	-2.480459000000	0.245709000000	2.813288000000
H	-1.251552000000	0.821965000000	3.990248000000
H	-1.686301000000	1.801718000000	2.558305000000
C	-0.517172000000	3.088068000000	-0.124848000000
H	-0.654453000000	2.946845000000	0.953289000000
H	-0.057644000000	4.070171000000	-0.299064000000
H	-1.510965000000	3.052153000000	-0.585333000000
C	0.971326000000	2.475954000000	-2.438191000000
H	1.488790000000	3.434941000000	-2.299723000000
H	1.612513000000	1.795098000000	-3.009396000000
H	0.062052000000	2.642209000000	-3.027529000000
C	-0.093277000000	-1.637368000000	2.907349000000
H	0.730133000000	-2.249840000000	2.520350000000
H	0.083428000000	-1.428788000000	3.971170000000
H	-1.020100000000	-2.214244000000	2.801754000000
C	2.770516000000	-1.145360000000	-2.030106000000
H	2.770437000000	-0.090206000000	-2.326851000000
H	3.807900000000	-1.478834000000	-1.890979000000
H	2.308651000000	-1.717499000000	-2.843498000000
H	-0.005090000000	-2.540333000000	-3.164067000000
B	-0.540343000000	-1.613462000000	-3.703824000000
H	-0.752451000000	-1.742096000000	-4.878715000000
H	-0.178422000000	-0.512341000000	-3.393943000000
H	-1.665547000000	-1.458751000000	-2.817905000000
C	-3.039710000000	-0.589300000000	-0.521574000000
F	-3.058237000000	0.839274000000	-0.407350000000
O	-2.014141000000	-1.065461000000	-1.067690000000
H	-1.877574000000	-1.778776000000	-3.561521000000
F	-4.246807000000	-0.889521000000	-1.160501000000
F	-3.255204000000	-1.004525000000	0.829208000000

2_TS2$_{BH}^{C}$_CF$_3$OH

E_{el} = -3539.80484994 Ha

E_{ZPVE} = -3539.377424 Ha

H = -3539.344545 Ha

G = -3539.447730 Ha

C	2.418002000000	0.897591000000	1.287048000000
C	2.159455000000	1.901111000000	0.128668000000
C	2.798888000000	-0.521663000000	0.776274000000
C	1.255192000000	0.865164000000	2.318286000000
H	2.981655000000	1.790151000000	-0.598853000000
H	2.243559000000	2.926548000000	0.528510000000
H	2.822364000000	-1.194619000000	1.649994000000
H	3.832488000000	-0.490139000000	0.390678000000
H	0.974860000000	1.908596000000	2.540807000000
H	1.633983000000	0.441107000000	3.264006000000
C	3.654243000000	1.426827000000	2.044997000000
H	3.966194000000	0.717853000000	2.823831000000
H	4.499652000000	1.575527000000	1.359504000000
H	3.432174000000	2.387992000000	2.527917000000
P	-0.309789000000	-0.045223000000	1.851868000000
P	1.746653000000	-1.356418000000	-0.531110000000
P	0.561003000000	1.804600000000	-0.842868000000
Cu	-0.255922000000	-0.291452000000	-0.446351000000
C	2.137795000000	-3.125416000000	-0.186953000000
H	3.219771000000	-3.286399000000	-0.085604000000
H	1.635736000000	-3.460488000000	0.727517000000
H	1.761904000000	-3.736437000000	-1.016344000000
C	-1.566270000000	0.823332000000	2.874296000000
H	-2.508251000000	0.274199000000	2.770454000000
H	-1.270342000000	0.864164000000	3.930919000000
H	-1.736384000000	1.840394000000	2.504902000000
C	-0.414028000000	3.196280000000	-0.133555000000
H	-0.717102000000	2.965234000000	0.893681000000
H	0.152203000000	4.137465000000	-0.142379000000
H	-1.332618000000	3.317470000000	-0.719024000000
C	1.100417000000	2.583157000000	-2.425891000000
H	1.625271000000	3.532786000000	-2.253502000000
H	1.758289000000	1.905006000000	-2.982095000000
H	0.216536000000	2.771546000000	-3.046365000000
C	-0.162619000000	-1.610297000000	2.810371000000
H	0.670777000000	-2.218367000000	2.438799000000
H	-0.015525000000	-1.420654000000	3.882299000000
H	-1.089076000000	-2.177647000000	2.664213000000
C	2.778880000000	-1.125883000000	-2.042526000000
H	2.804668000000	-0.070546000000	-2.338202000000
H	3.807067000000	-1.480010000000	-1.886963000000
H	2.323780000000	-1.692419000000	-2.864673000000
H	-0.069435000000	-2.370995000000	-3.278475000000
B	-0.596982000000	-1.411337000000	-3.746498000000
H	-1.168466000000	-1.502464000000	-4.781672000000
H	-0.418382000000	-0.344072000000	-3.256493000000
H	-2.740476000000	-2.327791000000	-2.778648000000
C	-2.995047000000	-0.659508000000	-0.418112000000
F	-3.112484000000	0.730452000000	-0.081171000000
O	-2.018973000000	-0.956758000000	-1.138729000000

H	-2.797532000000	-2.677170000000	-3.444026000000
F	-4.252691000000	-0.985649000000	-0.933292000000
F	-3.005097000000	-1.273902000000	0.891021000000

2_Product_CF_3OH

E_{el} = -3539.83626603 Ha

E_{ZPVE} = -3539.405205 Ha

H = -3539.373009 Ha

G = -3539.463506 Ha

C	2.414487000000	0.868577000000	1.273889000000
C	2.092179000000	1.880057000000	0.135979000000
C	2.829760000000	-0.532099000000	0.735265000000
C	1.278832000000	0.790321000000	2.336085000000
H	2.858664000000	1.764931000000	-0.649025000000
H	2.208962000000	2.903640000000	0.530894000000
H	2.896175000000	-1.216643000000	1.598310000000
H	3.851112000000	-0.461001000000	0.323591000000
H	0.947722000000	1.821069000000	2.547549000000
H	1.711093000000	0.411862000000	3.278241000000
C	3.650375000000	1.428838000000	2.010130000000
H	4.012300000000	0.717271000000	2.764734000000
H	4.468055000000	1.621911000000	1.302737000000
H	3.407970000000	2.372461000000	2.517445000000
P	-0.262986000000	-0.223257000000	1.989969000000
P	1.753694000000	-1.363402000000	-0.550344000000
P	0.416119000000	1.769149000000	-0.689241000000
Cu	-0.275360000000	-0.381005000000	-0.273676000000
C	2.206428000000	-3.130720000000	-0.313834000000
H	3.294868000000	-3.276583000000	-0.324193000000
H	1.800285000000	-3.513432000000	0.629023000000
H	1.758372000000	-3.708507000000	-1.131100000000
C	-1.503229000000	0.667835000000	3.017280000000
H	-2.420328000000	0.069312000000	3.060311000000
H	-1.138195000000	0.845238000000	4.037772000000
H	-1.761560000000	1.625072000000	2.550528000000
C	-0.484391000000	3.176641000000	0.088149000000
H	-0.583400000000	3.023797000000	1.169331000000
H	0.033131000000	4.129479000000	-0.087474000000
H	-1.491845000000	3.229615000000	-0.341185000000
C	0.749022000000	2.485754000000	-2.346921000000
H	1.296624000000	3.434807000000	-2.275856000000
H	1.307496000000	1.778719000000	-2.969404000000
H	-0.214255000000	2.655334000000	-2.841661000000
C	0.030990000000	-1.700015000000	3.054531000000
H	0.869444000000	-2.290039000000	2.666113000000
H	0.250550000000	-1.411566000000	4.091474000000
H	-0.860387000000	-2.337434000000	3.042724000000
C	2.660302000000	-1.008078000000	-2.109555000000
H	2.669318000000	0.070022000000	-2.305538000000
H	3.695124000000	-1.373447000000	-2.066674000000
H	2.129808000000	-1.490481000000	-2.939095000000
H	-0.582961000000	-2.357098000000	-2.659599000000
B	-1.126608000000	-1.312200000000	-2.944439000000
H	-1.997338000000	-1.419057000000	-3.765706000000
H	-0.340420000000	-0.418210000000	-3.188384000000
H	-3.245784000000	-3.243586000000	-1.472781000000
C	-2.834557000000	-0.064205000000	-1.528293000000
F	-2.557582000000	1.194452000000	-2.101813000000
O	-1.838205000000	-0.887027000000	-1.534352000000
H	-3.334947000000	-3.593122000000	-2.127499000000
F	-3.970609000000	-0.506826000000	-2.173592000000
F	-3.236440000000	0.234799000000	-0.219392000000

2_DHB_IIab_CF_3OH

E_{el} = -3539.82599041 Ha

E_{ZPVE} = -3539.390547 Ha

H = -3539.359184 Ha

G = -3539.448730 Ha

C	-3.417055000000	-0.712286000000	0.968775000000
C	-3.179631000000	-1.534483000000	-0.329109000000
C	-3.864658000000	0.745534000000	0.673903000000
C	-2.207501000000	-0.777851000000	1.943730000000
H	-4.007691000000	-1.320431000000	-1.025926000000
H	-3.255428000000	-2.606904000000	-0.082922000000
H	-3.897352000000	1.289028000000	1.633257000000
H	-4.902459000000	0.726484000000	0.298506000000
H	-1.861876000000	-1.824842000000	1.980931000000
H	-2.566096000000	-0.541381000000	2.960361000000
C	-4.598693000000	-1.385436000000	1.699002000000
H	-4.899093000000	-0.800167000000	2.578735000000
H	-5.468107000000	-1.473173000000	1.033300000000
H	-4.323869000000	-2.393833000000	2.036702000000
P	-0.695898000000	0.286765000000	1.627624000000
P	-2.854777000000	1.777214000000	-0.514897000000
P	-1.568757000000	-1.265330000000	-1.246200000000
Cu	-0.768706000000	0.812733000000	-0.626928000000
C	-3.319568000000	3.469536000000	0.052724000000
H	-4.407426000000	3.567135000000	0.169859000000
H	-2.833140000000	3.702444000000	1.006751000000
H	-2.974472000000	4.201739000000	-0.685925000000
C	0.584192000000	-0.691147000000	2.517956000000
H	1.505672000000	-0.099129000000	2.573910000000
H	0.258491000000	-0.952192000000	3.533832000000
H	0.822356000000	-1.604527000000	1.961666000000
C	-0.628690000000	-2.785182000000	-0.807817000000
H	-0.314122000000	-2.759206000000	0.241776000000
H	-1.224388000000	-3.689940000000	-0.988810000000
H	0.281138000000	-2.822474000000	-1.416828000000
C	-2.027029000000	-1.674022000000	-2.978732000000
H	-2.547651000000	-2.637881000000	-3.051154000000
H	-2.651977000000	-0.884792000000	-3.411509000000
H	-1.103124000000	-1.714411000000	-3.568623000000
C	-0.946975000000	1.647141000000	2.850125000000
H	-1.786380000000	2.285688000000	2.550336000000
H	-1.138585000000	1.254874000000	3.858256000000
H	-0.045645000000	2.270445000000	2.875967000000
C	-3.870595000000	1.684170000000	-2.050427000000
H	-3.939142000000	0.646429000000	-2.395626000000
H	-4.886045000000	2.070063000000	-1.888251000000
H	-3.381079000000	2.266335000000	-2.839903000000
H	0.534310000000	1.734945000000	-1.210425000000
B	0.797959000000	1.239353000000	-2.360298000000
H	-0.181895000000	1.041001000000	-3.052429000000
H	1.430165000000	0.186255000000	-2.245664000000
H	1.497142000000	2.116695000000	-2.807793000000
O	2.728301000000	0.444261000000	-0.121343000000
H	2.159694000000	0.557240000000	-0.935816000000
C	3.195431000000	-0.777098000000	-0.057484000000
F	4.040426000000	-1.121658000000	-1.097485000000
F	3.893079000000	-0.955393000000	1.110489000000
F	2.195639000000	-1.759372000000	-0.068672000000

2_ $TS1_{CuH}$_CF_3OH

E_{el} = -3539.78748242 Ha

E_{ZPVE} = -3539.360552 Ha

H = -3539.327886 Ha

G = -3539.420265 Ha

C	8.381987000000	-3.952687000000	-2.284580000000
C	7.074560000000	-4.598922000000	-2.826750000000
C	8.299794000000	-3.623227000000	-0.767732000000
C	8.828562000000	-2.726732000000	-3.130879000000
H	6.738518000000	-5.353018000000	-2.096725000000
H	7.317612000000	-5.154642000000	-3.748226000000
H	9.174516000000	-3.006335000000	-0.503167000000
H	8.408925000000	-4.562393000000	-0.199781000000
H	8.670581000000	-2.967620000000	-4.196095000000
H	9.916223000000	-2.589911000000	-3.006639000000
C	9.487239000000	-5.016827000000	-2.446508000000
H	10.423012000000	-4.679010000000	-1.981223000000
H	9.190266000000	-5.960633000000	-1.970066000000

H	9.685181000000	-5.216900000000	-3.508495000000
P	8.021699000000	-1.071919000000	-2.811024000000
P	6.764036000000	-2.768007000000	-0.115368000000
P	5.611054000000	-3.497469000000	-3.218679000000
Cu	5.949659000000	-1.617748000000	-1.935617000000
C	7.399353000000	-1.996687000000	1.422712000000
H	7.944329000000	-2.725218000000	2.037284000000
H	8.053905000000	-1.147414000000	1.195532000000
H	6.532510000000	-1.621822000000	1.978846000000
C	8.358597000000	-0.214874000000	-4.405674000000
H	8.094852000000	0.844464000000	-4.301137000000
H	9.416662000000	-0.292369000000	-4.689491000000
H	7.739701000000	-0.638806000000	-5.204865000000
C	5.686465000000	-3.464906000000	-5.062004000000
H	6.602515000000	-2.962806000000	-5.397156000000
H	5.669435000000	-4.481318000000	-5.477850000000
H	4.829767000000	-2.906376000000	-5.455498000000
C	4.192941000000	-4.632120000000	-2.953348000000
H	3.306004000000	-4.202459000000	-3.432843000000
H	4.384164000000	-5.627126000000	-3.376166000000
H	3.967053000000	-4.706923000000	-1.884291000000
C	9.267098000000	-0.239412000000	-1.739390000000
H	9.298766000000	-0.706520000000	-0.748273000000
H	10.269120000000	-0.277493000000	-2.187333000000
H	8.971938000000	0.807439000000	-1.601341000000
C	5.839131000000	-4.192512000000	0.583430000000
H	5.518280000000	-4.881379000000	-0.205731000000
H	6.467176000000	-4.736003000000	1.301786000000
H	4.944942000000	-3.804551000000	1.077714000000
H	4.902500000000	-0.284198000000	-2.315035000000
B	6.027905000000	1.371292000000	-0.655054000000
H	6.552096000000	0.740133000000	0.205630000000
H	5.015807000000	1.943462000000	-0.450199000000
H	6.594072000000	1.515980000000	-1.696153000000
H	4.529064000000	-0.448066000000	-1.616154000000
O	3.454179000000	-0.300188000000	-0.145656000000
C	3.279549000000	-1.397229000000	0.357354000000
F	2.006174000000	-1.740828000000	0.839458000000
F	4.140032000000	-1.744049000000	1.486915000000
F	3.576260000000	-2.558012000000	-0.542830000000

2_ INT$_{CuH}$_CF$_3$OH

E_{el} = -3539.82685108 Ha

E_{ZPVE} = -3539.395282 Ha

H = -3539.363795 Ha

G = -3539.453457 Ha

C	8.604893000000	-3.619030000000	-2.840976000000
C	7.546393000000	-4.511227000000	-3.546649000000
C	8.397481000000	-3.567880000000	-1.299955000000
C	8.710347000000	-2.205934000000	-3.484576000000
H	7.390515000000	-5.411000000000	-2.927413000000
H	7.963755000000	-4.868191000000	-4.503948000000
H	9.102649000000	-2.825875000000	-0.890178000000
H	8.699118000000	-4.540812000000	-0.876432000000
H	8.661183000000	-2.325309000000	-4.580005000000
H	9.711021000000	-1.796271000000	-3.267832000000
C	9.967665000000	-4.305308000000	-3.072374000000
H	10.759414000000	-3.796519000000	-2.506596000000
H	9.936599000000	-5.354334000000	-2.748384000000
H	10.239343000000	-4.282926000000	-4.136524000000
P	7.463733000000	-0.899126000000	-2.989863000000
P	6.702469000000	-3.154863000000	-0.605518000000
P	5.859304000000	-3.804048000000	-3.916423000000
Cu	5.629628000000	-2.141724000000	-2.361495000000
C	7.151113000000	-2.304717000000	0.956868000000
H	8.034633000000	-2.767154000000	1.416627000000
H	7.327909000000	-1.236716000000	0.778779000000
H	6.311338000000	-2.366574000000	1.657002000000
C	7.516592000000	0.230986000000	-4.439175000000
H	6.973996000000	1.146467000000	-4.174259000000
H	8.547939000000	0.492439000000	-4.710245000000
H	7.017638000000	-0.221816000000	-5.303730000000
C	6.007707000000	-3.374425000000	-5.703292000000
H	6.709583000000	-2.543559000000	-5.840420000000
H	6.354549000000	-4.232977000000	-6.293925000000
H	5.030974000000	-3.053181000000	-6.083091000000
C	4.877365000000	-5.356213000000	-4.041932000000
H	5.381033000000	-6.093012000000	-4.682020000000
H	4.726379000000	-5.787924000000	-3.046364000000
H	3.891164000000	-5.134830000000	-4.464971000000
C	8.435359000000	0.076657000000	-1.776325000000
H	8.679603000000	-0.530286000000	-0.896878000000
H	9.366711000000	0.437407000000	-2.233465000000
H	7.828573000000	0.919778000000	-1.427050000000
C	6.122532000000	-4.776406000000	0.041451000000
H	5.947631000000	-5.485807000000	-0.776190000000
H	6.844362000000	-5.211948000000	0.744995000000
H	5.171470000000	-4.603002000000	0.560643000000
H	3.939056000000	-1.562140000000	-2.569175000000
B	5.344381000000	0.966553000000	-0.231220000000
H	5.529723000000	1.096525000000	-1.431184000000
H	6.389030000000	0.946322000000	0.394013000000
H	4.548264000000	1.757357000000	0.209893000000
H	4.108611000000	-1.235454000000	-1.873242000000
O	4.720185000000	-0.486232000000	-0.123153000000
C	4.024294000000	-0.881402000000	0.870264000000
F	4.595720000000	-0.673037000000	2.131720000000
F	3.821777000000	-2.283632000000	0.805993000000
F	2.740449000000	-0.348335000000	0.968041000000

2_TS2$_{CuH}$_CF$_3$OH

E_{el} = -3539.82588120 Ha

E_{ZPVE} = -3539.395107 Ha

H = -3539.363972 Ha

G = -3539.452039 Ha

C	8.589512000000	-3.615758000000	-2.854434000000
C	7.567776000000	-4.536072000000	-3.579633000000
C	8.387381000000	-3.615254000000	-1.310243000000
C	8.626920000000	-2.185576000000	-3.466660000000
H	7.454538000000	-5.457427000000	-2.984106000000
H	8.001560000000	-4.850145000000	-4.544488000000
H	9.030127000000	-2.829166000000	-0.880700000000
H	8.768659000000	-4.570466000000	-0.911654000000
H	8.557945000000	-2.285915000000	-4.563352000000
H	9.615415000000	-1.740946000000	-3.263155000000
C	9.980516000000	-4.233682000000	-3.108796000000
H	10.750717000000	-3.704984000000	-2.531495000000
H	9.997766000000	-5.291489000000	-2.813151000000
H	10.246777000000	-4.170660000000	-4.172655000000
P	7.339499000000	-0.937570000000	-2.923570000000
P	6.657360000000	-3.367742000000	-0.629020000000
P	5.844180000000	-3.902870000000	-3.945482000000
Cu	5.573428000000	-2.271716000000	-2.333592000000
C	6.977157000000	-2.508738000000	0.958617000000
H	7.789789000000	-2.987498000000	1.520707000000
H	7.211212000000	-1.452255000000	0.780288000000
H	6.059744000000	-2.523334000000	1.558829000000
C	7.324837000000	0.217206000000	-4.353777000000
H	6.748934000000	1.104771000000	-4.065596000000
H	8.340644000000	0.524506000000	-4.635501000000
H	6.831398000000	-0.241613000000	-5.217982000000
C	5.969762000000	-3.522756000000	-5.747538000000
H	6.657270000000	-2.685412000000	-5.915305000000
H	6.327597000000	-4.392129000000	-6.315530000000
H	4.985029000000	-3.230553000000	-6.130097000000
C	4.928686000000	-5.499717000000	-4.027398000000
H	5.465368000000	-6.237824000000	-4.638605000000
H	4.783926000000	-5.902084000000	-3.018545000000
H	3.938210000000	-5.331086000000	-4.465037000000
C	8.298469000000	0.056835000000	-1.713417000000
H	8.560352000000	-0.543642000000	-0.834924000000
H	9.218549000000	0.439781000000	-2.175335000000

H	7.672999000000	0.885435000000	-1.363860000000
C	6.241880000000	-5.057514000000	-0.023759000000
H	6.177040000000	-5.769961000000	-0.854704000000
H	6.992393000000	-5.416543000000	0.693127000000
H	5.265374000000	-5.020768000000	0.472122000000
H	3.710623000000	-1.772357000000	-2.986281000000
B	5.076069000000	0.692970000000	-0.413785000000
H	5.337351000000	0.921224000000	-1.583292000000
H	6.063427000000	0.720063000000	0.296690000000
H	4.175057000000	1.373672000000	0.004411000000
H	3.692919000000	-1.425563000000	-2.305916000000
O	4.584679000000	-0.824979000000	-0.432612000000
C	3.738585000000	-1.263837000000	0.420516000000
F	4.058721000000	-1.028819000000	1.761726000000
F	3.618945000000	-2.670132000000	0.331997000000
F	2.432036000000	-0.798693000000	0.270034000000

2_DHB_IIa_MeOH

E_{el} = -3242.21759945 Ha

E_{ZPVE} = -3241.760816 Ha

H = -3241.730075 Ha

G = -3241.817991 Ha

C	2.435957000000	0.944997000000	1.327212000000
C	2.245023000000	2.004182000000	0.204805000000
C	3.010761000000	-0.395402000000	0.785832000000
C	1.152426000000	0.742429000000	2.175354000000
H	3.143385000000	1.978995000000	-0.435861000000
H	2.233160000000	3.005507000000	0.669380000000
H	2.991841000000	-1.129960000000	1.608383000000
H	4.073965000000	-0.245269000000	0.531842000000
H	0.773497000000	1.741133000000	2.452162000000
H	1.433629000000	0.252294000000	3.123595000000
C	3.505004000000	1.517318000000	2.282008000000
H	3.771660000000	0.780502000000	3.051646000000
H	4.417944000000	1.781957000000	1.731075000000
H	3.135385000000	2.420351000000	2.786507000000
P	-0.294863000000	-0.207929000000	1.450024000000
P	2.157975000000	-1.165164000000	-0.686940000000
P	0.761970000000	1.917404000000	-0.942545000000
Cu	0.034772000000	-0.285267000000	-0.852140000000
C	2.469556000000	-2.958816000000	-0.431123000000
H	3.530506000000	-3.165213000000	-0.237363000000
H	1.863975000000	-3.342534000000	0.397318000000
H	2.151149000000	-3.490495000000	-1.335886000000
C	-1.662688000000	0.489659000000	2.469485000000
H	-2.534676000000	-0.158279000000	2.323812000000
H	-1.391916000000	0.510355000000	3.533940000000
H	-1.922957000000	1.504612000000	2.146508000000
C	-0.343971000000	3.204665000000	-0.213239000000
H	-0.738380000000	2.874306000000	0.754108000000
H	0.179793000000	4.160779000000	-0.076694000000
H	-1.197866000000	3.359070000000	-0.883735000000
C	1.434601000000	2.899999000000	-2.354791000000
H	1.917920000000	3.823794000000	-2.007646000000
H	2.159770000000	2.306736000000	-2.922707000000
H	0.614350000000	3.161941000000	-3.032796000000
C	-0.131905000000	-1.845372000000	2.273897000000
H	0.754977000000	-2.378302000000	1.913531000000
H	-0.067502000000	-1.739502000000	3.365453000000
H	-1.017946000000	-2.438430000000	2.016568000000
C	3.362735000000	-0.846107000000	-2.046452000000
H	3.464676000000	0.228297000000	-2.238648000000
H	4.353531000000	-1.259568000000	-1.813635000000
H	2.981800000000	-1.317310000000	-2.960670000000
H	-0.715778000000	-2.511472000000	-0.925315000000
B	-1.029966000000	-2.046894000000	-2.017915000000
H	-0.271749000000	-2.447147000000	-2.876826000000
H	-1.056899000000	-0.761921000000	-2.060732000000
H	-2.404184000000	-2.048070000000	-0.215046000000
C	-3.766177000000	-0.655006000000	-0.168900000000
H	-3.159772000000	0.215294000000	-0.469750000000
O	-2.970217000000	-1.652809000000	0.469766000000
H	-2.193818000000	-2.305700000000	-2.260720000000
H	-4.269581000000	-1.048860000000	-1.060487000000
H	-4.523613000000	-0.330403000000	0.552208000000

2_TS1$_{BH}^{A}$_MeOH

E_{el} = -3242.19868518 Ha

E_{ZPVE} = -3241.742695 Ha

H = -3241.712785 Ha

G = -3241.798167 Ha

Cu	-0.529149000000	-0.513982000000	0.112912000000
P	-0.120366000000	1.780407000000	0.703584000000
P	0.455681000000	-1.304131000000	2.036434000000
P	1.378122000000	-0.571757000000	-1.179490000000
C	2.570361000000	0.587097000000	1.223835000000
C	1.561085000000	1.724836000000	1.544808000000
C	2.745091000000	0.353911000000	-0.302931000000
C	2.235793000000	-0.724942000000	1.992709000000
C	3.941665000000	1.060225000000	1.750111000000
H	2.841627000000	-1.540468000000	1.564527000000
H	2.571262000000	-0.611524000000	3.037570000000
H	1.366849000000	1.700866000000	2.631178000000
H	2.050243000000	2.694237000000	1.346596000000
H	2.851639000000	1.339775000000	-0.786580000000
H	3.697080000000	-0.177340000000	-0.473483000000
H	3.876608000000	1.350673000000	2.807740000000
H	4.688327000000	0.259532000000	1.660492000000
H	4.299456000000	1.926750000000	1.177599000000
H	-1.040491000000	-1.719844000000	-2.286894000000
H	-1.142928000000	-3.630457000000	-1.663420000000
B	-1.555795000000	-2.498818000000	-1.493150000000
H	-1.286888000000	-2.203041000000	-0.300633000000
H	-2.779076000000	-2.457388000000	-1.607301000000
C	2.084364000000	-2.259380000000	-1.368076000000
H	3.025518000000	-2.247517000000	-1.934315000000
H	2.264084000000	-2.711026000000	-0.385627000000
H	1.340118000000	-2.875736000000	-1.888719000000
C	1.552441000000	0.032417000000	-2.909301000000
H	2.590041000000	-0.033386000000	-3.262867000000
H	0.914097000000	-0.593979000000	-3.544417000000
H	1.204454000000	1.067995000000	-3.000747000000
C	0.218309000000	3.031371000000	-0.620209000000
H	0.654946000000	3.951049000000	-0.206403000000
H	0.907509000000	2.619209000000	-1.366788000000
H	-0.716737000000	3.285554000000	-1.133382000000
C	-0.993366000000	2.880231000000	1.907744000000
H	-1.941574000000	3.209720000000	1.465827000000
H	-1.230240000000	2.323903000000	2.822214000000
H	-0.393921000000	3.764256000000	2.167114000000
C	0.666207000000	-3.118101000000	2.249361000000
H	0.928364000000	-3.575032000000	1.287884000000
H	1.427968000000	-3.364306000000	3.001040000000
H	-0.294349000000	-3.548897000000	2.555367000000
C	-0.024299000000	-0.824532000000	3.754778000000
H	-0.034414000000	0.267615000000	3.856593000000
H	-1.035581000000	-1.191465000000	3.963766000000
H	0.668754000000	-1.242574000000	4.497837000000
H	-2.884882000000	-0.940450000000	-0.785039000000
O	-2.826770000000	-0.031741000000	-0.428225000000
C	-2.941988000000	0.880115000000	-1.519162000000
H	-3.924712000000	0.809086000000	-2.002315000000
H	-2.158984000000	0.707785000000	-2.274035000000
H	-2.828272000000	1.889790000000	-1.107930000000

2_INT$_{BH}^{A}$_MeOH

E_{el} = -3242.20265685 Ha

E_{ZPVE} = -3241.745899 Ha

H = -3241.715477 Ha

G = -3241.801790 Ha

Cu	-0.572090000000	-0.150083000000	0.263253000000

P	0.010952000000	1.992688000000	0.848943000000
P	0.362555000000	-1.199067000000	2.055780000000
P	1.223493000000	-0.513936000000	-1.147503000000
C	2.590511000000	0.577325000000	1.219316000000
C	1.716493000000	1.804537000000	1.597103000000
C	2.662714000000	0.357326000000	-0.317913000000
C	2.172009000000	-0.705860000000	1.994549000000
C	4.023920000000	0.911708000000	1.683739000000
H	2.726732000000	-1.557124000000	1.567262000000
H	2.518283000000	-0.609568000000	3.037609000000
H	1.586496000000	1.803578000000	2.693030000000
H	2.278469000000	2.724290000000	1.358384000000
H	2.788494000000	1.344186000000	-0.794796000000
H	3.578076000000	-0.212989000000	-0.550059000000
H	4.035798000000	1.195168000000	2.745183000000
H	4.686175000000	0.045380000000	1.553324000000
H	4.436039000000	1.746642000000	1.100962000000
H	-0.904414000000	-2.024120000000	-2.509650000000
H	-1.245753000000	-4.000177000000	-2.285125000000
B	-1.452135000000	-2.892296000000	-1.826250000000
H	-1.023513000000	-2.828479000000	-0.668740000000
H	-2.671937000000	-2.679928000000	-1.822335000000
C	1.909771000000	-2.207353000000	-1.353475000000
H	2.836316000000	-2.180017000000	-1.942902000000
H	2.122442000000	-2.660696000000	-0.378419000000
H	1.154445000000	-2.823884000000	-1.856357000000
C	1.378675000000	0.107099000000	-2.873235000000
H	2.413589000000	0.041633000000	-3.234808000000
H	0.734068000000	-0.514638000000	-3.506401000000
H	1.033137000000	1.145031000000	-2.948042000000
C	0.329456000000	3.206271000000	-0.505768000000
H	0.816881000000	4.116577000000	-0.130493000000
H	0.965809000000	2.755742000000	-1.276568000000
H	-0.622556000000	3.480192000000	-0.976642000000
C	-0.735428000000	3.128412000000	2.098922000000
H	-1.676915000000	3.532363000000	1.709689000000
H	-0.961023000000	2.581412000000	3.021571000000
H	-0.059688000000	3.962865000000	2.331537000000
C	0.489863000000	-3.023733000000	2.227713000000
H	0.745371000000	-3.476004000000	1.263091000000
H	1.229185000000	-3.311619000000	2.987100000000
H	-0.492441000000	-3.419315000000	2.510448000000
C	-0.073002000000	-0.743459000000	3.791269000000
H	-0.050481000000	0.345007000000	3.922970000000
H	-1.091130000000	-1.086758000000	4.007550000000
H	0.617811000000	-1.202341000000	4.511698000000
H	-2.408982000000	-1.412532000000	-0.822350000000
O	-2.461502000000	-0.487725000000	-0.469640000000
C	-2.858425000000	0.354737000000	-1.558975000000
H	-3.785358000000	-0.019162000000	-2.008323000000
H	-2.078469000000	0.392701000000	-2.332978000000
H	-3.029420000000	1.357418000000	-1.153104000000

2_TS$_{BH}^{B+C}$_MeOH

E_{el} = -3242.14492324 Ha

E_{ZPVE} = -3241.694952 Ha

H = -3241.663866 Ha

G = -3241.752770 Ha

Cu	-0.478649000000	-0.340367000000	0.018665000000
P	-0.070921000000	1.873851000000	0.536510000000
P	0.320246000000	-1.123127000000	2.003475000000
P	1.590036000000	-0.568927000000	-1.065009000000
C	2.531388000000	0.750451000000	1.397914000000
C	1.539747000000	1.942386000000	1.491564000000
C	2.868042000000	0.374238000000	-0.070379000000
C	2.066092000000	-0.477436000000	2.229790000000
C	3.849585000000	1.234020000000	2.037822000000
H	2.755536000000	-1.310061000000	2.010038000000
H	2.198474000000	-0.247031000000	3.301239000000
H	1.278681000000	2.077755000000	2.555074000000
H	2.067516000000	2.863523000000	1.188264000000
H	3.085006000000	1.308065000000	-0.616468000000
H	3.805395000000	-0.208758000000	-0.078793000000
H	3.673920000000	1.614527000000	3.053284000000
H	4.576473000000	0.412880000000	2.100736000000
H	4.296902000000	2.041561000000	1.442411000000
H	-0.405723000000	-2.023635000000	-2.780096000000
H	-0.561159000000	-4.057424000000	-2.576984000000
B	-1.088536000000	-2.993624000000	-2.700491000000
H	-1.302412000000	-3.491936000000	-0.555795000000
H	-2.230443000000	-2.946163000000	-3.015055000000
C	2.277090000000	-2.281205000000	-1.012265000000
H	3.320404000000	-2.309307000000	-1.355993000000
H	2.227029000000	-2.687610000000	0.004464000000
H	1.664335000000	-2.923107000000	-1.657606000000
C	2.113912000000	-0.108016000000	-2.775936000000
H	3.198810000000	-0.217337000000	-2.913090000000
H	1.594258000000	-0.764633000000	-3.484037000000
H	1.824278000000	0.923955000000	-3.005580000000
C	0.303432000000	2.966316000000	-0.905222000000
H	0.699411000000	3.940212000000	-0.585317000000
H	1.027376000000	2.491393000000	-1.576773000000
H	-0.620969000000	3.122555000000	-1.474117000000
C	-1.064341000000	3.072490000000	1.532190000000
H	-1.983434000000	3.309122000000	0.983339000000
H	-1.353758000000	2.630567000000	2.492554000000
H	-0.509138000000	4.002371000000	1.718174000000
C	0.547850000000	-2.870760000000	2.553612000000
H	1.062888000000	-3.454024000000	1.781529000000
H	1.115437000000	-2.931420000000	3.492513000000
H	-0.440043000000	-3.322044000000	2.703077000000
C	-0.504920000000	-0.458757000000	3.516123000000
H	-0.601435000000	0.631247000000	3.454918000000
H	-1.515713000000	-0.877786000000	3.580425000000
H	0.050184000000	-0.717335000000	4.428418000000
H	-1.639275000000	-2.804356000000	-0.644810000000
O	-2.027481000000	-0.929582000000	-0.957120000000
C	-2.444948000000	-0.044902000000	-1.951728000000
H	-3.261569000000	-0.484519000000	-2.554400000000
H	-1.630909000000	0.221910000000	-2.667760000000
H	-2.828417000000	0.914843000000	-1.541618000000

2_Product_MeOH

E_{el} = -3242.21548326 Ha

E_{ZPVE} = -3241.762462 Ha

H = -3241.732186 Ha

G = -3241.818040 Ha

Cu	-0.855413000000	-0.282696000000	-0.373148000000
P	-0.567868000000	1.910199000000	0.198370000000
P	-0.146100000000	-1.137226000000	1.611818000000
P	1.202154000000	-0.482206000000	-1.428101000000
C	2.044971000000	0.787167000000	1.079738000000
C	1.020642000000	1.949791000000	1.193287000000
C	2.430430000000	0.479815000000	-0.393713000000
C	1.593239000000	-0.484772000000	1.856111000000
C	3.331786000000	1.280504000000	1.774264000000
H	2.286903000000	-1.301404000000	1.594857000000
H	1.729464000000	-0.303061000000	2.936018000000
H	0.728212000000	2.036050000000	2.253716000000
H	1.534088000000	2.894707000000	0.942953000000
H	2.623772000000	1.440054000000	-0.901121000000
H	3.389406000000	-0.065968000000	-0.399724000000
H	3.118914000000	1.620426000000	2.797011000000
H	4.075612000000	0.474318000000	1.829993000000
H	3.776887000000	2.117856000000	1.219883000000
H	-0.808863000000	-1.997128000000	-2.966041000000
H	-1.186769000000	-3.012421000000	-1.255238000000
B	-1.681982000000	-2.351874000000	-2.160560000000
H	-3.294609000000	-2.602887000000	0.998098000000
H	-2.570331000000	-2.955827000000	-2.741171000000
C	1.958591000000	-2.159067000000	-1.428334000000
H	2.967304000000	-2.138171000000	-1.863088000000

H	2.020507000000	-2.556207000000	-0.408431000000
H	1.310070000000	-2.822951000000	-2.011363000000
C	1.662641000000	0.055578000000	-3.129103000000
H	2.745184000000	-0.022591000000	-3.298966000000
H	1.135256000000	-0.598455000000	-3.834097000000
H	1.340762000000	1.085809000000	-3.320549000000
C	-0.178992000000	3.066383000000	-1.187437000000
H	0.178479000000	4.038545000000	-0.821051000000
H	0.581697000000	2.632950000000	-1.846816000000
H	-1.085917000000	3.219219000000	-1.785390000000
C	-1.591040000000	3.042719000000	1.239525000000
H	-2.494223000000	3.325378000000	0.686652000000
H	-1.905681000000	2.535247000000	2.158802000000
H	-1.036598000000	3.953672000000	1.504300000000
C	0.077827000000	-2.917466000000	2.014029000000
H	0.600539000000	-3.424693000000	1.195710000000
H	0.628633000000	-3.060770000000	2.953341000000
H	-0.912876000000	-3.379983000000	2.098093000000
C	-0.973467000000	-0.564854000000	3.158762000000
H	-1.089214000000	0.525727000000	3.150389000000
H	-1.976156000000	-1.006187000000	3.205594000000
H	-0.411256000000	-0.858543000000	4.055742000000
H	-3.058437000000	-2.125689000000	0.463844000000
O	-2.269180000000	-1.091000000000	-1.516128000000
C	-2.860432000000	-0.219372000000	-2.462189000000
H	-3.616035000000	-0.762788000000	-3.048478000000
H	-2.102266000000	0.175356000000	-3.164909000000
H	-3.339480000000	0.618994000000	-1.937491000000

2_DHB_IIab_MeOH

E_{el} = -3242.21620909 Ha

E_{ZPVE} = -3241.759123 Ha

H = -3241.728334 Ha

G = -3241.816235 Ha

C	1.825161000000	-1.737243000000	-0.414783000000
C	0.347044000000	-2.156846000000	-0.642441000000
C	2.148540000000	-1.479296000000	1.083438000000
C	2.246532000000	-0.557794000000	-1.332551000000
H	0.086566000000	-2.905800000000	0.124369000000
H	0.275704000000	-2.676342000000	-1.613659000000
H	3.188256000000	-1.115165000000	1.147309000000
H	2.129406000000	-2.445404000000	1.616819000000
H	1.884547000000	-0.785620000000	-2.349723000000
H	3.348468000000	-0.539837000000	-1.398773000000
C	2.689807000000	-2.943555000000	-0.839241000000
H	3.750337000000	-2.761637000000	-0.617993000000
H	2.379083000000	-3.850720000000	-0.303530000000
H	2.591867000000	-3.133275000000	-1.916724000000
P	1.689813000000	1.192686000000	-0.944561000000
P	1.078546000000	-0.269563000000	2.023547000000
P	-0.985196000000	-0.836446000000	-0.602289000000
Cu	-0.117696000000	0.998701000000	0.522788000000
C	2.237004000000	0.280353000000	3.347122000000
H	2.699761000000	-0.573479000000	3.860262000000
H	3.024415000000	0.922952000000	2.937875000000
H	1.666874000000	0.871195000000	4.074021000000
C	1.816967000000	1.918601000000	-2.639864000000
H	1.757246000000	3.010560000000	-2.568351000000
H	2.765974000000	1.644568000000	-3.121127000000
H	0.985246000000	1.578502000000	-3.267019000000
C	-1.379196000000	-0.608023000000	-2.385347000000
H	-0.538947000000	-0.141300000000	-2.912700000000
H	-1.625709000000	-1.559820000000	-2.875091000000
H	-2.240849000000	0.070486000000	-2.437336000000
C	-2.434755000000	-1.850971000000	-0.098191000000
H	-3.334239000000	-1.272949000000	-0.332451000000
H	-2.463648000000	-2.806974000000	-0.638556000000
H	-2.425659000000	-2.040913000000	0.981238000000
C	3.233869000000	1.906259000000	-0.224449000000
H	3.450068000000	1.452306000000	0.748953000000
H	4.096971000000	1.754554000000	-0.887129000000
H	3.090027000000	2.980907000000	-0.063688000000
C	-0.003088000000	-1.369524000000	3.027545000000
H	-0.662114000000	-1.958459000000	2.380661000000
H	0.581668000000	-2.050135000000	3.660649000000
H	-0.640903000000	-0.734682000000	3.654749000000
H	-0.866031000000	2.466560000000	0.921769000000
B	-1.681895000000	2.138968000000	1.863094000000
H	-1.185214000000	2.505904000000	2.906832000000
H	-1.972973000000	0.949158000000	1.901084000000
H	-2.668131000000	2.789092000000	1.562523000000
H	-2.923327000000	1.758852000000	-0.060302000000
O	-3.544965000000	1.290368000000	-0.640577000000
C	-4.764038000000	1.173878000000	0.095568000000
H	-4.601291000000	0.680944000000	1.064738000000
H	-5.450696000000	0.570916000000	-0.507094000000
H	-5.222363000000	2.154605000000	0.278197000000

2_TS$_{CuH}$_MeOH

E_{el} = -3242.15425796 Ha

E_{ZPVE} = -3241.700601 Ha

H = -3241.670359 Ha

G = -3241.756088 Ha

C	8.408258000000	-4.029588000000	-2.249687000000
C	7.106527000000	-4.652988000000	-2.821110000000
C	8.266473000000	-3.619009000000	-0.759587000000
C	8.932193000000	-2.861309000000	-3.127633000000
H	6.747268000000	-5.406227000000	-2.099398000000
H	7.357454000000	-5.208193000000	-3.741680000000
H	9.170913000000	-3.052097000000	-0.480363000000
H	8.274732000000	-4.531985000000	-0.139343000000
H	8.872913000000	-3.175566000000	-4.183247000000
H	10.003630000000	-2.707393000000	-2.911399000000
C	9.482545000000	-5.134901000000	-2.302627000000
H	10.411068000000	-4.798395000000	-1.821592000000
H	9.137416000000	-6.040104000000	-1.784608000000
H	9.714067000000	-5.402710000000	-3.342718000000
P	8.068731000000	-1.207812000000	-2.979290000000
P	6.788688000000	-2.590077000000	-0.226558000000
P	5.668505000000	-3.515478000000	-3.208403000000
Cu	5.927259000000	-1.482423000000	-2.093427000000
C	7.481190000000	-1.854131000000	1.317355000000
H	8.011432000000	-2.608054000000	1.915348000000
H	8.160392000000	-1.026746000000	1.082587000000
H	6.655181000000	-1.439276000000	1.907242000000
C	8.519919000000	-0.465546000000	-4.607796000000
H	8.270522000000	0.601485000000	-4.589636000000
H	9.592254000000	-0.579181000000	-4.818301000000
H	7.944742000000	-0.927857000000	-5.418004000000
C	5.772006000000	-3.414046000000	-5.049557000000
H	6.650676000000	-2.835500000000	-5.356542000000
H	5.822873000000	-4.410521000000	-5.509570000000
H	4.884856000000	-2.890000000000	-5.423739000000
C	4.269720000000	-4.715531000000	-3.079226000000
H	3.369702000000	-4.251897000000	-3.499667000000
H	4.480380000000	-5.645828000000	-3.624702000000
H	4.060423000000	-4.955668000000	-2.030326000000
C	9.250424000000	-0.276078000000	-1.909520000000
H	9.299179000000	-0.722309000000	-0.909408000000
H	10.260541000000	-0.261188000000	-2.341334000000
H	8.888301000000	0.752520000000	-1.793829000000
C	5.735053000000	-3.892373000000	0.557008000000
H	5.328689000000	-4.578568000000	-0.194363000000
H	6.302054000000	-4.473011000000	1.297513000000
H	4.889655000000	-3.406060000000	1.057974000000
H	4.892125000000	-0.293030000000	-2.227647000000
B	5.686098000000	1.136974000000	0.156086000000
H	6.685868000000	0.857013000000	-0.428761000000
H	5.435603000000	0.564624000000	1.169443000000
H	5.085699000000	2.113374000000	-0.144047000000
H	3.829929000000	-0.117615000000	-1.145543000000
O	3.259363000000	0.016287000000	-0.354763000000

C	3.107800000000	-1.239812000000	0.284873000000
H	3.231055000000	-2.076998000000	-0.421776000000
H	2.103170000000	-1.293981000000	0.718267000000
H	3.841126000000	-1.366740000000	1.101071000000

2_INT$_{CuH}$_MeOH

E_{el} = -3242.19765916 Ha

E_{ZPVE} = -3241.741288 Ha

H = -3241.711606 Ha

G = -3241.796767 Ha

C	1.809719000000	-1.758966000000	-0.431111000000
C	0.644051000000	-2.533324000000	-1.101468000000
C	1.580888000000	-1.556485000000	1.092331000000
C	2.118723000000	-0.424766000000	-1.164687000000
H	0.386433000000	-3.392094000000	-0.458674000000
H	1.003504000000	-2.959430000000	-2.054199000000
H	2.373945000000	-0.887792000000	1.466380000000
H	1.731015000000	-2.524229000000	1.601643000000
H	2.078208000000	-0.614140000000	-2.250645000000
H	3.159989000000	-0.134058000000	-0.944229000000
C	3.065455000000	-2.642866000000	-0.571364000000
H	3.912791000000	-2.202515000000	-0.028311000000
H	2.883463000000	-3.647705000000	-0.165954000000
H	3.352531000000	-2.745868000000	-1.626782000000
P	1.034771000000	1.060508000000	-0.796289000000
P	-0.056153000000	-0.855921000000	1.686496000000
P	-0.935122000000	-1.592514000000	-1.447109000000
Cu	-1.046257000000	0.285985000000	-0.073409000000
C	0.473638000000	-0.153007000000	3.306069000000
H	1.120683000000	-0.849282000000	3.857235000000
H	0.992924000000	0.799932000000	3.152217000000
H	-0.417237000000	0.061645000000	3.908396000000
C	1.320824000000	2.064915000000	-2.315134000000
H	0.926067000000	3.072131000000	-2.135940000000
H	2.389843000000	2.136582000000	-2.557948000000
H	0.782494000000	1.639745000000	-3.169909000000
C	-0.767513000000	-1.260487000000	-3.256289000000
H	0.049278000000	-0.552822000000	-3.438835000000
H	-0.572132000000	-2.182090000000	-3.821770000000
H	-1.693669000000	-0.802789000000	-3.622523000000
C	-2.129446000000	-2.998711000000	-1.524942000000
H	-3.081164000000	-2.635424000000	-1.929094000000
H	-1.756033000000	-3.810245000000	-2.164546000000
H	-2.322223000000	-3.394308000000	-0.521062000000
C	2.122914000000	1.985331000000	0.368969000000
H	2.228951000000	1.446582000000	1.317792000000
H	3.118436000000	2.142081000000	-0.068768000000
H	1.653633000000	2.950038000000	0.593616000000
C	-0.891244000000	-2.388401000000	2.296065000000
H	-1.155698000000	-3.044418000000	1.458454000000
H	-0.254323000000	-2.945312000000	2.996916000000
H	-1.820827000000	-2.107376000000	2.804753000000
H	-2.421161000000	1.094030000000	-0.076019000000
B	-0.824429000000	3.620936000000	1.594208000000
H	-0.243042000000	2.720606000000	2.179345000000
H	-1.003589000000	4.589098000000	2.296498000000
H	-0.324655000000	3.884429000000	0.521322000000
H	-2.205460000000	2.260529000000	0.619923000000
O	-2.267252000000	3.074749000000	1.247216000000
C	-3.036848000000	2.664649000000	2.389686000000
H	-2.494601000000	1.890083000000	2.947490000000
H	-3.998598000000	2.278128000000	2.041791000000
H	-3.176635000000	3.546225000000	3.018438000000

2_INT1$_{CuH}$_MeOH

E_{el} = -3242.19375886 Ha

E_{ZPVE} = -3241.739435 Ha

H = -3241.709964 Ha

G = -3241.794151 Ha

C	8.602408000000	-3.629398000000	-2.848637000000
C	7.614735000000	-4.560249000000	-3.605266000000
C	8.354518000000	-3.647922000000	-1.312603000000
C	8.626776000000	-2.193457000000	-3.445868000000
H	7.501751000000	-5.487625000000	-3.018170000000
H	8.075245000000	-4.859162000000	-4.562563000000
H	9.000587000000	-2.884593000000	-0.850329000000
H	8.705848000000	-4.618301000000	-0.923260000000
H	8.569566000000	-2.280549000000	-4.544356000000
H	9.604555000000	-1.733124000000	-3.226075000000
C	10.009273000000	-4.223073000000	-3.068416000000
H	10.755458000000	-3.684065000000	-2.469501000000
H	10.037360000000	-5.282385000000	-2.778201000000
H	10.301053000000	-4.149070000000	-4.124864000000
P	7.303920000000	-0.994227000000	-2.883066000000
P	6.606200000000	-3.394482000000	-0.670259000000
P	5.892023000000	-3.944153000000	-3.994012000000
Cu	5.497344000000	-2.347323000000	-2.395686000000
C	6.864625000000	-2.440300000000	0.875196000000
H	7.798878000000	-2.716257000000	1.381241000000
H	6.828815000000	-1.363704000000	0.658110000000
H	6.020177000000	-2.640472000000	1.545807000000
C	7.286233000000	0.214395000000	-4.266317000000
H	6.684786000000	1.074654000000	-3.949193000000
H	8.298918000000	0.555913000000	-4.518155000000
H	6.816457000000	-0.221423000000	-5.155362000000
C	6.039329000000	-3.532560000000	-5.786252000000
H	6.697345000000	-2.666985000000	-5.926792000000
H	6.439660000000	-4.378885000000	-6.360649000000
H	5.051784000000	-3.269350000000	-6.182050000000
C	5.003120000000	-5.553921000000	-4.110266000000
H	5.549403000000	-6.269179000000	-4.739995000000
H	4.875322000000	-5.979571000000	-3.108065000000
H	4.007041000000	-5.393227000000	-4.537700000000
C	8.223702000000	-0.034115000000	-1.615080000000
H	8.528011000000	-0.674442000000	-0.779030000000
H	9.118691000000	0.423299000000	-2.058461000000
H	7.557194000000	0.735911000000	-1.208015000000
C	6.243137000000	-5.074546000000	0.004491000000
H	6.209660000000	-5.814998000000	-0.804484000000
H	6.999744000000	-5.383336000000	0.738196000000
H	5.261519000000	-5.060495000000	0.492185000000
H	3.855722000000	-1.785078000000	-2.436922000000
B	5.007938000000	0.700153000000	-0.360845000000
H	5.376343000000	0.837821000000	-1.529859000000
H	5.968466000000	0.849176000000	0.410791000000
H	4.127026000000	1.507824000000	-0.088768000000
H	4.052589000000	-1.433429000000	-1.715783000000
O	4.488103000000	-0.708894000000	-0.231962000000
C	3.786529000000	-0.966556000000	0.957912000000
H	4.425006000000	-0.784614000000	1.842285000000
H	3.460546000000	-2.020342000000	0.968448000000
H	2.900897000000	-0.317252000000	1.052338000000

2_TS2$_{CuH}$_MeOH

E_{el} = -3242.19298810 Ha

E_{ZPVE} = -3241.739307 Ha

H = -3241.710231 Ha

G = -3241.793891 Ha

C	8.583017000000	-3.631532000000	-2.867658000000
C	7.581018000000	-4.551014000000	-3.618079000000
C	8.348429000000	-3.655827000000	-1.330029000000
C	8.617442000000	-2.193495000000	-3.459335000000
H	7.468015000000	-5.479941000000	-3.033438000000
H	8.030007000000	-4.850328000000	-4.580750000000
H	8.993489000000	-2.889829000000	-0.870477000000
H	8.708247000000	-4.625047000000	-0.945416000000
H	8.558558000000	-2.277781000000	-4.557996000000
H	9.599835000000	-1.742634000000	-3.239885000000
C	9.982935000000	-4.236783000000	-3.101761000000
H	10.738742000000	-3.707479000000	-2.506153000000
H	10.003689000000	-5.297742000000	-2.816934000000
H	10.266935000000	-4.160153000000	-4.160116000000

P	7.306689000000	-0.978922000000	-2.896939000000
P	6.605568000000	-3.412314000000	-0.670346000000
P	5.856071000000	-3.927048000000	-3.992921000000
Cu	5.503150000000	-2.303559000000	-2.362312000000
C	6.898892000000	-2.494452000000	0.891697000000
H	7.808053000000	-2.834379000000	1.404940000000
H	6.942442000000	-1.416192000000	0.690061000000
H	6.035753000000	-2.650072000000	1.549965000000
C	7.306422000000	0.219694000000	-4.289550000000
H	6.717648000000	1.091573000000	-3.981009000000
H	8.324922000000	0.542286000000	-4.543423000000
H	6.831270000000	-0.216620000000	-5.175564000000
C	6.003703000000	-3.512720000000	-5.786380000000
H	6.666404000000	-2.650411000000	-5.925465000000
H	6.399202000000	-4.359539000000	-6.363636000000
H	5.017407000000	-3.243357000000	-6.181486000000
C	4.975667000000	-5.543149000000	-4.120812000000
H	5.527815000000	-6.252716000000	-4.752140000000
H	4.846651000000	-5.974819000000	-3.121194000000
H	3.980183000000	-5.386232000000	-4.551282000000
C	8.237063000000	-0.023936000000	-1.632577000000
H	8.551276000000	-0.672202000000	-0.806145000000
H	9.126968000000	0.439117000000	-2.080281000000
H	7.571433000000	0.741493000000	-1.215026000000
C	6.247350000000	-5.101272000000	-0.012991000000
H	6.190615000000	-5.829531000000	-0.831610000000
H	7.017253000000	-5.426545000000	0.699674000000
H	5.276382000000	-5.088250000000	0.496146000000
H	3.742740000000	-1.811218000000	-2.834136000000
B	4.950131000000	0.649989000000	-0.585864000000
H	5.350276000000	0.848513000000	-1.735871000000
H	5.865395000000	0.854064000000	0.227125000000
H	3.999113000000	1.380079000000	-0.330378000000
H	3.832863000000	-1.446027000000	-2.137902000000
O	4.532748000000	-0.798521000000	-0.511684000000
C	3.825588000000	-1.131844000000	0.656056000000
H	4.419093000000	-0.910092000000	1.562563000000
H	3.585949000000	-2.209124000000	0.643788000000
H	2.886086000000	-0.559903000000	0.733044000000

2_Product1_MeOH

E_{el} = -3242.21534274 Ha

E_{ZPVE} = -3241.761483 Ha

H = -3241.731296 Ha

G = -3241.816708 Ha

C	8.626385000000	-3.626653000000	-2.860798000000
C	7.506248000000	-4.500434000000	-3.488343000000
C	8.566646000000	-3.618487000000	-1.305680000000
C	8.676327000000	-2.197077000000	-3.468087000000
H	7.471307000000	-5.450292000000	-2.928074000000
H	7.804565000000	-4.766273000000	-4.517452000000
H	9.292291000000	-2.871623000000	-0.942185000000
H	8.925653000000	-4.595479000000	-0.938424000000
H	8.594372000000	-2.292716000000	-4.564124000000
H	9.672559000000	-1.764885000000	-3.272402000000
C	9.961403000000	-4.304415000000	-3.236768000000
H	10.803280000000	-3.803292000000	-2.740321000000
H	9.964387000000	-5.360325000000	-2.933493000000
H	10.129007000000	-4.258942000000	-4.321433000000
P	7.384520000000	-0.969829000000	-2.899605000000
P	6.934956000000	-3.261965000000	-0.455083000000
P	5.744130000000	-3.861187000000	-3.577546000000
Cu	5.636396000000	-2.192714000000	-2.034571000000
C	7.522368000000	-2.596083000000	1.157633000000
H	8.306986000000	-3.226532000000	1.598115000000
H	7.894524000000	-1.573335000000	1.032502000000
H	6.669917000000	-2.543230000000	1.845050000000
C	7.337751000000	0.200970000000	-4.318305000000
H	6.748791000000	1.073796000000	-4.011659000000
H	8.345323000000	0.526490000000	-4.609386000000
H	6.838569000000	-0.251726000000	-5.182604000000
C	5.618900000000	-3.351937000000	-5.345565000000
H	6.205587000000	-2.443902000000	-5.524463000000
H	5.966115000000	-4.145016000000	-6.021871000000
H	4.572265000000	-3.118133000000	-5.573795000000
C	4.859618000000	-5.480713000000	-3.684487000000
H	5.319353000000	-6.137652000000	-4.435794000000
H	4.870240000000	-5.987470000000	-2.712272000000
H	3.813866000000	-5.303611000000	-3.960386000000
C	8.334680000000	0.035365000000	-1.686577000000
H	8.695021000000	-0.597760000000	-0.867285000000
H	9.194279000000	0.528101000000	-2.160660000000
H	7.655732000000	0.782333000000	-1.257857000000
C	6.423600000000	-4.953409000000	0.082596000000
H	6.158424000000	-5.567679000000	-0.786260000000
H	7.214428000000	-5.461011000000	0.651647000000
H	5.530777000000	-4.866264000000	0.714234000000
H	3.859275000000	-0.629607000000	-4.395572000000
B	4.734270000000	0.230282000000	-0.788230000000
H	5.311711000000	0.779943000000	-1.720849000000
H	5.532704000000	-0.063163000000	0.111277000000
H	3.831120000000	0.925540000000	-0.350562000000
H	3.960072000000	-0.544643000000	-3.652501000000
O	4.139278000000	-1.069114000000	-1.347137000000
C	3.276758000000	-1.715370000000	-0.428950000000
H	3.821396000000	-2.008177000000	0.488520000000
H	2.851457000000	-2.613555000000	-0.897352000000
H	2.464264000000	-1.034687000000	-0.136453000000

2_DHB_IIab_TFE

E_{el} = -3579.08335691 Ha

E_{ZPVE} = -3578.618831 Ha

H = -3578.585945 Ha

G = -3578.678313 Ha

Cu	-0.387753000000	-0.658746000000	0.313146000000
P	-0.131839000000	1.561096000000	0.921843000000
P	0.762492000000	-1.483716000000	2.145421000000
P	1.458027000000	-0.627881000000	-1.059180000000
C	2.662375000000	0.614796000000	1.309340000000
C	1.585620000000	1.676404000000	1.671596000000
C	2.790958000000	0.378921000000	-0.222209000000
C	2.466486000000	-0.710668000000	2.095556000000
C	4.016180000000	1.193808000000	1.772152000000
H	3.160395000000	-1.460967000000	1.680478000000
H	2.783624000000	-0.549100000000	3.140322000000
H	1.464824000000	1.668274000000	2.768507000000
H	1.982014000000	2.674657000000	1.418560000000
H	2.819494000000	1.364573000000	-0.716389000000
H	3.767399000000	-0.093918000000	-0.423301000000
H	3.976671000000	1.481273000000	2.831689000000
H	4.818016000000	0.453048000000	1.648404000000
H	4.280211000000	2.084171000000	1.185628000000
H	-1.596722000000	-1.051690000000	-2.003334000000
H	-1.103876000000	-2.798082000000	-1.121887000000
B	-1.871619000000	-1.854615000000	-1.128422000000
H	-1.927468000000	-1.306191000000	0.045666000000
H	-3.029485000000	-2.208667000000	-1.208377000000
C	2.259815000000	-2.265662000000	-1.307237000000
H	3.211917000000	-2.181943000000	-1.847804000000
H	2.433361000000	-2.760264000000	-0.344694000000
H	1.566469000000	-2.893329000000	-1.880784000000
C	1.511785000000	0.011662000000	-2.780908000000
H	2.523191000000	-0.045819000000	-3.204636000000
H	0.825783000000	-0.591926000000	-3.387692000000
H	1.154711000000	1.046204000000	-2.824008000000
C	-0.026438000000	2.839765000000	-0.398416000000
H	0.389818000000	3.775584000000	-0.000851000000
H	0.594737000000	2.494837000000	-1.232542000000
H	-1.029948000000	3.030671000000	-0.794827000000
C	-1.106719000000	2.507244000000	2.166086000000
H	-2.106537000000	2.679329000000	1.749277000000
H	-1.219423000000	1.932362000000	3.092586000000

H	-0.639558000000	3.474752000000	2.394975000000
C	1.201671000000	-3.240711000000	2.486978000000
H	1.592451000000	-3.719616000000	1.582163000000
H	1.945585000000	-3.322259000000	3.291103000000
H	0.296054000000	-3.782827000000	2.781936000000
C	0.190716000000	-0.980329000000	3.826810000000
H	0.041271000000	0.105222000000	3.865133000000
H	-0.772796000000	-1.458049000000	4.038228000000
H	0.912208000000	-1.268126000000	4.603621000000
H	-2.550390000000	0.346703000000	-0.550531000000
O	-3.063684000000	1.154448000000	-0.726366000000
C	-3.538677000000	1.076226000000	-2.050897000000
H	-4.563992000000	1.459637000000	-2.095639000000
H	-3.519508000000	0.048945000000	-2.435518000000
C	-2.703742000000	1.928394000000	-2.959890000000
F	-1.381136000000	1.534003000000	-3.009129000000
F	-2.695148000000	3.255086000000	-2.571961000000
F	-3.187902000000	1.885854000000	-4.247792000000

2_TS1$_{BH}^{A}$_TFE

E_{el} = -3579.06821392 Ha

E_{ZPVE} = -3578.603743 Ha

H = -3578.572072 Ha

G = -3578.660463 Ha

Cu	-0.472566000000	-0.254761000000	0.132269000000
P	0.011898000000	1.957325000000	0.751174000000
P	0.392258000000	-1.219874000000	2.019327000000
P	1.384562000000	-0.479040000000	-1.185984000000
C	2.609086000000	0.584554000000	1.262122000000
C	1.668616000000	1.770154000000	1.618603000000
C	2.769918000000	0.386466000000	-0.272475000000
C	2.200263000000	-0.726662000000	1.994120000000
C	4.006173000000	0.961596000000	1.798901000000
H	2.763219000000	-1.561619000000	1.545653000000
H	2.534726000000	-0.660442000000	3.043239000000
H	1.462944000000	1.723897000000	2.701669000000
H	2.219046000000	2.712926000000	1.456901000000
H	2.905560000000	1.381030000000	-0.729986000000
H	3.704556000000	-0.169108000000	-0.460250000000
H	3.956902000000	1.230512000000	2.863014000000
H	4.704855000000	0.120950000000	1.690276000000
H	4.415330000000	1.818779000000	1.247158000000
H	-1.052524000000	-1.855831000000	-2.391451000000
H	-1.161666000000	-3.738698000000	-1.655380000000
B	-1.524770000000	-2.586308000000	-1.526361000000
H	-1.158691000000	-2.196105000000	-0.400235000000
H	-2.757651000000	-2.532040000000	-1.572554000000
C	2.057356000000	-2.176395000000	-1.407191000000
H	3.004255000000	-2.163553000000	-1.963662000000
H	2.221951000000	-2.656249000000	-0.435140000000
H	1.311099000000	-2.770024000000	-1.950152000000
C	1.584214000000	0.176700000000	-2.891292000000
H	2.625405000000	0.110262000000	-3.233409000000
H	0.945541000000	-0.419435000000	-3.554193000000
H	1.241326000000	1.215554000000	-2.948029000000
C	0.446532000000	3.241443000000	-0.502943000000
H	0.948186000000	4.097310000000	-0.031334000000
H	1.105796000000	2.820680000000	-1.271478000000
H	-0.468254000000	3.582764000000	-0.997197000000
C	-0.852576000000	3.027277000000	1.980635000000
H	-1.773567000000	3.406355000000	1.523022000000
H	-1.131698000000	2.441072000000	2.863973000000
H	-0.229792000000	3.877089000000	2.292295000000
C	0.517453000000	-3.045645000000	2.176989000000
H	0.797558000000	-3.482392000000	1.211404000000
H	1.241064000000	-3.343771000000	2.947247000000
H	-0.469847000000	-3.447668000000	2.432229000000
C	-0.070493000000	-0.764240000000	3.747993000000
H	-0.029067000000	0.324108000000	3.878415000000
H	-1.097659000000	-1.089231000000	3.948492000000
H	0.601468000000	-1.234070000000	4.479221000000
H	-2.645773000000	-1.127906000000	-0.667326000000
O	-2.763729000000	-0.159493000000	-0.511621000000
C	-3.334160000000	0.354935000000	-1.693701000000
H	-4.398377000000	0.585333000000	-1.551816000000
H	-3.230414000000	-0.354213000000	-2.526949000000
C	-2.664765000000	1.631315000000	-2.091796000000
F	-1.342447000000	1.478492000000	-2.456316000000
F	-2.682674000000	2.579101000000	-1.079529000000
F	-3.315235000000	2.187768000000	-3.169435000000

2_INT$_{BH}^{A}$_TFE

E_{el} = -3579.07087817 Ha

E_{ZPVE} = -3578.604996 Ha

H = -3578.573120 Ha

G = -3578.661704 Ha

Cu	-0.495625000000	0.008043000000	0.171845000000
P	0.131326000000	2.088717000000	0.807527000000
P	0.283798000000	-1.140563000000	1.986990000000
P	1.312877000000	-0.459455000000	-1.177589000000
C	2.620633000000	0.550521000000	1.264401000000
C	1.793299000000	1.818297000000	1.622334000000
C	2.746141000000	0.342774000000	-0.272073000000
C	2.113958000000	-0.723828000000	2.001451000000
C	4.048426000000	0.810754000000	1.789487000000
H	2.646317000000	-1.591480000000	1.578373000000
H	2.422584000000	-0.661832000000	3.058889000000
H	1.624323000000	1.817463000000	2.712826000000
H	2.409663000000	2.709432000000	1.411953000000
H	2.928398000000	1.328008000000	-0.733452000000
H	3.647462000000	-0.260478000000	-0.473692000000
H	4.031020000000	1.082626000000	2.853840000000
H	4.674086000000	-0.084491000000	1.674639000000
H	4.521782000000	1.631491000000	1.233832000000
H	-0.888841000000	-1.862886000000	-2.660247000000
H	-1.002039000000	-3.870163000000	-2.456417000000
B	-1.430775000000	-2.799419000000	-2.075091000000
H	-1.180556000000	-2.710905000000	-0.856735000000
H	-2.645457000000	-2.739685000000	-2.248970000000
C	1.927305000000	-2.182476000000	-1.372096000000
H	2.877864000000	-2.193600000000	-1.922739000000
H	2.080437000000	-2.656654000000	-0.395702000000
H	1.169555000000	-2.760557000000	-1.916753000000
C	1.571990000000	0.165286000000	-2.885515000000
H	2.611056000000	0.018029000000	-3.209395000000
H	0.902125000000	-0.394136000000	-3.549387000000
H	1.314416000000	1.227400000000	-2.958354000000
C	0.532449000000	3.308371000000	-0.512126000000
H	1.027913000000	4.199765000000	-0.104676000000
H	1.181725000000	2.850058000000	-1.267299000000
H	-0.398914000000	3.603514000000	-1.008675000000
C	-0.661932000000	3.206805000000	2.038039000000
H	-1.585071000000	3.612200000000	1.608129000000
H	-0.927843000000	2.651085000000	2.944536000000
H	0.002210000000	4.039164000000	2.307356000000
C	0.327844000000	-2.972890000000	2.129634000000
H	0.564474000000	-3.419305000000	1.157273000000
H	1.052989000000	-3.306171000000	2.883970000000
H	-0.670463000000	-3.329470000000	2.408656000000
C	-0.195716000000	-0.692186000000	3.712195000000
H	-0.108189000000	0.390071000000	3.865673000000
H	-1.241497000000	-0.972420000000	3.881939000000
H	0.435268000000	-1.206551000000	4.449728000000
H	-2.141838000000	-1.458955000000	-0.831169000000
O	-2.410493000000	-0.545576000000	-0.531910000000
C	-3.237071000000	0.011108000000	-1.533282000000
H	-4.262703000000	0.127030000000	-1.161258000000
H	-3.247655000000	-0.637079000000	-2.420448000000
C	-2.771291000000	1.370284000000	-1.952940000000
F	-1.518266000000	1.381413000000	-2.527465000000
F	-2.722951000000	2.272351000000	-0.897299000000
F	-3.646290000000	1.894264000000	-2.876060000000

2_TS2$_{BH}^{B+C}$_TFE

E_{el} = -3579.02596629 Ha

E_{ZPVE} = -3578.573297 Ha

H = -3578.538287 Ha

G = -3578.637230 Ha

Cu	-0.396617000000	-0.211501000000	-0.147311000000
P	0.057538000000	1.954224000000	0.448266000000
P	0.288556000000	-1.081463000000	1.899285000000
P	1.685943000000	-0.549892000000	-1.107777000000
C	2.562796000000	0.731650000000	1.420254000000
C	1.606562000000	1.953093000000	1.502175000000
C	2.931324000000	0.364994000000	-0.043762000000
C	2.034153000000	-0.488358000000	2.222561000000
C	3.877683000000	1.162791000000	2.103407000000
H	2.708179000000	-1.339131000000	2.024172000000
H	2.125761000000	-0.268957000000	3.300627000000
H	1.290035000000	2.064836000000	2.553087000000
H	2.179137000000	2.864614000000	1.258037000000
H	3.177050000000	1.302325000000	-0.571668000000
H	3.860298000000	-0.231362000000	-0.033408000000
H	3.684450000000	1.535060000000	3.118715000000
H	4.575243000000	0.317258000000	2.175819000000
H	4.368314000000	1.963423000000	1.533329000000
H	-0.602822000000	-1.627126000000	-2.894182000000
H	-0.234462000000	-3.648756000000	-2.898693000000
B	-1.009643000000	-2.742857000000	-2.859921000000
H	-0.903779000000	-3.530837000000	-0.730025000000
H	-2.163996000000	-2.968116000000	-3.015459000000
C	2.325782000000	-2.279398000000	-1.012916000000
H	3.393271000000	-2.330399000000	-1.268542000000
H	2.178747000000	-2.689204000000	-0.006996000000
H	1.756196000000	-2.903076000000	-1.713963000000
C	2.331082000000	-0.106168000000	-2.781395000000
H	3.418599000000	-0.249322000000	-2.846638000000
H	1.840786000000	-0.746934000000	-3.524206000000
H	2.090510000000	0.935103000000	-3.024860000000
C	0.556721000000	3.069847000000	-0.933819000000
H	0.931216000000	4.032488000000	-0.559579000000
H	1.333859000000	2.601651000000	-1.548887000000
H	-0.317989000000	3.244425000000	-1.569969000000
C	-0.997342000000	3.127510000000	1.402557000000
H	-1.864236000000	3.383085000000	0.783624000000
H	-1.372280000000	2.653970000000	2.317067000000
H	-0.451297000000	4.043845000000	1.664757000000
C	0.424522000000	-2.824567000000	2.495822000000
H	1.005359000000	-3.430232000000	1.790573000000
H	0.894065000000	-2.877765000000	3.487721000000
H	-0.581886000000	-3.255499000000	2.551906000000
C	-0.627258000000	-0.359449000000	3.329888000000
H	-0.642631000000	0.734144000000	3.260850000000
H	-1.666606000000	-0.706029000000	3.291162000000
H	-0.181263000000	-0.650749000000	4.290735000000
H	-1.315676000000	-2.887687000000	-0.660170000000
O	-2.053183000000	-1.042787000000	-0.744488000000
C	-3.043248000000	-0.455194000000	-1.484855000000
H	-3.979095000000	-1.045606000000	-1.455733000000
H	-2.787571000000	-0.322767000000	-2.559607000000
C	-3.441413000000	0.923200000000	-1.017296000000
F	-2.482794000000	1.900272000000	-1.300806000000
F	-3.671296000000	1.012495000000	0.340220000000
F	-4.595856000000	1.351620000000	-1.645362000000

2_Product_TFE

E_{el} = -3579.08903483 Ha

E_{ZPVE} = -3578.628028 Ha

H = -3578.595337 Ha

G =-3578.686098 Ha

Cu	-0.135660000000	-0.365219000000	-0.320947000000
P	0.193445000000	1.791417000000	0.317437000000
P	0.425541000000	-1.313476000000	1.695875000000
P	1.935858000000	-0.658064000000	-1.275687000000
C	2.694557000000	0.536753000000	1.320449000000
C	1.711341000000	1.737525000000	1.416529000000
C	3.132377000000	0.229726000000	-0.139979000000
C	2.163908000000	-0.721488000000	2.062137000000
C	3.972998000000	0.969762000000	2.070347000000
H	2.848689000000	-1.557536000000	1.842274000000
H	2.236317000000	-0.545655000000	3.149296000000
H	1.354924000000	1.793025000000	2.459566000000
H	2.277678000000	2.668597000000	1.240372000000
H	3.394348000000	1.186939000000	-0.621987000000
H	4.065176000000	-0.359215000000	-0.107615000000
H	3.733030000000	1.303757000000	3.088955000000
H	4.682775000000	0.134675000000	2.143003000000
H	4.471420000000	1.797185000000	1.547212000000
H	-0.662709000000	-2.345690000000	-2.965207000000
H	-0.338070000000	-3.084994000000	-1.102370000000
B	-1.162539000000	-2.624978000000	-1.876575000000
H	-2.890930000000	-2.711015000000	1.143990000000
H	-2.124307000000	-3.365199000000	-2.006776000000
C	2.598720000000	-2.373409000000	-1.279959000000
H	3.661128000000	-2.396384000000	-1.557543000000
H	2.470140000000	-2.835963000000	-0.295091000000
H	2.009244000000	-2.963999000000	-1.991356000000
C	2.536941000000	-0.098245000000	-2.925420000000
H	3.623080000000	-0.226473000000	-3.027332000000
H	2.031048000000	-0.698832000000	-3.690857000000
H	2.280159000000	0.952789000000	-3.099148000000
C	0.722144000000	2.985769000000	-0.983800000000
H	1.105588000000	3.916694000000	-0.544186000000
H	1.498899000000	2.545593000000	-1.619208000000
H	-0.138879000000	3.219098000000	-1.620620000000
C	-0.887139000000	2.902862000000	1.314521000000
H	-1.742195000000	3.205900000000	0.699998000000
H	-1.277769000000	2.373550000000	2.191184000000
H	-0.344839000000	3.799353000000	1.644680000000
C	0.558715000000	-3.094029000000	2.136732000000
H	1.134992000000	-3.633729000000	1.377488000000
H	1.024418000000	-3.232614000000	3.121813000000
H	-0.448189000000	-3.526928000000	2.145792000000
C	-0.502979000000	-0.689769000000	3.161606000000
H	-0.492017000000	0.406657000000	3.178425000000
H	-1.548099000000	-1.011662000000	3.075691000000
H	-0.082815000000	-1.065117000000	4.104681000000
H	-2.466854000000	-2.287247000000	0.687239000000
O	-1.659865000000	-1.308855000000	-1.232312000000
C	-2.831821000000	-0.830272000000	-1.805660000000
H	-3.655749000000	-1.547579000000	-1.653373000000
H	-2.727078000000	-0.668797000000	-2.892627000000
C	-3.248511000000	0.470797000000	-1.192734000000
F	-2.407927000000	1.526767000000	-1.525055000000
F	-3.293515000000	0.437129000000	0.187830000000
F	-4.503584000000	0.829213000000	-1.629124000000

2_DHB_IIab_TFE

E_{el} = -3579.08192399 Ha

E_{ZPVE} = -3578.617167 Ha

H = -3578.584500 Ha

G = -3578.675969 Ha

C	2.272712000000	-1.888521000000	-0.980633000000
C	0.852559000000	-2.382297000000	-1.372932000000
C	2.382784000000	-1.537185000000	0.531483000000
C	2.775999000000	-0.729328000000	-1.883755000000
H	0.529314000000	-3.107739000000	-0.606720000000
H	0.930005000000	-2.952088000000	-2.315127000000
H	3.322356000000	-0.981389000000	0.686247000000
H	2.485160000000	-2.474187000000	1.104244000000
H	2.574293000000	-0.997070000000	-2.934548000000
H	3.873207000000	-0.659992000000	-1.789963000000
C	3.227014000000	-3.076003000000	-1.225075000000
H	4.238024000000	-2.840027000000	-0.866331000000

H	2.877680000000	-3.972908000000	-0.695798000000
H	3.290702000000	-3.312406000000	-2.295958000000
P	2.042582000000	0.956809000000	-1.570672000000
P	0.995274000000	-0.551771000000	1.313997000000
P	-0.566245000000	-1.169545000000	-1.594376000000
Cu	0.062678000000	0.723297000000	-0.384906000000
C	1.854566000000	0.245379000000	2.728700000000
H	2.440203000000	-0.474580000000	3.315185000000
H	2.509096000000	1.047778000000	2.369879000000
H	1.096960000000	0.708420000000	3.372319000000
C	2.238071000000	1.766998000000	-3.211974000000
H	1.993512000000	2.829672000000	-3.097285000000
H	3.264539000000	1.670896000000	-3.590249000000
H	1.542369000000	1.341721000000	-3.943884000000
C	-0.654595000000	-1.060242000000	-3.435935000000
H	0.232499000000	-0.554230000000	-3.834020000000
H	-0.732421000000	-2.055091000000	-3.895246000000
H	-1.531686000000	-0.466998000000	-3.719272000000
C	-1.976785000000	-2.324108000000	-1.299178000000
H	-2.910175000000	-1.843038000000	-1.616138000000
H	-1.853593000000	-3.261161000000	-1.859406000000
H	-2.065984000000	-2.547005000000	-0.229785000000
C	3.374173000000	1.823066000000	-0.641890000000
H	3.558994000000	1.329773000000	0.319348000000
H	4.311917000000	1.858420000000	-1.212313000000
H	3.029597000000	2.842991000000	-0.430685000000
C	0.090011000000	-1.892401000000	2.198435000000
H	-0.427642000000	-2.543391000000	1.483755000000
H	0.775505000000	-2.499288000000	2.805052000000
H	-0.668048000000	-1.444405000000	2.847488000000
H	-0.969999000000	2.094145000000	-0.509404000000
B	-0.284754000000	3.002449000000	0.084253000000
H	0.559939000000	2.568511000000	0.853265000000
H	-1.106295000000	3.625071000000	0.734003000000
H	0.208859000000	3.685678000000	-0.789808000000
H	-2.576513000000	2.878312000000	0.840024000000
O	-3.470673000000	2.498849000000	0.947480000000
C	-3.406257000000	1.120448000000	0.718326000000
H	-2.640524000000	0.846201000000	-0.024379000000
H	-4.383677000000	0.770706000000	0.366273000000
C	-3.094248000000	0.357100000000	1.973075000000
F	-4.054210000000	0.489956000000	2.942008000000
F	-2.995281000000	-1.000148000000	1.687744000000
F	-1.891110000000	0.725286000000	2.547018000000

2_TS1$_{CuH}$_TFE

E_{el} = -3579.02493248 Ha

E_{ZPVE} = -3578.564841 Ha

H = -3578.531853 Ha

G = -3578.624902 Ha

C	8.438464000000	-4.042913000000	-2.271507000000
C	7.130575000000	-4.674199000000	-2.819784000000
C	8.334251000000	-3.689017000000	-0.765089000000
C	8.918578000000	-2.837306000000	-3.124053000000
H	6.810319000000	-5.453284000000	-2.107343000000
H	7.359496000000	-5.197628000000	-3.764363000000
H	9.245997000000	-3.133804000000	-0.486700000000
H	8.360704000000	-4.626329000000	-0.183204000000
H	8.852029000000	-3.123882000000	-4.187288000000
H	9.988998000000	-2.664416000000	-2.918084000000
C	9.529198000000	-5.126796000000	-2.396110000000
H	10.466714000000	-4.790746000000	-1.932800000000
H	9.215837000000	-6.054945000000	-1.899196000000
H	9.732125000000	-5.354988000000	-3.451480000000
P	8.018449000000	-1.209739000000	-2.925093000000
P	6.869020000000	-2.688453000000	-0.143082000000
P	5.656469000000	-3.559897000000	-3.125612000000
Cu	5.929030000000	-1.560605000000	-1.960000000000
C	7.632343000000	-1.985614000000	1.381268000000
H	8.087407000000	-2.776828000000	1.992752000000
H	8.398877000000	-1.245101000000	1.124971000000
H	6.857980000000	-1.473641000000	1.961549000000
C	8.386262000000	-0.433081000000	-4.558645000000
H	8.087738000000	0.620755000000	-4.520420000000
H	9.456477000000	-0.492579000000	-4.799378000000
H	7.812731000000	-0.912374000000	-5.360015000000
C	5.697066000000	-3.395336000000	-4.964282000000
H	6.562256000000	-2.801681000000	-5.279860000000
H	5.738681000000	-4.375426000000	-5.458941000000
H	4.795691000000	-2.864674000000	-5.292211000000
C	4.288686000000	-4.794851000000	-2.991494000000
H	3.367961000000	-4.345180000000	-3.381537000000
H	4.508604000000	-5.706635000000	-3.563823000000
H	4.110554000000	-5.065175000000	-1.944224000000
C	9.196713000000	-0.235292000000	-1.893545000000
H	9.201551000000	-0.596689000000	-0.859776000000
H	10.218101000000	-0.271859000000	-2.296222000000
H	8.854114000000	0.806286000000	-1.870280000000
C	5.855643000000	-4.023617000000	0.636406000000
H	5.391704000000	-4.660727000000	-0.125143000000
H	6.471091000000	-4.651717000000	1.295112000000
H	5.056454000000	-3.569021000000	1.232287000000
H	4.907121000000	-0.352362000000	-2.085062000000
B	5.807676000000	1.288641000000	0.179662000000
H	6.741161000000	0.550634000000	0.136311000000
H	5.174105000000	1.377917000000	1.177087000000
H	5.623373000000	2.042003000000	-0.719317000000
H	3.913405000000	0.055053000000	-1.146387000000
O	3.244041000000	0.182002000000	-0.419242000000
C	2.854898000000	-1.099293000000	-0.022186000000
H	3.414624000000	-1.883639000000	-0.565306000000
H	1.780216000000	-1.262935000000	-0.182183000000
C	3.112607000000	-1.304247000000	1.440059000000
F	2.506551000000	-0.370636000000	2.238627000000
F	2.642758000000	-2.548562000000	1.831095000000
F	4.462299000000	-1.289018000000	1.757814000000

2_INT$_{CuH}$_TFE

E_{el} = -3579.05618692 Ha

E_{ZPVE} = -3578.596601 Ha

H = -3578.563777 Ha

G = -3578.657554 Ha

C	3.203497000000	0.117511000000	0.809206000000
C	3.202619000000	-1.166188000000	-0.061674000000
C	2.227518000000	0.012007000000	2.013831000000
C	2.962227000000	1.395377000000	-0.042138000000
H	3.246497000000	-2.038519000000	0.611963000000
H	4.133453000000	-1.190904000000	-0.654234000000
H	2.177381000000	1.002683000000	2.495403000000
H	2.667829000000	-0.670009000000	2.761456000000
H	3.544229000000	1.299941000000	-0.974285000000
H	3.383330000000	2.262430000000	0.494362000000
C	4.620722000000	0.243295000000	1.404081000000
H	4.670785000000	1.078085000000	2.116197000000
H	4.905769000000	-0.676155000000	1.933533000000
H	5.359558000000	0.425498000000	0.611773000000
P	1.197887000000	1.828059000000	-0.505105000000
P	0.460533000000	-0.545404000000	1.719770000000
P	1.772720000000	-1.424789000000	-1.237763000000
Cu	-0.031396000000	-0.153278000000	-0.511244000000
C	-0.358931000000	0.211477000000	3.186038000000
H	0.214731000000	0.035184000000	4.106196000000
H	-0.493795000000	1.288115000000	3.030772000000
H	-1.358903000000	-0.224663000000	3.299117000000
C	1.485910000000	2.898842000000	-1.976391000000
H	0.548005000000	3.415469000000	-2.212332000000
H	2.267317000000	3.645953000000	-1.782237000000
H	1.767084000000	2.297619000000	-2.848385000000
C	2.528352000000	-0.924730000000	-2.845632000000
H	2.721880000000	0.154053000000	-2.858107000000
H	3.470679000000	-1.457737000000	-3.032196000000
H	1.823915000000	-1.146500000000	-3.655542000000

C	1.849840000000	-3.257128000000	-1.440716000000
H	1.210179000000	-3.550381000000	-2.280841000000
H	2.875959000000	-3.595691000000	-1.638614000000
H	1.473432000000	-3.759978000000	-0.542800000000
C	0.836963000000	3.134608000000	0.742227000000
H	0.805042000000	2.710820000000	1.752641000000
H	1.599496000000	3.924746000000	0.708414000000
H	-0.152406000000	3.556887000000	0.533495000000
C	0.537470000000	-2.298312000000	2.297140000000
H	1.115039000000	-2.911924000000	1.596392000000
H	0.988594000000	-2.376243000000	3.295756000000
H	-0.479897000000	-2.705718000000	2.333893000000
H	-1.429242000000	-0.375820000000	-1.271203000000
B	-2.612729000000	2.339911000000	0.232181000000
H	-1.943932000000	2.016501000000	1.200450000000
H	-3.636716000000	2.896197000000	0.545413000000
H	-1.973392000000	2.918884000000	-0.616463000000
H	-2.207023000000	0.430654000000	-0.851587000000
O	-3.061560000000	0.979057000000	-0.457644000000
C	-3.778692000000	0.091450000000	0.373300000000
H	-3.920112000000	0.529369000000	1.367515000000
H	-3.229963000000	-0.858418000000	0.462499000000
C	-5.119247000000	-0.190251000000	-0.229825000000
F	-5.021161000000	-0.774236000000	-1.471401000000
F	-5.810184000000	-1.068821000000	0.583806000000
F	-5.889217000000	0.936320000000	-0.364525000000

2_INT1$_{CuH}$_TFE

E_{el} = -3579.07170756 Ha

E_{ZPVE} = −3578.610642 Ha

H = -3578.578227 Ha

G = -3578.669799 Ha

C	2.216639000000	-1.813089000000	-1.098699000000
C	0.969415000000	-2.472727000000	-1.748675000000
C	2.055237000000	-1.658740000000	0.440095000000
C	2.614064000000	-0.484229000000	-1.803478000000
H	0.636108000000	-3.293770000000	-1.091520000000
H	1.273147000000	-2.945187000000	-2.698539000000
H	2.900868000000	-1.060843000000	0.816205000000
H	2.164550000000	-2.656181000000	0.898490000000
H	2.492958000000	-0.623991000000	-2.891182000000
H	3.688906000000	-0.301888000000	-1.636513000000
C	3.386987000000	-2.794293000000	-1.318217000000
H	4.284463000000	-2.451991000000	-0.785894000000
H	3.131641000000	-3.796664000000	-0.948155000000
H	3.632747000000	-2.875123000000	-2.385916000000
P	1.696760000000	1.070362000000	-1.309622000000
P	0.476105000000	-0.908783000000	1.129173000000
P	-0.535639000000	-1.426807000000	-2.117546000000
Cu	-0.373497000000	0.314215000000	-0.616735000000
C	1.088048000000	-0.104841000000	2.656444000000
H	1.819461000000	-0.738272000000	3.175816000000
H	1.521223000000	0.875104000000	2.421596000000
H	0.231072000000	0.077091000000	3.312479000000
C	1.958918000000	2.144892000000	-2.778510000000
H	1.638119000000	3.159913000000	-2.514419000000
H	3.015903000000	2.170898000000	-3.075187000000
H	1.351864000000	1.807974000000	-3.626138000000
C	-0.358669000000	-1.153359000000	-3.933708000000
H	0.508997000000	-0.517199000000	-4.143621000000
H	-0.236439000000	-2.105009000000	-4.468751000000
H	-1.250177000000	-0.642874000000	-4.315448000000
C	-1.834562000000	-2.732776000000	-2.125148000000
H	-2.760297000000	-2.326459000000	-2.547699000000
H	-1.522504000000	-3.601255000000	-2.720882000000
H	-2.048694000000	-3.056126000000	-1.100320000000
C	2.891968000000	1.836719000000	-0.143853000000
H	3.066386000000	1.188701000000	0.721797000000
H	3.850101000000	2.025069000000	-0.646752000000
H	2.462925000000	2.772123000000	0.233681000000
C	-0.343639000000	-2.409536000000	1.817891000000
H	-0.585262000000	-3.120423000000	1.018202000000
H	0.305249000000	-2.909184000000	2.549738000000
H	-1.275013000000	-2.112472000000	2.310181000000
H	-1.750318000000	1.387650000000	-0.816731000000
B	0.000709000000	3.314726000000	1.394710000000
H	0.972730000000	3.107004000000	2.130686000000
H	-0.500736000000	4.400289000000	1.658225000000
H	0.332376000000	3.268335000000	0.213446000000
H	-1.593810000000	1.556955000000	-0.047810000000
O	-1.025595000000	2.216722000000	1.606821000000
C	-1.789682000000	2.384232000000	2.747502000000
H	-2.368909000000	3.323990000000	2.734867000000
H	-1.180112000000	2.393678000000	3.671558000000
C	-2.758551000000	1.248783000000	2.862090000000
F	-2.127253000000	0.019418000000	3.025778000000
F	-3.586341000000	1.403287000000	3.951439000000
F	-3.567487000000	1.110320000000	1.753238000000

2_TS2$_{CuH}$_TFE

E_{el} = -3579.06989162 Ha

E_{ZPVE} = -3578.608824 Ha

H = -3578.577263 Ha

G = -3578.666017 Ha

C	8.456513000000	-3.663614000000	-2.846426000000
C	7.364247000000	-4.497033000000	-3.571212000000
C	8.249516000000	-3.646881000000	-1.303908000000
C	8.608074000000	-2.238210000000	-3.448865000000
H	7.180681000000	-5.407918000000	-2.976700000000
H	7.767132000000	-4.842254000000	-4.538815000000
H	8.947570000000	-2.911402000000	-0.872935000000
H	8.558343000000	-4.627248000000	-0.904027000000
H	8.524685000000	-2.317877000000	-4.546098000000
H	9.630666000000	-1.877551000000	-3.246978000000
C	9.793047000000	-4.392615000000	-3.097476000000
H	10.601720000000	-3.929783000000	-2.516051000000
H	9.723257000000	-5.449305000000	-2.805074000000
H	10.067057000000	-4.347895000000	-4.160346000000
P	7.419357000000	-0.911029000000	-2.868773000000
P	6.536597000000	-3.288530000000	-0.617139000000
P	5.694382000000	-3.727747000000	-3.922650000000
Cu	5.521901000000	-2.082999000000	-2.291797000000
C	6.939571000000	-2.453466000000	0.969608000000
H	7.829342000000	-2.884878000000	1.446988000000
H	7.082761000000	-1.378490000000	0.797269000000
H	6.085882000000	-2.565401000000	1.647335000000
C	7.505310000000	0.279823000000	-4.265712000000
H	6.991539000000	1.198333000000	-3.958468000000
H	8.545002000000	0.516508000000	-4.528478000000
H	6.989743000000	-0.120372000000	-5.146122000000
C	5.852751000000	-3.328167000000	-5.718610000000
H	6.603138000000	-2.542718000000	-5.867382000000
H	6.145670000000	-4.211281000000	-6.302633000000
H	4.894828000000	-2.953528000000	-6.097522000000
C	4.671419000000	-5.257789000000	-4.028614000000
H	5.149738000000	-6.017950000000	-4.661189000000
H	4.514218000000	-5.669819000000	-3.024998000000
H	3.688607000000	-5.014474000000	-4.447797000000
C	8.455934000000	-0.035768000000	-1.628829000000
H	8.685183000000	-0.688152000000	-0.778162000000
H	9.396631000000	0.301107000000	-2.085289000000
H	7.889282000000	0.819039000000	-1.243734000000
C	6.062791000000	-4.970665000000	-0.025361000000
H	5.979673000000	-5.662674000000	-0.872776000000
H	6.805759000000	-5.365549000000	0.680560000000
H	5.088635000000	-4.916013000000	0.469690000000
H	3.821378000000	-1.396406000000	-3.049329000000
B	5.200393000000	0.905889000000	-0.657505000000
H	5.647774000000	0.986170000000	-1.795619000000
H	6.110038000000	0.933408000000	0.179806000000
H	4.403412000000	1.807700000000	-0.435913000000
H	3.781480000000	-1.060743000000	-2.356124000000

O	4.484410000000	-0.433820000000	-0.555234000000
C	3.767105000000	-0.547538000000	0.624840000000
H	3.075867000000	0.301524000000	0.768013000000
H	4.416378000000	-0.587471000000	1.520570000000
C	2.946567000000	-1.797672000000	0.604891000000
F	2.063017000000	-1.851355000000	-0.450887000000
F	3.722318000000	-2.950130000000	0.510983000000
F	2.207528000000	-1.927592000000	1.760006000000

2_DHB_IIbc_HFIP

E_{el} = -3915.93709832 Ha

E_{ZPVE} = -3915.468490 Ha

H = -3915.432138 Ha

G = -3915.532549 Ha

Cu	-0.373529000000	-0.524184000000	0.309626000000
P	-0.064264000000	1.652019000000	0.995881000000
P	0.816620000000	-1.445306000000	2.084392000000
P	1.433464000000	-0.495109000000	-1.109512000000
C	2.724800000000	0.640715000000	1.274889000000
C	1.673747000000	1.704899000000	1.702207000000
C	2.805373000000	0.452762000000	-0.265700000000
C	2.533499000000	-0.705775000000	2.026494000000
C	4.098676000000	1.189562000000	1.715169000000
H	3.207086000000	-1.451876000000	1.572953000000
H	2.877802000000	-0.578164000000	3.067123000000
H	1.579615000000	1.656974000000	2.800631000000
H	2.079298000000	2.706002000000	1.476715000000
H	2.841690000000	1.454165000000	-0.727160000000
H	3.765666000000	-0.032466000000	-0.510861000000
H	4.091940000000	1.447725000000	2.782864000000
H	4.886904000000	0.442673000000	1.549185000000
H	4.358333000000	2.092702000000	1.146570000000
H	-1.450303000000	-1.422310000000	-1.832976000000
H	-1.326863000000	-2.993467000000	-0.565963000000
B	-1.910847000000	-1.968360000000	-0.846200000000
H	-1.920465000000	-1.209793000000	0.205978000000
H	-3.108992000000	-2.130625000000	-0.970170000000
C	2.186176000000	-2.146127000000	-1.414804000000
H	3.112682000000	-2.072378000000	-1.999615000000
H	2.398770000000	-2.658201000000	-0.469774000000
H	1.454911000000	-2.753823000000	-1.962355000000
C	1.508466000000	0.190358000000	-2.814447000000
H	2.528026000000	0.143979000000	-3.219587000000
H	0.839350000000	-0.400728000000	-3.451420000000
H	1.151303000000	1.225144000000	-2.835747000000
C	0.027078000000	2.986882000000	-0.268328000000
H	0.419291000000	3.914669000000	0.169592000000
H	0.668673000000	2.683524000000	-1.103488000000
H	-0.974475000000	3.171776000000	-0.671711000000
C	-0.983178000000	2.546824000000	2.318749000000
H	-1.988445000000	2.780410000000	1.948291000000
H	-1.090578000000	1.913593000000	3.207142000000
H	-0.479953000000	3.481809000000	2.600054000000
C	1.196898000000	-3.232257000000	2.310681000000
H	1.563322000000	-3.667951000000	1.374425000000
H	1.939425000000	-3.393728000000	3.103519000000
H	0.270749000000	-3.756783000000	2.572545000000
C	0.295259000000	-1.016870000000	3.802075000000
H	0.174946000000	0.068637000000	3.900993000000
H	-0.675254000000	-1.481758000000	4.010299000000
H	1.025089000000	-1.363044000000	4.546540000000
H	-2.762853000000	0.284214000000	-0.108152000000
O	-3.214568000000	1.050911000000	-0.502639000000
C	-3.506038000000	0.715643000000	-1.832179000000
H	-3.243710000000	-0.331141000000	-2.057137000000
C	-2.665394000000	1.587582000000	-2.735679000000
F	-1.328749000000	1.368855000000	-2.472831000000
F	-2.893155000000	2.929862000000	-2.547161000000
F	-2.864258000000	1.315587000000	-4.065148000000
C	-4.996371000000	0.865948000000	-2.039091000000
F	-5.365848000000	0.548593000000	-3.324917000000
F	-5.665364000000	0.015627000000	-1.197876000000
F	-5.441579000000	2.139269000000	-1.785305000000

2_TS1$_{BH}^{A}$_HFIP

E_{el} = -3915.92037750 Ha

E_{ZPVE} = -3915.451405 Ha

H = -3915.416199 Ha

G = -3915.513522 Ha

Cu	-0.451140000000	-0.164477000000	0.121832000000
P	0.065663000000	2.016632000000	0.759312000000
P	0.355418000000	-1.190223000000	1.998923000000
P	1.392296000000	-0.451088000000	-1.200609000000
C	2.628077000000	0.554127000000	1.264792000000
C	1.722085000000	1.768903000000	1.615171000000
C	2.799311000000	0.354400000000	-0.267654000000
C	2.176368000000	-0.748626000000	1.987507000000
C	4.030133000000	0.888648000000	1.817025000000
H	2.717632000000	-1.596851000000	1.537088000000
H	2.505440000000	-0.699109000000	3.039164000000
H	1.515442000000	1.731627000000	2.698441000000
H	2.302673000000	2.693208000000	1.452875000000
H	2.982723000000	1.342958000000	-0.721162000000
H	3.712680000000	-0.238532000000	-0.445345000000
H	3.977656000000	1.155910000000	2.881304000000
H	4.704590000000	0.027914000000	1.713441000000
H	4.470706000000	1.734732000000	1.272512000000
H	-1.119677000000	-1.721666000000	-2.465920000000
H	-1.211839000000	-3.634338000000	-1.811316000000
B	-1.556864000000	-2.488059000000	-1.612667000000
H	-1.132488000000	-2.146217000000	-0.494006000000
H	-2.790132000000	-2.428734000000	-1.601744000000
C	2.000513000000	-2.170414000000	-1.434233000000
H	2.948312000000	-2.186819000000	-1.989005000000
H	2.147473000000	-2.663918000000	-0.466098000000
H	1.235333000000	-2.734231000000	-1.982761000000
C	1.633327000000	0.216754000000	-2.895302000000
H	2.669575000000	0.090690000000	-3.235845000000
H	0.962369000000	-0.326033000000	-3.571494000000
H	1.363140000000	1.277649000000	-2.935195000000
C	0.501577000000	3.330722000000	-0.463311000000
H	1.082102000000	4.131685000000	0.014155000000
H	1.080951000000	2.918738000000	-1.296889000000
H	-0.418492000000	3.759573000000	-0.874901000000
C	-0.767207000000	3.070390000000	2.023380000000
H	-1.685364000000	3.481187000000	1.588451000000
H	-1.049945000000	2.469557000000	2.895273000000
H	-0.122481000000	3.898413000000	2.348444000000
C	0.419352000000	-3.020320000000	2.134289000000
H	0.691043000000	-3.455838000000	1.165925000000
H	1.127809000000	-3.349400000000	2.905826000000
H	-0.582073000000	-3.392167000000	2.379987000000
C	-0.105372000000	-0.738193000000	3.727787000000
H	-0.001971000000	0.343107000000	3.879107000000
H	-1.151594000000	-1.006911000000	3.911306000000
H	0.530091000000	-1.258306000000	4.457381000000
H	-2.622456000000	-1.102916000000	-0.644003000000
O	-2.748842000000	-0.126347000000	-0.500202000000
C	-3.327569000000	0.351518000000	-1.679014000000
H	-3.102326000000	-0.315134000000	-2.528341000000
C	-2.730025000000	1.705699000000	-1.990044000000
F	-1.421454000000	1.570402000000	-2.399783000000
F	-2.721825000000	2.550838000000	-0.900826000000
F	-3.400335000000	2.348991000000	-2.997486000000
C	-4.839416000000	0.394024000000	-1.523317000000
F	-5.465184000000	0.581974000000	-2.730924000000
F	-5.289985000000	-0.793433000000	-1.010726000000
F	-5.251291000000	1.396492000000	-0.678755000000

2_INT$_{BH}^{A}$_HFIP

E_{el} = -3915.92217388 Ha

E_{ZPVE} = -3915.453620 Ha

H = -3915.417960 Ha
G = -3915.515724 Ha

Cu	0.231174000000	-0.333863000000	0.106458000000
P	0.552922000000	1.844442000000	0.633595000000
P	0.880739000000	-1.275228000000	2.079341000000
P	2.228894000000	-0.659958000000	-0.985223000000
C	3.093899000000	0.623506000000	1.530810000000
C	2.091513000000	1.801372000000	1.696756000000
C	3.440930000000	0.340857000000	0.040710000000
C	2.636485000000	-0.655936000000	2.290082000000
C	4.405316000000	1.075675000000	2.207249000000
H	3.308080000000	-1.480523000000	1.998994000000
H	2.798654000000	-0.497068000000	3.369713000000
H	1.763022000000	1.824114000000	2.749707000000
H	2.632360000000	2.748591000000	1.527634000000
H	3.592289000000	1.310083000000	-0.463633000000
H	4.414629000000	-0.175839000000	0.001013000000
H	4.219884000000	1.403135000000	3.239378000000
H	5.131944000000	0.252621000000	2.234677000000
H	4.857870000000	1.912348000000	1.658051000000
H	0.438478000000	-2.410391000000	-2.743426000000
H	-0.033286000000	-4.363262000000	-2.453914000000
B	-0.213819000000	-3.219716000000	-2.096921000000
H	0.058549000000	-3.103725000000	-0.898109000000
H	-1.425518000000	-2.969537000000	-2.271728000000
C	3.062549000000	-2.298027000000	-1.034523000000
H	4.061537000000	-2.212336000000	-1.483139000000
H	3.162716000000	-2.717192000000	-0.026189000000
H	2.441286000000	-2.979563000000	-1.628097000000
C	2.599805000000	-0.052434000000	-2.679098000000
H	3.680351000000	-0.031403000000	-2.872825000000
H	2.114819000000	-0.732648000000	-3.389677000000
H	2.177970000000	0.948067000000	-2.830866000000
C	1.035787000000	3.054770000000	-0.668952000000
H	1.350544000000	4.010661000000	-0.229034000000
H	1.859576000000	2.655291000000	-1.272195000000
H	0.181734000000	3.226291000000	-1.333605000000
C	-0.556414000000	2.893704000000	1.658612000000
H	-1.425425000000	3.180295000000	1.055112000000
H	-0.923242000000	2.323061000000	2.519564000000
H	-0.046442000000	3.800428000000	2.010597000000
C	1.101171000000	-3.084136000000	2.312498000000
H	1.540267000000	-3.524491000000	1.410400000000
H	1.727618000000	-3.311421000000	3.185292000000
H	0.116268000000	-3.546463000000	2.445278000000
C	0.129016000000	-0.820640000000	3.701430000000
H	0.049168000000	0.268634000000	3.798956000000
H	-0.883983000000	-1.235596000000	3.755257000000
H	0.718759000000	-1.210468000000	4.542081000000
H	-1.260582000000	-1.942125000000	-1.213042000000
O	-1.513918000000	-1.082148000000	-0.734369000000
C	-2.578047000000	-0.475057000000	-1.383988000000
H	-3.109985000000	-1.204755000000	-2.015941000000
C	-3.544413000000	0.006773000000	-0.318848000000
F	-2.918350000000	0.745082000000	0.659436000000
F	-4.135605000000	-1.062551000000	0.297419000000
F	-4.540377000000	0.786004000000	-0.854851000000
C	-2.134437000000	0.646016000000	-2.316141000000
F	-3.119200000000	0.930601000000	-3.227409000000
F	-1.852382000000	1.825696000000	-1.650268000000
F	-1.009393000000	0.292953000000	-3.007625000000

2_TS1$_{BH}^{B+C}$_HFIP

E_{el} = -3915.89525686 Ha
E_{ZPVE} = -3915.432575 Ha
H = -3915.396030 Ha
G = -3915.496016 Ha

Cu	-0.420059000000	-0.266414000000	-0.081534000000
P	-0.048858000000	1.910465000000	0.483287000000
P	0.268406000000	-1.129051000000	1.938612000000
P	1.640899000000	-0.545173000000	-1.095610000000
C	2.493049000000	0.745076000000	1.431388000000
C	1.497398000000	1.934390000000	1.537822000000
C	2.866129000000	0.404191000000	-0.039152000000
C	2.008450000000	-0.501257000000	2.222234000000
C	3.796904000000	1.210050000000	2.113368000000
H	2.697185000000	-1.332482000000	1.995291000000
H	2.119118000000	-0.299033000000	3.301716000000
H	1.181118000000	2.016149000000	2.591563000000
H	2.039646000000	2.868546000000	1.310235000000
H	3.078229000000	1.352474000000	-0.561779000000
H	3.814669000000	-0.159852000000	-0.036804000000
H	3.596184000000	1.568657000000	3.132057000000
H	4.519993000000	0.385565000000	2.176983000000
H	4.261275000000	2.029261000000	1.547803000000
H	-0.308248000000	-1.924832000000	-2.944401000000
H	-0.496768000000	-3.971510000000	-2.975150000000
B	-0.997977000000	-2.890605000000	-2.960015000000
H	-0.970392000000	-3.655724000000	-0.784539000000
H	-2.162285000000	-2.793532000000	-3.167523000000
C	2.377376000000	-2.235886000000	-1.095192000000
H	3.434619000000	-2.219168000000	-1.393686000000
H	2.293245000000	-2.693312000000	-0.102449000000
H	1.812666000000	-2.859063000000	-1.799909000000
C	2.163368000000	0.001160000000	-2.778143000000
H	3.251546000000	-0.073353000000	-2.910617000000
H	1.665819000000	-0.636698000000	-3.518545000000
H	1.843899000000	1.032504000000	-2.965370000000
C	0.429984000000	3.060887000000	-0.875122000000
H	0.711431000000	4.048355000000	-0.484801000000
H	1.275142000000	2.651563000000	-1.439978000000
H	-0.418128000000	3.167345000000	-1.559799000000
C	-1.150420000000	3.022541000000	1.451856000000
H	-2.010504000000	3.286609000000	0.826308000000
H	-1.533146000000	2.508898000000	2.341027000000
H	-0.629690000000	3.940425000000	1.756723000000
C	0.465255000000	-2.889707000000	2.452978000000
H	1.042863000000	-3.445317000000	1.705026000000
H	0.962146000000	-2.974886000000	3.429126000000
H	-0.527145000000	-3.351523000000	2.514362000000
C	-0.611428000000	-0.482332000000	3.425361000000
H	-0.686780000000	0.610152000000	3.379687000000
H	-1.632229000000	-0.882134000000	3.434605000000
H	-0.102994000000	-0.767280000000	4.356721000000
H	-1.312719000000	-2.977715000000	-0.711373000000
O	-1.974677000000	-1.087187000000	-0.941916000000
C	-3.075441000000	-0.469970000000	-1.413524000000
H	-3.685800000000	-1.137360000000	-2.060214000000
C	-4.015904000000	-0.073598000000	-0.277215000000
F	-3.405767000000	0.670822000000	0.712511000000
F	-4.509144000000	-1.200785000000	0.334189000000
F	-5.102093000000	0.656690000000	-0.715775000000
C	-2.781134000000	0.740184000000	-2.312467000000
F	-3.822989000000	1.008425000000	-3.171348000000
F	-2.542768000000	1.920622000000	-1.618031000000
F	-1.667824000000	0.523602000000	-3.089556000000

2_Product_HFIP

E_{el} = -3915.94785535 Ha
E_{ZPVE} = -3915.480998 Ha
H = -3915.445594 Ha
G = -3915.541603 Ha

Cu	0.231771000000	-0.369734000000	0.072724000000
P	0.535327000000	1.810791000000	0.617857000000
P	0.900162000000	-1.270667000000	2.064658000000
P	2.264900000000	-0.634433000000	-0.981873000000
C	3.103288000000	0.646277000000	1.541184000000
C	2.095521000000	1.825143000000	1.653564000000
C	3.489593000000	0.314836000000	0.070749000000
C	2.632283000000	-0.608099000000	2.328749000000
C	4.399156000000	1.124077000000	2.230628000000
H	3.330176000000	-1.430441000000	2.098606000000

H	2.744960000000	-0.407380000000	3.408164000000
H	1.786071000000	1.900982000000	2.709784000000
H	2.629376000000	2.764140000000	1.426729000000
H	3.705354000000	1.265618000000	-0.445102000000
H	4.438928000000	-0.247460000000	0.079172000000
H	4.191516000000	1.476963000000	3.249917000000
H	5.130712000000	0.307274000000	2.293899000000
H	4.856944000000	1.949642000000	1.669074000000
H	-0.108590000000	-2.142383000000	-2.700321000000
H	-0.043126000000	-3.055634000000	-0.894553000000
B	-0.743795000000	-2.497740000000	-1.717441000000
H	-1.931492000000	-3.077738000000	1.533713000000
H	-1.724333000000	-3.154934000000	-2.015300000000
C	2.992420000000	-2.323483000000	-1.006769000000
H	4.021593000000	-2.313178000000	-1.390322000000
H	2.988230000000	-2.764460000000	-0.003547000000
H	2.360807000000	-2.952831000000	-1.645352000000
C	2.727402000000	-0.087420000000	-2.677629000000
H	3.803797000000	-0.203664000000	-2.862044000000
H	2.166369000000	-0.706950000000	-3.388246000000
H	2.439900000000	0.955767000000	-2.848697000000
C	0.979850000000	2.999958000000	-0.717725000000
H	1.335342000000	3.952999000000	-0.303386000000
H	1.760454000000	2.577639000000	-1.361276000000
H	0.096655000000	3.182838000000	-1.337873000000
C	-0.570691000000	2.870551000000	1.639060000000
H	-1.459423000000	3.121243000000	1.048531000000
H	-0.908843000000	2.320469000000	2.524981000000
H	-0.072371000000	3.797461000000	1.953288000000
C	1.159577000000	-3.036675000000	2.515266000000
H	1.707430000000	-3.557575000000	1.722508000000
H	1.709579000000	-3.129279000000	3.461659000000
H	0.184516000000	-3.525535000000	2.616363000000
C	0.026550000000	-0.687123000000	3.579537000000
H	-0.078000000000	0.404215000000	3.564032000000
H	-0.982353000000	-1.118117000000	3.587583000000
H	0.552607000000	-0.984032000000	4.497019000000
H	-1.788953000000	-2.434248000000	1.173935000000
O	-1.274267000000	-1.206924000000	-0.995036000000
C	-2.358942000000	-0.595977000000	-1.575600000000
H	-2.796440000000	-1.246663000000	-2.353343000000
C	-3.435375000000	-0.404092000000	-0.519460000000
F	-2.967565000000	0.207071000000	0.625115000000
F	-3.945140000000	-1.619430000000	-0.144963000000
F	-4.482556000000	0.355868000000	-0.988716000000
C	-2.013152000000	0.717848000000	-2.267823000000
F	-2.968011000000	1.057679000000	-3.195638000000
F	-1.918859000000	1.788669000000	-1.390305000000
F	-0.813352000000	0.646009000000	-2.926108000000

2_DHB_Ia_HFIP

E_{el} = -3915.93946897 Ha

E_{ZPVE} = -3915.468917 Ha

H = -3915.433402 Ha

G = -3915.530886 Ha

C	2.823656000000	-1.962497000000	-1.114690000000
C	1.469493000000	-2.471972000000	-1.685041000000
C	2.751340000000	-1.641265000000	0.406582000000
C	3.405839000000	-0.774962000000	-1.930498000000
H	1.080961000000	-3.234395000000	-0.988792000000
H	1.668813000000	-3.001005000000	-2.632790000000
H	3.652103000000	-1.067055000000	0.679447000000
H	2.813290000000	-2.588024000000	0.968862000000
H	3.300805000000	-1.009478000000	-3.003272000000
H	4.489142000000	-0.705650000000	-1.733691000000
C	3.824042000000	-3.127035000000	-1.269155000000
H	4.780692000000	-2.881977000000	-0.788227000000
H	3.433378000000	-4.043174000000	-0.805923000000
H	4.018683000000	-3.335351000000	-2.329966000000
P	2.631172000000	0.892615000000	-1.630575000000
P	1.260181000000	-0.719152000000	1.068699000000
P	0.059745000000	-1.270653000000	-2.014607000000
Cu	0.537289000000	0.586929000000	-0.719803000000
C	1.939531000000	0.032665000000	2.602530000000
H	2.541718000000	-0.681797000000	3.179018000000
H	2.544522000000	0.912063000000	2.352326000000
H	1.101065000000	0.375672000000	3.221892000000
C	2.972283000000	1.769279000000	-3.210096000000
H	2.666035000000	2.815304000000	-3.091584000000
H	4.037569000000	1.730461000000	-3.473096000000
H	2.383611000000	1.338738000000	-4.027948000000
C	0.149530000000	-1.106892000000	-3.849835000000
H	1.051042000000	-0.554275000000	-4.139210000000
H	0.156737000000	-2.087141000000	-4.345414000000
H	-0.717600000000	-0.535582000000	-4.200440000000
C	-1.375078000000	-2.420411000000	-1.875546000000
H	-2.267031000000	-1.923482000000	-2.274592000000
H	-1.202293000000	-3.351132000000	-2.432645000000
H	-1.578120000000	-2.654390000000	-0.823931000000
C	3.838977000000	1.735363000000	-0.529294000000
H	3.907510000000	1.219409000000	0.435778000000
H	4.838882000000	1.788455000000	-0.979992000000
H	3.466454000000	2.749322000000	-0.337616000000
C	0.304500000000	-2.128224000000	1.779382000000
H	-0.060844000000	-2.785352000000	0.980642000000
H	0.931638000000	-2.715171000000	2.463991000000
H	-0.566396000000	-1.750028000000	2.322097000000
H	-0.501166000000	1.941658000000	-0.909872000000
B	0.130851000000	2.883790000000	-0.305065000000
H	0.722001000000	2.517058000000	0.699951000000
H	-0.773580000000	3.644066000000	0.005006000000
H	0.869443000000	3.437647000000	-1.091572000000
H	-2.118937000000	3.064097000000	0.611473000000
O	-2.806866000000	2.554713000000	1.084946000000
C	-2.245222000000	1.325426000000	1.424618000000
H	-1.234673000000	1.191702000000	0.997927000000
C	-2.095194000000	1.258757000000	2.929232000000
F	-3.272331000000	1.409212000000	3.604355000000
F	-1.543733000000	0.052660000000	3.336883000000
F	-1.234891000000	2.239986000000	3.349734000000
C	-3.107580000000	0.227851000000	0.836971000000
F	-4.375363000000	0.201569000000	1.348441000000
F	-3.208251000000	0.381340000000	-0.522194000000
F	-2.557821000000	-1.026276000000	1.051141000000

2_TS1$_{CuH}$_HFIP

E_{el} = -3915.88205585 Ha

E_{ZPVE} = -3915.416405 Ha

H = -3915.380771 Ha

G = -3915.478336 Ha

C	8.311805000000	-4.069369000000	-2.263111000000
C	6.949201000000	-4.621823000000	-2.763899000000
C	8.280295000000	-3.681702000000	-0.759162000000
C	8.845406000000	-2.910382000000	-3.149794000000
H	6.600541000000	-5.369932000000	-2.031766000000
H	7.117654000000	-5.171534000000	-3.706015000000
H	9.225966000000	-3.164455000000	-0.525091000000
H	8.282448000000	-4.606812000000	-0.157996000000
H	8.718890000000	-3.200612000000	-4.206391000000
H	9.932511000000	-2.811946000000	-2.986233000000
C	9.325922000000	-5.224063000000	-2.397605000000
H	10.296217000000	-4.943141000000	-1.966115000000
H	8.966886000000	-6.121821000000	-1.876415000000
H	9.483383000000	-5.481697000000	-3.453772000000
P	8.070091000000	-1.224463000000	-2.923664000000
P	6.886797000000	-2.603285000000	-0.112962000000
P	5.539539000000	-3.420480000000	-3.042355000000
Cu	5.990629000000	-1.446367000000	-1.921090000000
C	7.696624000000	-1.879532000000	1.375050000000
H	8.201841000000	-2.649228000000	1.973923000000
H	8.421089000000	-1.110921000000	1.082735000000
H	6.929744000000	-1.390537000000	1.987006000000

C	8.421903000000	-0.460631000000	-4.563815000000
H	8.223270000000	0.615256000000	-4.499603000000
H	9.467389000000	-0.613981000000	-4.863542000000
H	7.762244000000	-0.874399000000	-5.334619000000
C	5.533287000000	-3.264149000000	-4.880257000000
H	6.433548000000	-2.746489000000	-5.229665000000
H	5.473568000000	-4.245751000000	-5.369608000000
H	4.666932000000	-2.661537000000	-5.176668000000
C	4.090789000000	-4.544305000000	-2.847303000000
H	3.185305000000	-4.000206000000	-3.141248000000
H	4.194017000000	-5.444993000000	-3.467195000000
H	3.958939000000	-4.838839000000	-1.800262000000
C	9.345261000000	-0.351936000000	-1.914865000000
H	9.479882000000	-0.848517000000	-0.946910000000
H	10.315223000000	-0.316163000000	-2.429399000000
H	8.999548000000	0.670101000000	-1.718996000000
C	5.834942000000	-3.875134000000	0.720036000000
H	5.308403000000	-4.494113000000	-0.016211000000
H	6.442375000000	-4.528514000000	1.361207000000
H	5.079224000000	-3.387603000000	1.347459000000
H	5.056700000000	-0.156229000000	-2.032489000000
B	5.511742000000	1.515529000000	0.262118000000
H	6.365528000000	0.700374000000	0.427998000000
H	4.743402000000	1.752551000000	1.132379000000
H	5.537006000000	2.189629000000	-0.714857000000
H	3.959587000000	0.052487000000	-1.224038000000
O	3.271367000000	0.063769000000	-0.480866000000
C	3.199240000000	-1.246071000000	-0.039379000000
H	4.115756000000	-1.805290000000	-0.319851000000
C	3.113210000000	-1.246436000000	1.470509000000
F	2.166707000000	-0.399210000000	1.965888000000
F	2.842421000000	-2.507417000000	1.967433000000
F	4.329681000000	-0.877440000000	2.007136000000
C	2.053463000000	-1.990075000000	-0.698229000000
F	0.823007000000	-1.614524000000	-0.232114000000
F	2.071818000000	-1.787573000000	-2.056850000000
F	2.171102000000	-3.355413000000	-0.508856000000

2_INT1$_{CuH}$_HFIP

E_{el} = -3915.92864076 Ha

E_{ZPVE} = -3915.463346 Ha

H = -3915.427480 Ha

G = -3915.526850 Ha

C	2.149412000000	-1.840688000000	-1.163966000000
C	0.870008000000	-2.407800000000	-1.839394000000
C	2.004005000000	-1.734203000000	0.380576000000
C	2.617168000000	-0.508463000000	-1.816876000000
H	0.502502000000	-3.245067000000	-1.222517000000
H	1.149117000000	-2.845514000000	-2.813173000000
H	2.881655000000	-1.190947000000	0.768082000000
H	2.064072000000	-2.750176000000	0.806201000000
H	2.517420000000	-0.610715000000	-2.910686000000
H	3.694223000000	-0.377762000000	-1.619021000000
C	3.266846000000	-2.872423000000	-1.424457000000
H	4.181299000000	-2.598214000000	-0.881853000000
H	2.959608000000	-3.873283000000	-1.091746000000
H	3.507428000000	-2.925451000000	-2.494950000000
P	1.758852000000	1.072821000000	-1.299795000000
P	0.482401000000	-0.918628000000	1.112306000000
P	-0.586175000000	-1.277048000000	-2.147476000000
Cu	-0.325537000000	0.378294000000	-0.591510000000
C	1.140995000000	-0.231339000000	2.673643000000
H	1.845189000000	-0.926388000000	3.149897000000
H	1.613575000000	0.743007000000	2.498398000000
H	0.301591000000	-0.043718000000	3.349900000000
C	2.056919000000	2.153462000000	-2.757483000000
H	1.766583000000	3.175826000000	-2.486673000000
H	3.114915000000	2.149748000000	-3.051497000000
H	1.442424000000	1.841298000000	-3.609669000000
C	-0.391248000000	-0.889163000000	-3.939847000000
H	0.495153000000	-0.265366000000	-4.103898000000
H	-0.296229000000	-1.805264000000	-4.538143000000
H	-1.265701000000	-0.327063000000	-4.287165000000
C	-1.941471000000	-2.520527000000	-2.242352000000
H	-2.846470000000	-2.047159000000	-2.639106000000
H	-1.662805000000	-3.358660000000	-2.895136000000
H	-2.174454000000	-2.905254000000	-1.243162000000
C	2.978735000000	1.779601000000	-0.124393000000
H	3.098660000000	1.130297000000	0.750002000000
H	3.953399000000	1.908883000000	-0.613918000000
H	2.600347000000	2.740120000000	0.242930000000
C	-0.456654000000	-2.370641000000	1.745762000000
H	-0.807032000000	-3.006000000000	0.923543000000
H	0.161154000000	-2.975230000000	2.423378000000
H	-1.331784000000	-2.004553000000	2.294380000000
H	-1.668478000000	1.499378000000	-0.617978000000
B	0.234521000000	3.248845000000	1.627155000000
H	1.257346000000	2.851892000000	2.173493000000
H	-0.087768000000	4.345951000000	2.046262000000
H	0.380198000000	3.283491000000	0.407256000000
H	-1.404339000000	1.608086000000	0.130094000000
O	-0.897645000000	2.244801000000	1.924593000000
C	-1.916776000000	2.651941000000	2.743491000000
H	-1.661062000000	3.554077000000	3.328188000000
C	-2.194913000000	1.546607000000	3.746777000000
F	-1.123658000000	1.416522000000	4.604563000000
F	-3.303269000000	1.784964000000	4.522206000000
F	-2.376288000000	0.309912000000	3.159704000000
C	-3.157213000000	3.015917000000	1.933482000000
F	-2.838119000000	3.884841000000	0.922689000000
F	-3.745645000000	1.911484000000	1.343717000000
F	-4.123696000000	3.624459000000	2.699313000000

2_TS2$_{CuH}$_HFIP

E_{el} = -3915.92504960 Ha

E_{ZPVE} = -3915.460444 Ha

H = -3915.424746 Ha

G = -3915.523741 Ha

C	8.634815000000	-3.617870000000	-2.982194000000
C	7.580345000000	-4.540578000000	-3.648598000000
C	8.520703000000	-3.628009000000	-1.433596000000
C	8.633575000000	-2.182640000000	-3.585273000000
H	7.549105000000	-5.485783000000	-3.081405000000
H	7.927001000000	-4.803003000000	-4.662925000000
H	9.220949000000	-2.873215000000	-1.039193000000
H	8.891537000000	-4.601016000000	-1.067444000000
H	8.494592000000	-2.272344000000	-4.675960000000
H	9.633066000000	-1.738743000000	-3.441094000000
C	10.012253000000	-4.227924000000	-3.319138000000
H	10.812621000000	-3.695664000000	-2.787981000000
H	10.053547000000	-5.286284000000	-3.027969000000
H	10.214168000000	-4.161030000000	-4.396874000000
P	7.381593000000	-0.943624000000	-2.947942000000
P	6.872154000000	-3.323654000000	-0.578906000000
P	5.822707000000	-3.932714000000	-3.801888000000
Cu	5.633857000000	-2.247346000000	-2.215086000000
C	7.500691000000	-2.717678000000	1.037540000000
H	8.309960000000	-3.363603000000	1.404949000000
H	7.853362000000	-1.685014000000	0.942550000000
H	6.681475000000	-2.706077000000	1.761841000000
C	7.326861000000	0.265019000000	-4.332721000000
H	6.776733000000	1.148818000000	-3.987547000000
H	8.335039000000	0.570513000000	-4.642391000000
H	6.793202000000	-0.149374000000	-5.195228000000
C	5.749798000000	-3.440101000000	-5.578077000000
H	6.400935000000	-2.578147000000	-5.762787000000
H	6.059487000000	-4.264475000000	-6.234731000000
H	4.724466000000	-3.148276000000	-5.833925000000
C	4.923989000000	-5.539481000000	-3.897317000000
H	5.402347000000	-6.220098000000	-4.614513000000
H	4.889806000000	-6.020138000000	-2.913219000000
H	3.891197000000	-5.357564000000	-4.215281000000

C	8.392805000000	0.001730000000	-1.740633000000
H	8.681806000000	-0.632440000000	-0.895514000000
H	9.296269000000	0.401162000000	-2.220712000000
H	7.781479000000	0.816040000000	-1.336203000000
C	6.378545000000	-5.037573000000	-0.110704000000
H	6.113832000000	-5.622661000000	-0.999243000000
H	7.182047000000	-5.553906000000	0.431685000000
H	5.493678000000	-4.980494000000	0.533244000000
H	3.948552000000	-1.693421000000	-2.881512000000
B	5.241739000000	0.366463000000	-0.079850000000
H	5.588755000000	0.783781000000	-1.177134000000
H	6.181317000000	-0.149952000000	0.518947000000
H	4.740000000000	1.253283000000	0.587083000000
H	3.882069000000	-1.375683000000	-2.174300000000
O	4.181579000000	-0.714271000000	-0.362369000000
C	3.219186000000	-0.921928000000	0.590196000000
H	3.420724000000	-0.382547000000	1.533421000000
C	1.875797000000	-0.415626000000	0.080282000000
F	1.965856000000	0.893020000000	-0.305390000000
F	1.432439000000	-1.132208000000	-1.013276000000
F	0.889008000000	-0.487639000000	1.037654000000
C	3.188114000000	-2.401925000000	0.930565000000
F	3.045175000000	-3.212099000000	-0.174567000000
F	4.381042000000	-2.771091000000	1.527837000000
F	2.192829000000	-2.742228000000	1.813291000000

2_Product1_HFIP

E_{el} = -3915.94256876 Ha

E_{ZPVE} = -3915.474689 Ha

H = -3915.439145 Ha

G = -3915.536286 Ha

C	8.307342000000	-3.999888000000	-2.191353000000
C	6.921357000000	-4.475382000000	-2.706243000000
C	8.313441000000	-3.748749000000	-0.657528000000
C	8.854604000000	-2.785784000000	-2.990789000000
H	6.545995000000	-5.240435000000	-2.005616000000
H	7.064961000000	-4.992184000000	-3.670504000000
H	9.270453000000	-3.268376000000	-0.393082000000
H	8.310952000000	-4.724733000000	-0.143798000000
H	8.688128000000	-2.979662000000	-4.063704000000
H	9.949028000000	-2.740415000000	-2.856782000000
C	9.288724000000	-5.163466000000	-2.444918000000
H	10.271279000000	-4.947118000000	-2.004006000000
H	8.912095000000	-6.094449000000	-2.000223000000
H	9.426226000000	-5.330367000000	-3.521832000000
P	8.173222000000	-1.086564000000	-2.611969000000
P	6.940624000000	-2.714750000000	0.086660000000
P	5.548807000000	-3.220567000000	-2.944357000000
Cu	6.118038000000	-1.376931000000	-1.639275000000
C	7.780490000000	-1.976060000000	1.544279000000
H	8.338958000000	-2.725053000000	2.120558000000
H	8.457654000000	-1.175940000000	1.224773000000
H	7.020715000000	-1.517904000000	2.186688000000
C	8.463776000000	-0.235805000000	-4.217785000000
H	8.308221000000	0.840761000000	-4.086268000000
H	9.483479000000	-0.408832000000	-4.586995000000
H	7.743332000000	-0.587201000000	-4.965422000000
C	5.520861000000	-3.050833000000	-4.781133000000
H	6.423982000000	-2.542317000000	-5.139142000000
H	5.442115000000	-4.028492000000	-5.275644000000
H	4.657816000000	-2.437403000000	-5.064481000000
C	4.072305000000	-4.295267000000	-2.710209000000
H	3.175473000000	-3.737932000000	-3.004561000000
H	4.142556000000	-5.213273000000	-3.309004000000
H	3.956740000000	-4.561436000000	-1.652610000000
C	9.533420000000	-0.357388000000	-1.604446000000
H	9.679232000000	-0.939592000000	-0.686842000000
H	10.479995000000	-0.337282000000	-2.161190000000
H	9.261087000000	0.663957000000	-1.314265000000
C	5.920008000000	-4.007623000000	0.920194000000
H	5.422476000000	-4.647868000000	0.181438000000
H	6.536151000000	-4.638322000000	1.575310000000
H	5.139431000000	-3.532826000000	1.527906000000
H	3.467863000000	-0.386869000000	-4.402935000000
B	4.937835000000	0.527996000000	-0.749612000000
H	5.012785000000	-0.099677000000	-1.872716000000
H	5.855093000000	0.266338000000	0.022195000000
H	4.970875000000	1.682908000000	-1.085859000000
H	3.364615000000	-0.296617000000	-3.665759000000
O	3.601289000000	0.207876000000	-0.167139000000
C	3.384682000000	-1.079077000000	0.238721000000
H	4.206158000000	-1.771137000000	-0.041333000000
C	3.286141000000	-1.130856000000	1.754074000000
F	2.318522000000	-0.318785000000	2.267614000000
F	3.035624000000	-2.413019000000	2.220184000000
F	4.488287000000	-0.753077000000	2.310528000000
C	2.151224000000	-1.641221000000	-0.446411000000
F	0.982164000000	-1.051330000000	-0.056279000000
F	2.256954000000	-1.492209000000	-1.811708000000
F	2.025321000000	-3.002097000000	-0.222680000000