

SUPPLEMENTARY INFORMATION for

**A comprehensive Density Functional Theory study of the key role of
fluorination and dual hydrogen bonding in the activation of the
epoxide/CO₂ coupling by fluorinated alcohols**

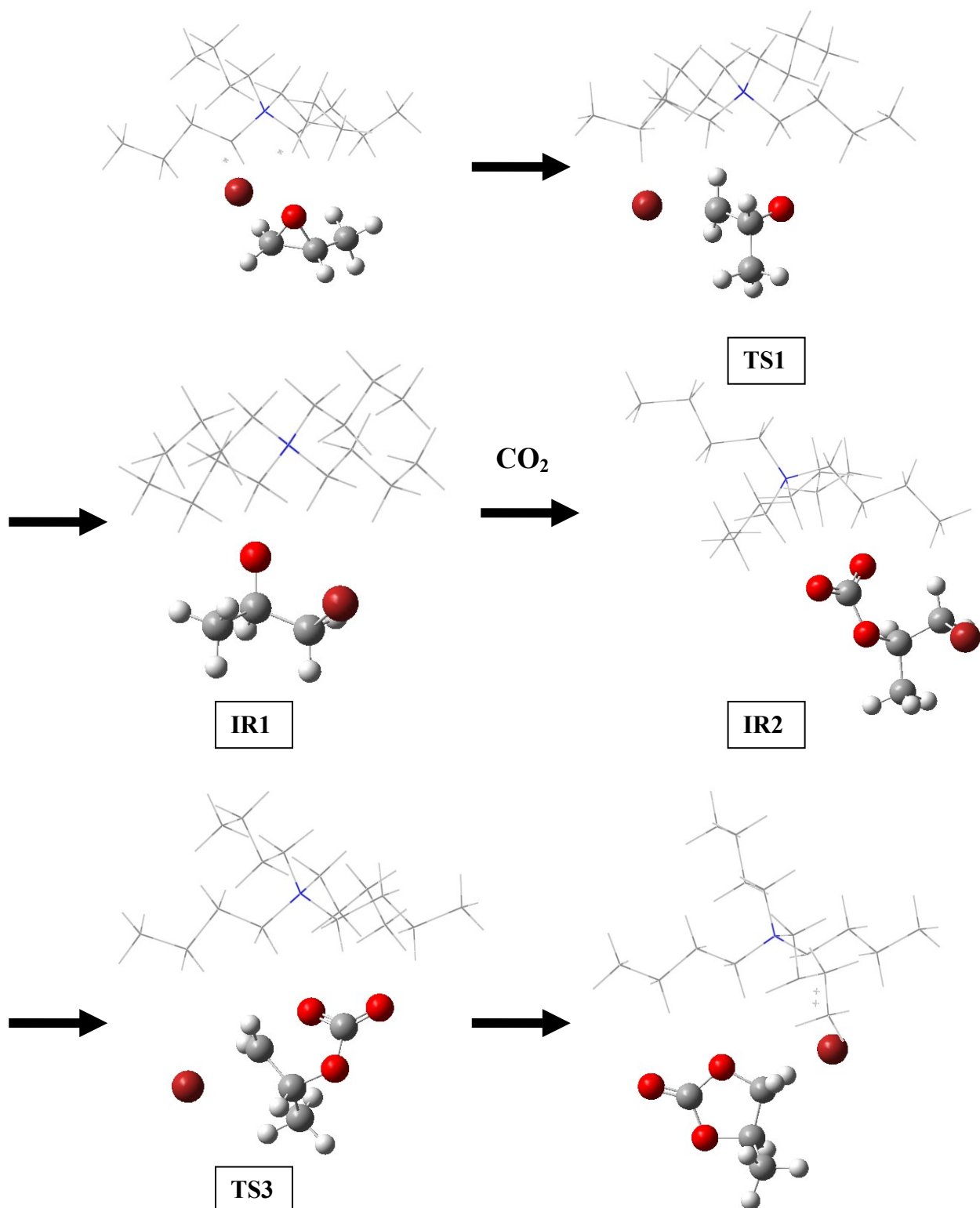
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TASSAING^{1,*}

- I. Cycloaddition of CO₂ onto propylene oxide catalyzed by TBABr
- II. Cycloaddition of CO₂ onto propylene oxide catalyzed by TBABr plus PFB
- III. Cycloaddition of CO₂ onto propylene oxide catalyzed by TBABr plus 2 molecules of *Tert*-Butanol
- IV. Key role of trifluoromethyl groups
- V. Optimized Cartesian coordinates (Å) from M06-2X/6-311G(d) calculations

Although CO₂, PO, the bromine ion and the different hydrogen bond donor activators will be represented using the Ball-and-Stick model, the tetrabutylammonium cation will be represented using the skeleton model in order to improve the visualization of those complex systems described below.

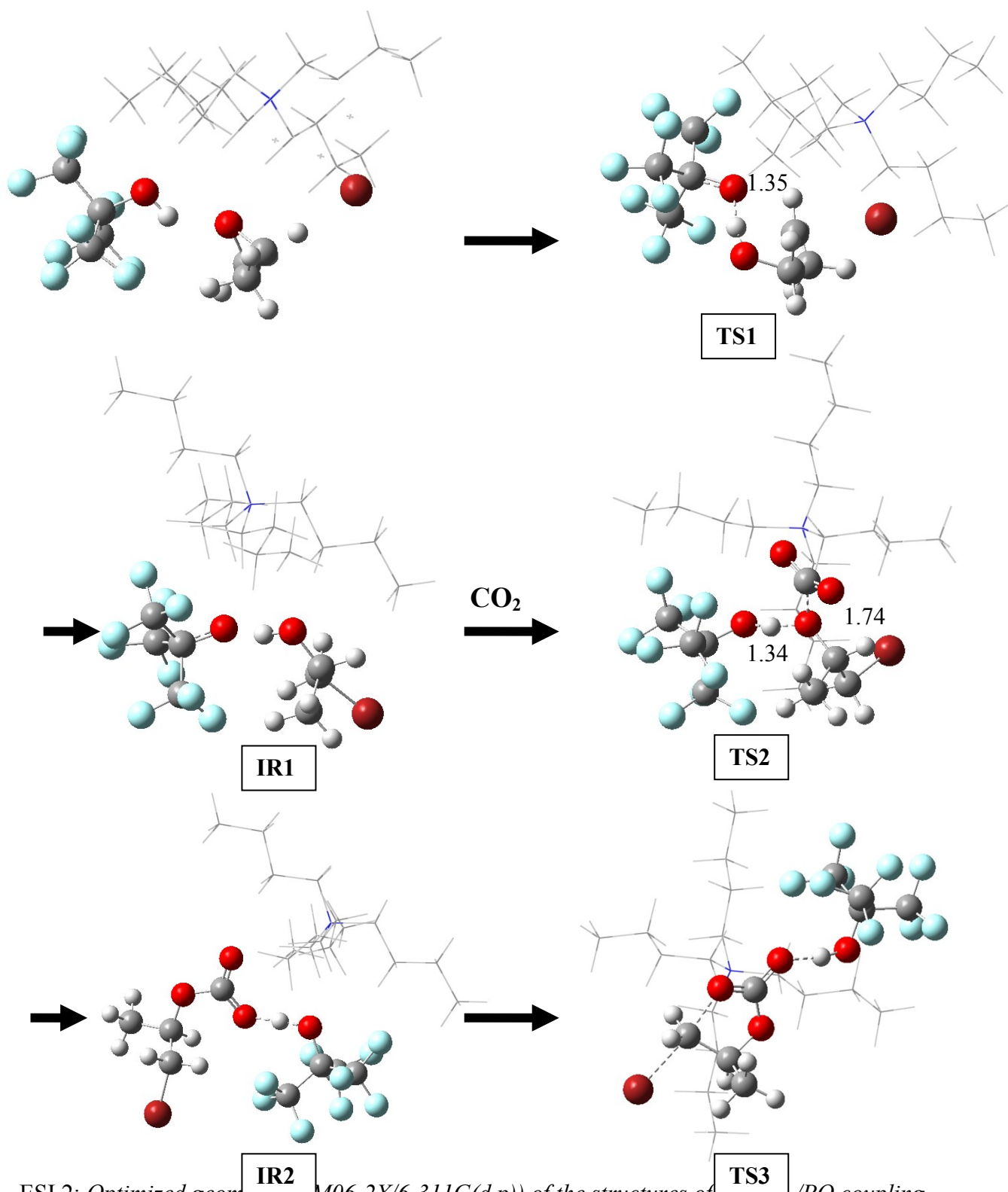
Dashed lines represent hydrogen bonds and distances are given in angstrom.

1- CYCLOADDITION OF CO₂ ONTO PROPYLENE OXIDE CATALYZED BY TBABr



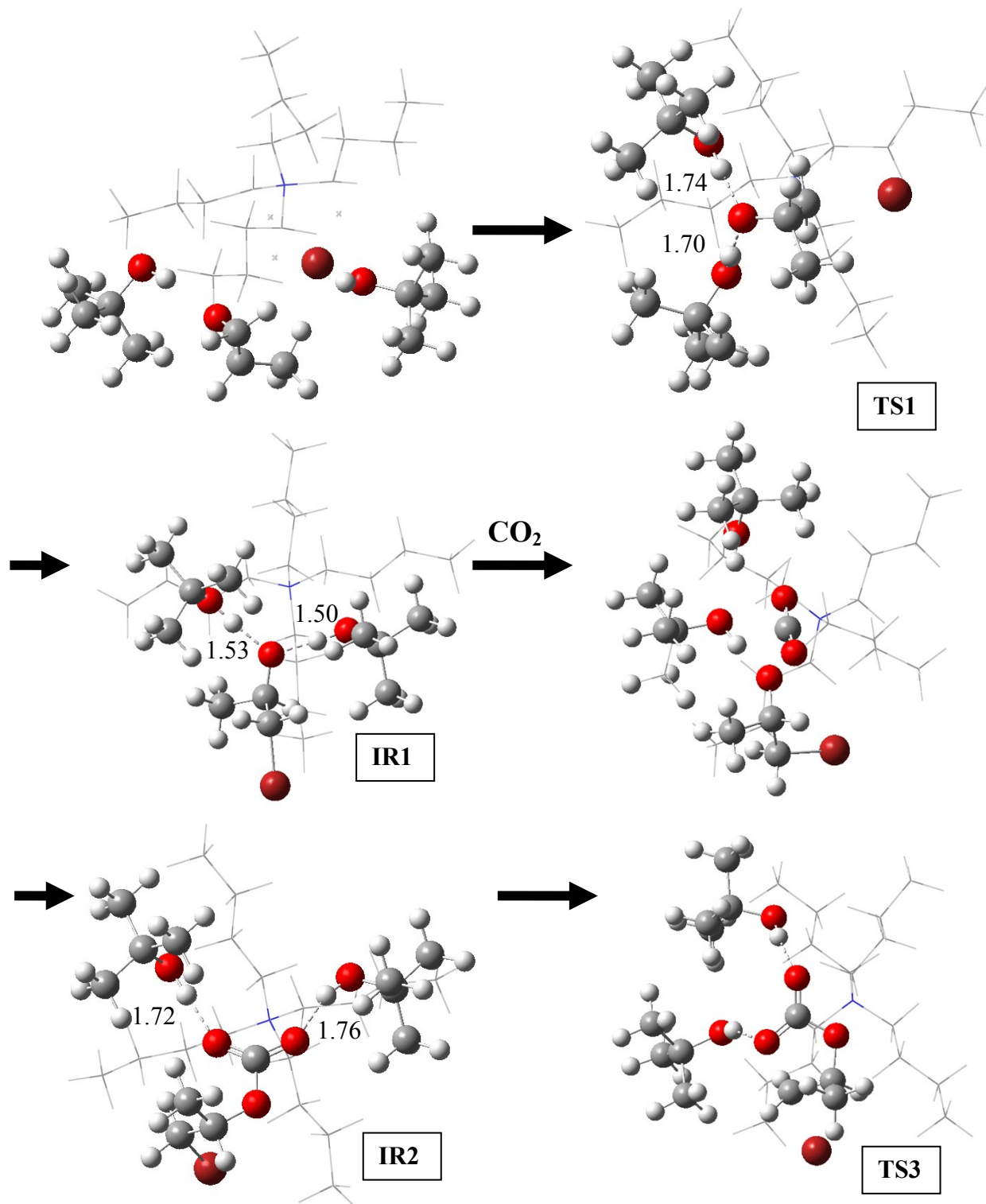
ESI 1: *Optimized geometries (M06-2X/6-311G(d,p)) of the structures of the CO₂/PO coupling in the presence of TBABr.*

2- CYCLOADDITION OF CO₂ ONTO PROPYLENE OXIDE CATALYZED BY TBABr PLUS PFB



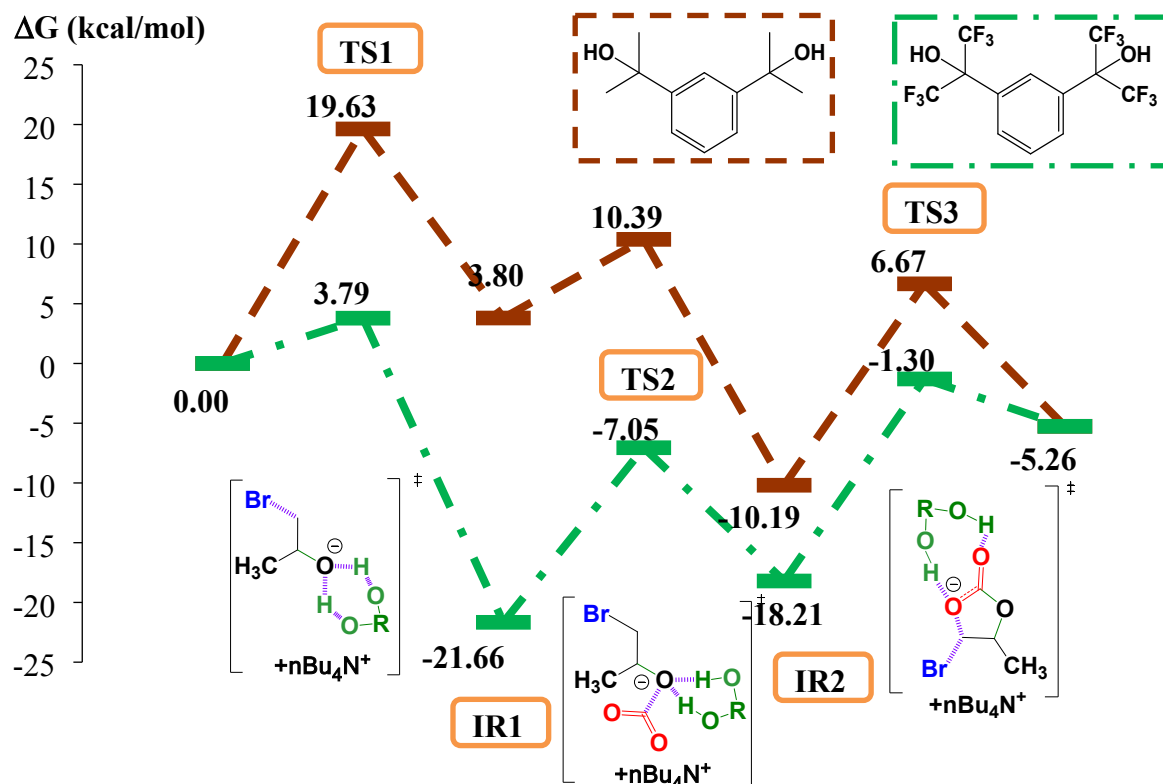
ESI 2: Optimized geometries (M06-2X/6-311G(d,p)) of the structures of the CO₂/PO coupling in the presence of TBABr plus PFB as catalysts. The dashed lines depict the intermolecular distances in angström.

3- CYCLOADDITION OF CO₂ ONTO PROPYLENE OXIDE
CATALYZED BY TBABr PLUS 2 MOLECULES OF *TERT*-
BUTANOL



ESI 3: Optimized geometries (M06-2X/6-311G(d,p)) of the structures of the CO₂/PO coupling in the presence of TBABr plus two molecules of *tert*-butanol as catalysts. The dashed lines depict the intermolecular distances in angström

4- KEY ROLE OF TRIFLUOROMETHYL GROUPS



ESI 4: Free energy profiles (M06-2X/6-311G(d,p)) and Lewis structures of the transition states for the propylene oxide/ CO_2 coupling catalyzed by TBABr plus 1,3-bis-HFAB or α, α' -dihydroxy-1,3-diisopropylbenzene

5- OPTIMIZED CARTESIAN COORDINATES (Å) FROM M06-2X/6-311G(D) CALCULATIONS

CO₂/PO COUPLING WITHOUT HBDS

TS1

N	1.41021600	-0.05089200	0.55704600
C	1.06333000	0.40745600	1.95441900
C	-0.32235800	1.01075600	2.10314100
H	1.83675300	1.12521600	2.23543900
H	1.17170700	-0.46601300	2.60022000
C	-0.47360600	1.68907100	3.46541200
H	-0.52767200	1.73951100	1.31095400
H	-1.07539900	0.21975500	2.01997300
C	-1.88098900	2.25327100	3.64353500
H	-0.25379100	0.97299000	4.26510200
H	0.26329600	2.49522000	3.55251200
H	-1.99047200	2.74912200	4.60909800
H	-2.10579600	2.97824100	2.85789200
H	-2.62763700	1.45793700	3.58439200
C	2.81863500	-0.59512200	0.61265700
C	3.28158000	-1.39253900	-0.59837400
H	2.88460100	-1.21665900	1.50667800
H	3.46654700	0.26836600	0.76916600
C	4.77277400	-1.71474400	-0.47234500
H	2.72047000	-2.32870100	-0.67494600
H	3.11493300	-0.83848100	-1.52621200
C	5.26969200	-2.57378600	-1.63163500
H	5.34303400	-0.78118000	-0.43231000
H	4.95392600	-2.23301700	0.47523600

H	6.33418200	-2.79007600	-1.53337800
H	4.73502900	-3.52564000	-1.66886000
H	5.11676400	-2.06635600	-2.58696400
C	1.32577000	1.10862900	-0.42530200
C	2.02931800	2.39707300	-0.03108800
H	0.26799500	1.35718100	-0.56267300
H	1.71468800	0.72820100	-1.37102500
C	1.82804900	3.41042200	-1.16523800
H	1.57549400	2.81204500	0.87469500
H	3.09982200	2.26452800	0.16202700
C	2.37626800	4.78622900	-0.80094600
H	2.32448900	3.04116800	-2.06930600
H	0.75583100	3.46429200	-1.38210900
H	2.23344700	5.49383600	-1.61875300
H	1.86299500	5.18703600	0.07657000
H	3.44581900	4.74403000	-0.57593700
C	0.42994200	-1.10356300	0.07535400
C	0.33081200	-2.35012900	0.94148800
H	0.73795500	-1.35453600	-0.94082200
H	-0.54815700	-0.62775900	-0.00560700
C	-0.38747700	-3.45952900	0.16695600
H	1.31819100	-2.70899700	1.25391700
H	-0.23739800	-2.12658700	1.85037900
C	-0.64702100	-4.68321300	1.03885200
H	-1.33255900	-3.06720800	-0.21988500
H	0.22332000	-3.73976700	-0.69901200
H	-1.13862900	-5.47139800	0.46735400
H	0.28369800	-5.09037300	1.44492200
H	-1.29965900	-4.42694500	1.87663800

Br	-3.50176000	-1.23059400	-0.68007500
C	-1.77287500	1.27726300	-1.77373000
H	-1.00584000	0.50148800	-1.95868300
C	-2.61206200	1.00367900	-0.60526100
H	-2.13905600	0.74650300	0.32104500
H	-3.54912700	1.53997100	-0.53679200
O	-1.35019000	2.37135900	-1.03891100
C	-2.50093000	1.59298400	-3.06401600
H	-2.97149000	0.69608700	-3.47350900
H	-3.26569100	2.34850400	-2.87094300
H	-1.79811200	1.99938200	-3.79515800

TS2

N	-1.98397000	0.44081000	0.46520300
C	-2.28273800	-0.35789000	1.71749200
C	-1.35502400	-1.53356300	1.98322600
H	-3.31482800	-0.69738700	1.61141700
H	-2.25854800	0.35200900	2.54609500
C	-1.94541600	-2.43457200	3.06864000
H	-1.18147200	-2.12560200	1.07971400
H	-0.36830700	-1.18264900	2.29430600
C	-0.99961300	-3.58743700	3.39529900
H	-2.15218500	-1.85198800	3.97367600
H	-2.90722100	-2.83210600	2.72485900
H	-1.43151900	-4.25898900	4.13887500
H	-0.77699000	-4.16569700	2.49579700
H	-0.05206700	-3.21047200	3.78645200
C	-3.02035500	1.53182200	0.38768000
C	-2.91258600	2.47432700	-0.80062100

H	-2.94001200	2.09256100	1.32085600
H	-3.99220200	1.03522600	0.38658200
C	-3.91644600	3.62110100	-0.65110100
H	-1.90523300	2.89333900	-0.87894100
H	-3.11904400	1.94322400	-1.73387100
C	-3.88916500	4.56361900	-1.85074700
H	-4.92346700	3.20894700	-0.52745400
H	-3.69188400	4.17951800	0.26367200
H	-4.60584300	5.37644200	-1.72769000
H	-2.89812500	5.00521100	-1.97816100
H	-4.14010500	4.03121500	-2.77100200
C	-2.02063300	-0.45402100	-0.75994700
C	-3.25182700	-1.32601900	-0.92992900
H	-1.14527600	-1.10018800	-0.70013100
H	-1.89182500	0.20582200	-1.61840500
C	-3.10876200	-2.12204000	-2.23218000
H	-3.32844100	-2.03724000	-0.10173800
H	-4.17685400	-0.73798200	-0.95473700
C	-4.26276300	-3.10014000	-2.42889000
H	-3.06426200	-1.42688200	-3.07736700
H	-2.15491200	-2.65735000	-2.20535200
H	-4.15192300	-3.65196800	-3.36314400
H	-4.29681800	-3.82777800	-1.61465100
H	-5.22407600	-2.57976900	-2.45784900
C	-0.57724500	1.00616300	0.51427000
C	-0.30180600	2.07948100	1.55282200
H	-0.37531000	1.39522700	-0.48599900
H	0.07495700	0.14362700	0.66112600
C	1.20005800	2.39134300	1.54075300

H	-0.86380000	2.99566600	1.33872500
H	-0.58772000	1.74541000	2.55576800
C	1.57009700	3.52407800	2.49108000
H	1.75462300	1.48731200	1.80970600
H	1.52210500	2.64560700	0.52523500
H	2.64288800	3.71523000	2.45272400
H	1.05251700	4.44861400	2.22230000
H	1.30555900	3.27661900	3.52260600
Br	4.41842700	1.29315900	-0.69619300
C	3.17663400	-1.45318300	-1.18496500
H	3.58164400	-1.00113900	-2.08640100
C	2.71393900	-0.36252900	-0.23036600
H	3.06014400	-0.32662500	0.78702200
H	2.00607500	0.37620400	-0.56901200
O	2.02853600	-2.20015500	-1.61905600
C	4.18923200	-2.37137600	-0.52861300
H	3.76086000	-2.80554800	0.37803400
H	4.46083900	-3.17582900	-1.21202800
H	5.08187600	-1.79994100	-0.26892500
C	1.03483000	-2.23062200	-0.69118500
O	1.28217200	-1.51205300	0.34196200
O	0.01636400	-2.86246300	-0.92398900

CO₂/PO COUPLING USING (MULTI)PHENOLIC HBDs

TBABr PLUS PHENOL

TS1

C	0.86256800	-2.60443200	-1.79324100
H	1.36178200	-3.30933700	-2.44027100
C	-0.06374400	-1.65993900	-2.41763100
H	-0.42932500	-0.88479600	-1.72959200
C	0.30417000	-1.08474100	-3.76275600
H	-0.57046100	-0.61413700	-4.21764100
H	1.10389200	-0.34738600	-3.65923400
H	0.64603600	-1.88569400	-4.42092700
O	-0.89808300	-2.78059800	-2.45871400
H	0.67358300	-2.89211400	-0.76885700
C	-3.38329100	-1.08139300	-1.30931900
C	-2.87185700	-1.73396200	-0.17304100
C	-3.40906300	-1.40991900	1.08531300
C	-4.43950100	-0.48595100	1.19790000
C	-4.95578100	0.14493100	0.06825800
C	-4.41791100	-0.16247800	-1.17953000
H	-2.98072200	-1.34626100	-2.28169500
H	-4.85862800	-0.27241000	2.17572600
H	-5.77382300	0.84933300	0.15812500
H	-4.81732400	0.31098300	-2.07031700
O	-1.89278400	-2.62778500	-0.24234800
H	-1.53513100	-2.76764900	-1.24908200
Br	2.95058800	-1.48957100	-1.20519700
N	0.41600800	1.19650300	0.98341300
C	0.07775700	-0.28277200	1.10156000
C	-0.19320600	-0.79778700	2.50786200

H	0.92012200	-0.81218000	0.65007000
H	-0.79483800	-0.44939700	0.46954800
C	-0.10640300	-2.32858500	2.51072700
H	0.53286400	-0.41251900	3.23031200
H	-1.18900800	-0.49221100	2.84466400
C	-0.49869600	-2.91384600	3.86341400
H	-0.74724800	-2.72853200	1.72076900
H	0.92020900	-2.61935500	2.25998500
H	-0.40849700	-4.00087400	3.86065100
H	0.13683700	-2.52564200	4.66427000
H	-1.53533200	-2.66717600	4.11018500
C	0.78952400	1.42387800	-0.46705400
C	1.28466100	2.81680100	-0.81566600
H	-0.10382800	1.18007300	-1.04284600
H	1.54408500	0.67471100	-0.71747000
C	1.41539900	2.93215300	-2.33713600
H	0.60613300	3.59493700	-0.44717700
H	2.26681500	2.99795300	-0.36784000
C	1.98508100	4.28107800	-2.76448300
H	2.05778500	2.12216400	-2.69742700
H	0.43250300	2.77976500	-2.79583100
H	2.07048800	4.34578200	-3.85001000
H	1.34600200	5.10168700	-2.42833700
H	2.98067400	4.43489200	-2.34120800
C	1.56363000	1.56780200	1.89422900
C	2.81135400	0.71675000	1.74295600
H	1.17585100	1.51962000	2.91291200
H	1.78647400	2.61540100	1.68761400
C	3.91944100	1.22329300	2.66707100

H	2.59939100	-0.33093500	1.97593000
H	3.16748100	0.72397900	0.70948700
C	5.17946700	0.37114100	2.53763200
H	4.15068700	2.26649900	2.42455800
H	3.56874000	1.21373000	3.70521700
H	5.97332900	0.73583600	3.19110100
H	4.97194900	-0.66846900	2.80070100
H	5.54866200	0.38004600	1.50990700
C	-0.76314600	2.05331600	1.39100300
C	-1.90856300	2.15429900	0.39463200
H	-0.36395700	3.05122300	1.58552600
H	-1.11592200	1.64919500	2.34198200
C	-3.05912200	2.95221300	1.02036300
H	-1.57196700	2.67506800	-0.50729000
H	-2.27790700	1.16890300	0.09097400
C	-4.00622500	3.50439600	-0.04199200
H	-3.60421000	2.30301300	1.71136800
H	-2.65711800	3.78386000	1.61106400
H	-4.87782400	3.97908300	0.41188000
H	-3.49931100	4.25070000	-0.65907500
H	-4.35471000	2.70451600	-0.69707400
H	-3.03022400	-1.93682800	1.95475500

TS2

Br	5.84062000	-0.18422100	0.10868500
C	-1.11105800	-4.10798800	-1.09360900
C	-0.90091500	-2.86896400	-1.68263600
C	0.04450000	-1.96693500	-1.15486700
C	0.76449900	-2.36996800	-0.01006600

C	0.54595000	-3.61411100	0.56831800
C	-0.39326800	-4.49497100	0.03723600
H	-1.83753800	-4.78729500	-1.52752500
H	1.12425000	-3.90141000	1.44031800
H	-0.54838700	-5.47019400	0.48236000
O	0.19075500	-0.77834800	-1.70666100
H	1.01108300	-0.14991500	-1.25454900
C	3.21324500	0.34452400	-1.06060400
H	3.71211400	1.22048900	-1.49586000
C	3.89749900	0.04808500	0.27477100
H	3.76582400	0.88135800	0.96089100
H	3.52942400	-0.87392600	0.72439900
O	1.88051400	0.66757600	-0.76707200
C	3.32593800	-0.81217900	-2.05057100
H	2.76268500	-0.56604200	-2.95244500
H	4.36619000	-0.99614800	-2.32337200
H	2.90801400	-1.73172100	-1.62972500
C	1.23129700	2.39123800	-1.75344500
O	2.18722500	2.71951400	-2.32961000
O	0.11992400	2.41725600	-1.36623800
N	-2.32879500	0.62874100	0.78793000
C	-0.84698100	0.47643700	1.09227400
C	-0.38937900	0.90308100	2.47775400
H	-0.30637900	1.03685000	0.32992000
H	-0.62069200	-0.57551200	0.92839400
C	1.07365100	0.47315900	2.63343400
H	-0.45487000	1.99029600	2.59238100
H	-0.98713100	0.45418900	3.27826500
C	1.72688800	1.05600300	3.88145600

H	1.11672500	-0.62115000	2.66420900
H	1.61539900	0.77527900	1.73191400
H	2.76095600	0.71977000	3.97494600
H	1.73348200	2.14826200	3.84418800
H	1.19329300	0.75415200	4.78698500
C	-2.47648700	0.42685300	-0.70726300
C	-3.88812900	0.58790800	-1.24589000
H	-2.08680500	-0.56899300	-0.91420000
H	-1.78582500	1.12238600	-1.18376300
C	-3.92221700	0.13711600	-2.70871200
H	-4.60889200	-0.00888100	-0.67559000
H	-4.21073200	1.63301000	-1.18583500
C	-5.28551500	0.37060000	-3.35181100
H	-3.14635100	0.66982200	-3.26694800
H	-3.66045700	-0.92481300	-2.75659100
H	-5.29617800	0.02916800	-4.38777800
H	-6.07069800	-0.16665000	-2.81352300
H	-5.54280200	1.43275400	-3.34714300
C	-2.83324800	1.98453900	1.20891000
C	-2.14301200	3.16819500	0.55377900
H	-2.72331600	2.02594200	2.29490100
H	-3.90217300	1.99945700	0.98826300
C	-2.66743100	4.47587800	1.14893600
H	-1.06035400	3.11325200	0.68412800
H	-2.31433000	3.16419600	-0.52603100
C	-2.01664600	5.69245600	0.49620400
H	-3.75498100	4.52725300	1.02599900
H	-2.47416000	4.48771800	2.22725500
H	-2.39469900	6.62184700	0.92464600

H	-0.93311200	5.67189700	0.63208800
H	-2.21484400	5.70907400	-0.57778600
C	-3.12880400	-0.39947400	1.55694200
C	-2.99752400	-1.84719600	1.10397200
H	-4.17364600	-0.08917400	1.49758200
H	-2.82178200	-0.30093100	2.59931300
C	-3.77455200	-2.74775300	2.06833500
H	-3.40250400	-1.97431300	0.09569300
H	-1.95336800	-2.17413800	1.06423700
C	-3.74154800	-4.20970300	1.63363200
H	-3.35069300	-2.65299900	3.07374900
H	-4.81305000	-2.40334900	2.13310300
H	-4.30806400	-4.83825500	2.32262100
H	-4.17071700	-4.32785500	0.63528600
H	-2.71368700	-4.57414400	1.59421900
H	-1.43716200	-2.57223200	-2.57784400
H	1.49295600	-1.68080600	0.40254500

TS3

O	3.13000300	0.38907300	2.19429000
H	2.22362900	0.41727000	2.58125300
C	-2.73477100	-0.01337200	1.66486400
H	-2.38272800	0.63414400	0.88473500
H	-3.61318800	0.29825300	2.20590600
C	-1.95242900	-1.24420800	2.09751500
H	-1.91970000	-1.97349000	1.29248800
C	-2.54041500	-1.86051700	3.35245400
H	-3.55133600	-2.21596300	3.14370500
H	-1.92650400	-2.70098500	3.67625200

H	-2.57789800	-1.11623100	4.15015300
O	-0.59191600	-0.85452000	2.29681000
Br	-4.10173200	-1.06141800	-0.02637900
N	0.32093300	0.89164100	-1.38622100
C	-0.15804300	-0.52412500	-1.11061700
C	-0.82263500	-1.25343400	-2.26694000
H	-0.86177500	-0.45720000	-0.28030400
H	0.71607100	-1.06691500	-0.74584000
C	-1.07324200	-2.70804800	-1.85887400
H	-1.78763900	-0.79330100	-2.50200900
H	-0.20645600	-1.23636700	-3.17211500
C	-1.89047000	-3.45547600	-2.90683700
H	-0.11302400	-3.20729300	-1.69103300
H	-1.62053800	-2.71499000	-0.91171600
H	-2.04022700	-4.49663300	-2.61820400
H	-2.87468700	-2.99432200	-3.01666800
H	-1.39254900	-3.44334100	-3.88027100
C	0.63885400	1.50740200	-0.03643800
C	1.19632400	2.91961500	-0.07076800
H	1.33122600	0.82475100	0.45928800
H	-0.29147800	1.49222100	0.53154300
C	1.52442500	3.37769100	1.35472300
H	2.10627400	2.97044700	-0.67838500
H	0.46815200	3.61133500	-0.50850400
C	2.01434100	4.82187700	1.37867100
H	0.64086600	3.25963700	1.98854200
H	2.28277600	2.71138100	1.77314500
H	2.25607400	5.13270300	2.39577500
H	2.91495000	4.94225100	0.77013600

H	1.25371000	5.50552800	0.99193500
C	-0.72962900	1.69419600	-2.12209800
C	-2.06161600	1.84589100	-1.41271700
H	-0.86582200	1.19707100	-3.08434800
H	-0.28594000	2.67109100	-2.31785900
C	-3.08444300	2.51276900	-2.33598300
H	-2.46516400	0.87129000	-1.12390400
H	-1.94914000	2.45244700	-0.50748900
C	-4.41178600	2.73688900	-1.61593300
H	-2.68931700	3.46476700	-2.70808000
H	-3.24361000	1.87144700	-3.20962900
H	-5.15509900	3.16942800	-2.28727200
H	-4.80091300	1.79111600	-1.23166400
H	-4.28327900	3.41850300	-0.77140900
C	1.53834800	0.87587500	-2.28264000
C	2.83321000	0.30864300	-1.71770100
H	1.70025800	1.91214100	-2.58496400
H	1.24441100	0.32175700	-3.17546600
C	3.91648300	0.48737600	-2.79000800
H	3.13309900	0.83409300	-0.80619700
H	2.74119100	-0.75108100	-1.45707600
C	5.25541500	-0.12634800	-2.39880700
H	3.57250900	0.03761100	-3.72825300
H	4.04581800	1.55701700	-2.98889600
H	6.00311200	0.04947900	-3.17415400
H	5.62369300	0.29939300	-1.46285100
H	5.15660200	-1.20344500	-2.25240200
C	-0.47923200	0.42477100	2.80216000
O	-1.57767700	1.04232600	2.86265500

O	0.65070800	0.81707800	3.06670500
C	3.36104800	-0.77100300	1.54924500
C	4.64772300	-0.99706300	1.05411800
C	2.36274000	-1.72698800	1.33566900
C	4.92501700	-2.15500800	0.34156700
C	2.65488000	-2.87986000	0.61212700
C	3.93023700	-3.10102300	0.10159000
H	5.93014900	-2.32063600	-0.03015900
H	1.87579200	-3.62036000	0.46389600
H	4.15413900	-4.00539000	-0.45026400
H	5.41223900	-0.25383300	1.24835700
H	1.37439700	-1.56945900	1.75336900

TBABr PLUS PYROCATECHOL

TS1

C	-2.64608400	-1.22947500	1.77590100
H	-3.57567300	-1.51823200	2.24160700
C	-1.97192300	-0.03784800	2.28286000
H	-1.12320700	0.29404300	1.67008700
C	-2.81626700	1.11632400	2.75828600
H	-2.20745200	1.81079200	3.34136900
H	-3.25448400	1.64238200	1.90675100
H	-3.62008200	0.74254100	3.39478000
O	-1.59154900	-0.94705600	3.28464300
H	-2.04537600	-1.99125100	1.30191200
C	1.40961900	0.20601300	3.09979300
C	1.42500000	-0.99747800	2.39451900
C	2.56663700	-1.31961500	1.63049200
C	3.65476300	-0.46775200	1.57240800
C	3.62304700	0.74020300	2.27520400

C	2.50571000	1.06750200	3.03508400
H	0.53934500	0.44115200	3.70356100
H	4.51675400	-0.76127400	0.98317300
H	4.47821200	1.40436200	2.24343100
H	2.48625200	1.99352900	3.59805200
O	2.54192400	-2.48133500	0.91290400
H	1.74938300	-2.95268200	1.21237600
O	0.42776700	-1.88268300	2.34806400
H	-0.47512000	-1.50577800	2.85896700
Br	-3.77390800	-0.70970600	-0.36050700
N	0.47713400	0.53443000	-1.43696400
C	-0.05748100	-0.75077400	-0.80776700
C	-0.18254600	-1.94758000	-1.73869400
H	-1.04281700	-0.50282300	-0.40876200
H	0.60204700	-0.99773500	0.02128700
C	-0.83383300	-3.10988500	-0.98236600
H	-0.79750400	-1.71281000	-2.61430300
H	0.80135500	-2.27003900	-2.09424100
C	-0.78316800	-4.40462700	-1.78736200
H	-0.32417700	-3.24233100	-0.02120700
H	-1.87228100	-2.84564200	-0.76591300
H	-1.27289100	-5.21871600	-1.25132300
H	-1.29262900	-4.28435300	-2.74686100
H	0.24885900	-4.70489100	-1.98791100
C	0.99338100	1.41083200	-0.31683500
C	1.59895700	2.72983800	-0.77548100
H	1.72584600	0.82276100	0.23764500
H	0.14771800	1.57847800	0.35043900
C	1.73478900	3.68863300	0.40873900

H	2.58929600	2.55918300	-1.21036900
H	0.98509100	3.20234100	-1.54953600
C	2.42482100	4.99067700	0.01504600
H	0.73831200	3.89981300	0.81201200
H	2.29332900	3.18920400	1.20555500
H	2.49682700	5.67115000	0.86454800
H	3.43778000	4.80072000	-0.34844500
H	1.87512700	5.50320700	-0.77878700
C	-0.65682400	1.21248200	-2.18980400
C	-1.63597800	1.99847000	-1.32925100
H	-1.18555300	0.41252900	-2.71108000
H	-0.20154600	1.86213200	-2.93959800
C	-2.86687100	2.38032400	-2.15284800
H	-1.97986600	1.39556300	-0.48453800
H	-1.16432800	2.90507300	-0.93588300
C	-3.88682100	3.13147400	-1.30335600
H	-2.56657200	2.98696100	-3.01511300
H	-3.32628600	1.46410000	-2.53428800
H	-4.75709500	3.41843600	-1.89556500
H	-4.23154500	2.48984900	-0.48898000
H	-3.45465000	4.04045300	-0.87554600
C	1.58507500	0.23820500	-2.41648900
C	2.80315100	-0.42366700	-1.79011000
H	1.85618200	1.18814200	-2.87998100
H	1.14564300	-0.39048200	-3.19247000
C	3.71464300	-1.03427000	-2.85414700
H	3.36881300	0.31057200	-1.20818500
H	2.50779000	-1.21004800	-1.09004400
C	4.95352300	-1.65796600	-2.21615200

H	3.15960400	-1.79924400	-3.40812800
H	4.00924000	-0.27025000	-3.58189700
H	5.58623100	-2.14259800	-2.96091600
H	5.55262800	-0.89675800	-1.70975700
H	4.66325600	-2.40445800	-1.47231700

TS2

Br	-5.91428300	-0.00103400	0.44993700
C	-0.45623400	4.15531100	-0.25254700
C	-0.76764200	3.06939800	-1.06333200
C	-0.96606000	1.79090600	-0.53877300
C	-0.83746400	1.60129900	0.86119500
C	-0.52766100	2.70429600	1.66045400
C	-0.33516700	3.97214400	1.11982100
H	-0.32180700	5.13648800	-0.69248900
H	-0.46146200	2.53214000	2.72921400
H	-0.11013900	4.80852600	1.77118800
O	-0.95052900	0.39959600	1.46311800
H	-1.40330000	-0.30743600	0.87194000
O	-1.21714800	0.78739500	-1.40399600
H	-1.51179800	-0.08468000	-0.94094400
C	-3.39767400	-1.29796600	-0.23674800
H	-3.76979500	-2.11498600	0.39468100
C	-3.95871000	0.01835000	0.30526300
H	-3.59238000	0.20894500	1.31149500
H	-3.71172700	0.85567800	-0.34744000
O	-1.99556900	-1.22663900	-0.13367800
C	-3.80286700	-1.55724400	-1.68242700
H	-3.34985000	-2.49318300	-2.01410000

H	-4.88578400	-1.63205900	-1.79468600
H	-3.43474000	-0.74445000	-2.31606800
C	-1.07200000	-3.09307600	0.10861800
O	-1.99000400	-3.80363700	0.06157800
O	0.04197800	-2.72941600	0.20319900
N	2.77404800	-0.14672600	-0.08467900
C	2.02330400	-0.17715500	1.23501900
C	2.85335800	-0.36219600	2.49329200
H	1.28029600	-0.96907000	1.14638900
H	1.46988500	0.75863400	1.28365200
C	1.91777800	-0.27634800	3.70459300
H	3.35422300	-1.33590000	2.50121200
H	3.62842500	0.40529200	2.59095500
C	2.66274500	-0.47956700	5.01975300
H	1.41614300	0.69594500	3.69903000
H	1.12606300	-1.02331300	3.59689200
H	1.98238800	-0.41485400	5.86992500
H	3.14367000	-1.46059100	5.05132000
H	3.43882900	0.27858800	5.15346100
C	1.70865300	-0.20490300	-1.16412400
C	2.22838100	-0.25436100	-2.59000400
H	1.08917300	0.67493000	-1.01090300
H	1.08481300	-1.07029300	-0.94017900
C	1.05716300	-0.10903100	-3.56636300
H	2.94948700	0.54924300	-2.77967100
H	2.74054700	-1.20298200	-2.78571300
C	1.51748600	-0.19529800	-5.01780400
H	0.31462500	-0.88476700	-3.35608000
H	0.54698800	0.83904800	-3.37660800

H	0.67609600	-0.08815200	-5.70357900
H	2.23931300	0.59313300	-5.24811100
H	1.99560500	-1.15682200	-5.22308400
C	3.73292500	-1.30208000	-0.19570100
C	3.10021300	-2.67803600	-0.08085400
H	4.48479800	-1.15257900	0.58237500
H	4.23425200	-1.19453500	-1.15897700
C	4.17261300	-3.76396200	-0.17514400
H	2.55502000	-2.78038100	0.86090600
H	2.36084100	-2.82859700	-0.87122800
C	3.56918000	-5.16127500	-0.05959800
H	4.70510100	-3.66912300	-1.12780300
H	4.91721500	-3.61614900	0.61482600
H	4.33595100	-5.93229400	-0.14759900
H	3.06809900	-5.28931300	0.90247500
H	2.82747800	-5.32960500	-0.84358500
C	3.58593600	1.12433100	-0.20070300
C	2.80261900	2.41702600	-0.39023500
H	4.26863100	0.98062800	-1.04026500
H	4.19401000	1.17623400	0.70398100
C	3.76631800	3.60472700	-0.31503300
H	2.30242300	2.42628700	-1.36306400
H	2.01623100	2.53957700	0.36158100
C	3.04962600	4.93438800	-0.52857500
H	4.26329000	3.60839300	0.66118200
H	4.55464100	3.48250000	-1.06641000
H	3.75035900	5.76984700	-0.48833400
H	2.54857600	4.95490900	-1.49950800
H	2.28527100	5.08395000	0.23612700

H	-0.88514400	3.18400600	-2.13545800
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TS3

O	-3.11162500	1.45409400	-0.96942800
H	-2.42066300	1.29683700	-1.63871900
C	2.60204200	0.23397700	-1.98103900
H	2.43029400	0.80546700	-1.08652900
H	3.29957800	0.63796900	-2.69581400
C	1.87117700	-1.07239000	-2.26204600
H	2.06821400	-1.79655000	-1.47642900
C	2.25002100	-1.63434000	-3.61827700
H	3.31077700	-1.89136000	-3.61899200
H	1.66339200	-2.52853400	-3.82822700
H	2.05947100	-0.89195300	-4.39649300
O	0.46242700	-0.82011400	-2.19027100
Br	4.47002000	-0.75348000	-0.75858100
N	0.25879300	0.40935900	1.63777600
C	0.72775900	-0.90244400	1.03068400
C	1.00139100	-2.04213300	1.99795200
H	1.64108700	-0.66904900	0.47944600
H	-0.03559200	-1.19301000	0.30549700
C	1.64383800	-3.19848600	1.22396500
H	1.68367900	-1.74076700	2.79871200
H	0.07338000	-2.38902500	2.46434400
C	1.89285700	-4.41205600	2.11373300
H	0.99086500	-3.47712000	0.38952600
H	2.58726000	-2.85097000	0.78946200
H	2.36577500	-5.21851800	1.55197500
H	2.55221700	-4.15566900	2.94671200

H	0.95712100	-4.79486700	2.52914000
C	-0.16548200	1.27704700	0.47324600
C	-0.75324200	2.63505300	0.81519600
H	-0.89484600	0.69312300	-0.08642200
H	0.71708900	1.39214400	-0.15442600
C	-0.70423200	3.51893300	-0.43804000
H	-1.79396600	2.51606000	1.13078400
H	-0.20729200	3.13111200	1.62485700
C	-1.62451000	4.72737800	-0.31683300
H	0.33057100	3.83555300	-0.60762500
H	-0.98265500	2.92804800	-1.31475000
H	-1.54257000	5.37409500	-1.19146800
H	-2.66276200	4.39738300	-0.23655500
H	-1.38299800	5.32358600	0.56771700
C	1.36996200	1.05966400	2.43592900
C	2.54976500	1.58855600	1.63738100
H	1.70493800	0.30940100	3.15316700
H	0.90785400	1.86823300	3.00408600
C	3.66289200	2.05188400	2.58076600
H	2.97307000	0.81729200	0.98732200
H	2.24093300	2.43219500	1.01106900
C	4.84647300	2.61524100	1.79887000
H	3.27489800	2.80439700	3.27646200
H	3.99397100	1.20081000	3.18478700
H	5.65295900	2.91795200	2.46826000
H	5.23603600	1.86636400	1.10523100
H	4.54615300	3.49044600	1.21707000
C	-0.89486500	0.19563000	2.58745500
C	-2.14307600	-0.41889600	1.97918700

H	-1.13053500	1.17904600	2.99923500
H	-0.50735400	-0.42008100	3.40198400
C	-3.17815000	-0.66425200	3.07942200
H	-2.56749200	0.25541200	1.22999100
H	-1.92032300	-1.35699800	1.46271000
C	-4.48033200	-1.22286200	2.51440500
H	-2.76466100	-1.35592900	3.82223100
H	-3.37777200	0.27641700	3.60474700
H	-5.21787400	-1.37768000	3.30383700
H	-4.90680400	-0.54207500	1.77366400
H	-4.30956900	-2.17852600	2.01386500
C	0.14154300	0.44672700	-2.58596100
O	1.12781000	1.19521100	-2.80079500
O	-1.06588500	0.70621700	-2.63147200
C	-4.00936900	0.42105000	-0.95265900
C	-5.35776900	0.71239800	-0.78653600
C	-3.59263600	-0.91817800	-1.02884100
C	-6.29750300	-0.30894700	-0.69191800
C	-4.54010300	-1.93160800	-0.94570600
C	-5.88761900	-1.63436600	-0.77375100
H	-7.34498900	-0.06615400	-0.56298000
H	-4.18834400	-2.95422200	-1.01482700
H	-6.61186400	-2.43696000	-0.70812900
O	-2.27175500	-1.25461400	-1.12007200
H	-1.81993000	-0.69448000	-1.78234100
H	-5.64575100	1.75560400	-0.73445900

TBABR PLUS PYROGALLOL

TS1

C	2.66072800	0.50098100	2.04206200
H	3.60274100	0.57894300	2.56160900
C	1.98759300	-0.79054500	2.02238700
H	1.13217600	-0.84842400	1.33751600
C	2.81043300	-2.05143900	2.01563500
H	2.18500800	-2.89788900	2.30747500
H	3.22537900	-2.22895000	1.02068000
H	3.63071600	-1.95736400	2.72912000
O	1.62089000	-0.32031000	3.30290200
H	2.07768300	1.39470100	1.87855600
C	-1.53820300	-1.24797000	2.72910400
C	-1.48475900	0.13319100	2.48770900
C	-2.57479000	0.75413300	1.86020300
C	-3.69813600	0.04328400	1.46429600
C	-3.73396800	-1.32916600	1.69990700
C	-2.66811600	-1.96396900	2.32327100
H	-4.51982300	0.57331800	0.99838000
H	-4.60676200	-1.90364100	1.41333500
H	-2.68423800	-3.02607500	2.53491800
O	-2.48258300	2.09287100	1.60473600
H	-1.70284700	2.40798100	2.08407400
O	-0.45906200	0.96043500	2.80332700
H	0.39788700	0.46777800	3.10091500
Br	3.79982000	0.84672900	-0.16698400
N	-0.43366200	0.06824700	-1.61800700
C	0.08683500	1.04584800	-0.56749300
C	0.26369900	2.48660100	-1.02331300
H	1.05326400	0.65418600	-0.24608100

H	-0.60524600	1.00755800	0.27139400
C	0.88030400	3.30206200	0.11787900
H	0.92582400	2.55239200	-1.89303100
H	-0.69879800	2.93234900	-1.29366300
C	0.88663700	4.79556200	-0.19153700
H	0.31940300	3.11064900	1.03972900
H	1.90319000	2.95181800	0.27909700
H	1.35461800	5.35970500	0.61642300
H	1.44820900	4.99868600	-1.10676900
H	-0.12906800	5.17708200	-0.32526900
C	-0.99342200	-1.13426900	-0.88850200
C	-1.59231000	-2.20273900	-1.79273300
H	-1.74251400	-0.76299000	-0.18777500
H	-0.17230900	-1.53976700	-0.29667000
C	-1.80294300	-3.49823000	-1.00657300
H	-2.55723200	-1.86620700	-2.18620300
H	-0.94645100	-2.40646700	-2.65339900
C	-2.48096100	-4.57383400	-1.84910200
H	-0.83407600	-3.86006200	-0.64610000
H	-2.40120000	-3.27842900	-0.11797900
H	-2.62109600	-5.49214500	-1.27737000
H	-3.46356700	-4.23963900	-2.19142600
H	-1.88400000	-4.81757500	-2.73186800
C	0.71831700	-0.32496000	-2.53089700
C	1.66840300	-1.37487800	-1.97457200
H	1.26746500	0.59747500	-2.72801500
H	0.27931700	-0.66653100	-3.47003500
C	2.90248600	-1.48918100	-2.87146200
H	2.01200000	-1.09360800	-0.97590900

H	1.17582000	-2.35032300	-1.90936100
C	3.91203700	-2.47878300	-2.29832900
H	2.60138900	-1.79177900	-3.88106100
H	3.37298600	-0.50456600	-2.94565700
H	4.77055100	-2.59201700	-2.96200000
H	4.27773900	-2.11521300	-1.33516600
H	3.46336800	-3.46588900	-2.15483700
C	-1.50601300	0.70347900	-2.46596900
C	-2.73693600	1.14603900	-1.68938200
H	-1.77465200	-0.02919800	-3.22831700
H	-1.03349900	1.54536900	-2.97466300
C	-3.60977600	2.07796100	-2.52945200
H	-3.32483500	0.27315300	-1.38939300
H	-2.45852800	1.66130100	-0.76542800
C	-4.86691700	2.48882900	-1.76713000
H	-3.03202000	2.96921100	-2.79791100
H	-3.88420300	1.58719500	-3.46965300
H	-5.47711000	3.18209000	-2.34767100
H	-5.48075300	1.61521200	-1.53311200
H	-4.60147600	2.97239700	-0.82354700
O	-0.54823400	-1.94293500	3.33575900
H	0.21207400	-1.37757000	3.57275400

TS2

Br	-6.03724600	-0.06523900	-0.08960500
C	-0.14464300	-3.89033500	0.54844200
C	-0.36703600	-2.67214900	1.17139800
C	-0.79255400	-1.53916800	0.46087900
C	-0.96313900	-1.63786000	-0.93103900

C	-0.72383100	-2.86478000	-1.56078100
C	-0.33023800	-3.97766600	-0.82896200
H	0.16031400	-4.74019700	1.14582200
H	-0.88116500	-2.91622300	-2.63132800
H	-0.17616400	-4.92426300	-1.33331700
O	-1.27940900	-0.57573600	-1.70790900
H	-1.61700400	0.20093800	-1.16957300
O	-0.94465600	-0.41588900	1.19956100
H	-1.46121000	0.36892100	0.68389500
O	-0.13665300	-2.51917900	2.50722700
H	-0.48943500	-1.64456100	2.72971100
C	-3.49655700	1.32865000	0.17338100
H	-3.95555200	2.10608500	-0.44914600
C	-4.08280000	-0.02559500	-0.22588500
H	-3.85461800	-0.25945900	-1.26299600
H	-3.71590200	-0.82118500	0.42360100
O	-2.11578900	1.27260400	-0.10632100
C	-3.72588000	1.65593800	1.64380000
H	-3.27134500	2.62149800	1.87083100
H	-4.78841700	1.70472500	1.88547300
H	-3.25548600	0.88890300	2.26654700
C	-1.18844400	3.08610600	-0.21471500
O	-2.09071700	3.82154800	-0.24511600
O	-0.06553700	2.72939800	-0.20554200
N	2.80878300	0.26346400	-0.09478700
C	1.80740600	0.25724000	-1.23834800
C	2.39366800	0.12840600	-2.63366100
H	1.22362600	1.17109200	-1.13528700
H	1.13100100	-0.56958900	-1.03590400

C	1.27729200	0.29965500	-3.66907400
H	3.16597600	0.88432400	-2.81707600
H	2.85509600	-0.85532000	-2.77317000
C	1.79511800	0.12503700	-5.09312800
H	0.47683700	-0.41382200	-3.45720600
H	0.83177700	1.29265500	-3.54953600
H	0.99387400	0.25777500	-5.82123700
H	2.57881400	0.85285400	-5.32096500
H	2.21441100	-0.87423700	-5.23678500
C	1.98028300	0.31215600	1.17418100
C	2.74891700	0.52627100	2.46643500
H	1.43433800	-0.62794600	1.20864500
H	1.23022100	1.08948600	1.02735900
C	1.81448700	0.25957100	3.65099600
H	3.60999900	-0.14691800	2.54128900
H	3.12829600	1.55199300	2.52871800
C	2.46830300	0.59987600	4.98626900
H	0.89595200	0.84094500	3.52053900
H	1.52147300	-0.79463200	3.63209700
H	1.79844800	0.38180300	5.81903200
H	3.38358200	0.02052400	5.13316400
H	2.73043500	1.65975600	5.03557600
C	3.73923200	1.44580100	-0.18653200
C	3.06353100	2.80472800	-0.25656500
H	4.36394400	1.28260700	-1.06626200
H	4.39074600	1.38747100	0.68760300
C	4.10650500	3.91774300	-0.14212800
H	2.51656800	2.91339100	-1.19722700
H	2.32310900	2.91723900	0.53898500

C	3.47238100	5.29996500	-0.27143100
H	4.61932800	3.83459000	0.82242100
H	4.87208200	3.78781900	-0.91496700
H	4.21776300	6.08887100	-0.16122300
H	2.99521200	5.41907600	-1.24672100
H	2.70560700	5.44788700	0.49230900
C	3.67037600	-0.97634800	-0.12672900
C	2.94598900	-2.30616600	0.02442100
H	4.41281100	-0.85762000	0.66467400
H	4.20553400	-0.94244600	-1.07703800
C	3.93204100	-3.44807900	-0.23803400
H	2.53356900	-2.41577600	1.03189700
H	2.10264400	-2.38994000	-0.66930600
C	3.28223000	-4.81659500	-0.05827400
H	4.32710200	-3.35817400	-1.25595600
H	4.78851000	-3.35350500	0.43900000
H	3.99799100	-5.61868000	-0.24546400
H	2.89685000	-4.93175100	0.95739800
H	2.44083100	-4.93424800	-0.74388900

TS3

O	-2.81738400	0.46151900	-1.18842500
H	-2.23080100	0.24238000	-1.95877000
C	2.50620500	-0.60840300	-2.04555500
H	2.50093600	0.29025700	-1.45339900
H	3.23815000	-0.67597800	-2.83288900
C	1.48806700	-1.72273800	-1.83855000
H	1.56030600	-2.13419100	-0.83569600
C	1.64471700	-2.81622600	-2.87653500

H	2.62509000	-3.28210500	-2.76179700
H	0.87166600	-3.57264300	-2.74116600
H	1.56203000	-2.39377500	-3.87999300
O	0.17915400	-1.13371300	-1.90752900
Br	4.17190700	-1.42740300	-0.47231300
N	0.46763500	1.19709800	1.35484100
C	0.83622500	-0.27441300	1.27855700
C	1.50071900	-0.87481100	2.50626300
H	1.51603300	-0.37252500	0.43378500
H	-0.08181200	-0.80585800	1.02856500
C	1.59611600	-2.39319100	2.32409000
H	2.51272900	-0.47418400	2.62816400
H	0.93868200	-0.66065500	3.42141500
C	2.30823300	-3.05967100	3.49667600
H	0.58880700	-2.80492800	2.20274300
H	2.14942900	-2.60012700	1.40305900
H	2.35915200	-4.14064900	3.36027500
H	3.33113000	-2.68624500	3.58587300
H	1.78986000	-2.86315400	4.43908500
C	0.02714900	1.59878400	-0.03919500
C	-0.43804900	3.03553100	-0.20017200
H	-0.76424600	0.90423300	-0.32120200
H	0.87816300	1.41129700	-0.69316700
C	-0.79415500	3.29681500	-1.66741300
H	-1.31944300	3.23334700	0.41859100
H	0.34588700	3.73745500	0.10550900
C	-1.18113100	4.75330900	-1.90209800
H	0.05351900	3.02304600	-2.30433200
H	-1.61126300	2.63393300	-1.95860600

H	-1.43916100	4.92394700	-2.94797700
H	-2.04572500	5.03304700	-1.29423000
H	-0.35899700	5.42712200	-1.64644000
C	1.64976800	2.01716000	1.81656100
C	2.87248600	1.95220300	0.91545300
H	1.89231800	1.65569400	2.81734100
H	1.29663100	3.04423100	1.91647200
C	4.07866200	2.60872200	1.59034600
H	3.14336800	0.91691600	0.68477800
H	2.67423000	2.46420800	-0.03246900
C	5.30669900	2.55698300	0.68483200
H	3.84331100	3.64607300	1.85311300
H	4.29106600	2.08410000	2.52802600
H	6.17828400	2.99231900	1.17558200
H	5.53912500	1.52334700	0.41731500
H	5.12956900	3.11108100	-0.24023600
C	-0.65249400	1.42282700	2.34838700
C	-1.98574500	0.78571400	1.99189300
H	-0.76430000	2.50521300	2.43461300
H	-0.28801100	1.05592100	3.30901700
C	-3.03219200	1.08885900	3.06640900
H	-2.34899600	1.16105200	1.03133500
H	-1.89035600	-0.29867900	1.88776700
C	-4.40718300	0.57558500	2.64444900
H	-2.73184200	0.62850100	4.01373400
H	-3.07873500	2.16951200	3.24269100
H	-5.14762800	0.73209000	3.43050500
H	-4.75358400	1.09074600	1.74471700
H	-4.37201200	-0.49271200	2.41272700

C	0.11861500	-0.08940700	-2.81997400
O	1.24650100	0.25348900	-3.25449300
O	-0.99309700	0.37370800	-3.03881700
C	-3.57745200	-0.57854000	-0.70858000
C	-4.96153900	-0.38169200	-0.68766500
C	-3.03613000	-1.73136400	-0.13990900
C	-5.80424100	-1.32885000	-0.11928000
C	-3.87724100	-2.68212700	0.43390100
C	-5.25125000	-2.47520400	0.43836900
H	-6.87077000	-1.14642100	-0.12095700
H	-3.43060900	-3.57186400	0.85832900
H	-5.90174700	-3.22013600	0.88021400
O	-5.46967700	0.77081700	-1.18481200
H	-4.72193100	1.27279000	-1.53462100
O	-1.68747600	-1.92855800	-0.07118400
H	-1.22103100	-1.57084500	-0.84578500

CO₂/PO COUPLING USING FLUORINATED MONOALCOHOLS AS HBDs

TBABr PLUS TFE

TS1

C	3.67551100	-0.87700900	-0.19972100
C	2.73406500	-1.91390700	-0.79165000
C	2.89749800	-3.23563000	-0.03995200
H	3.90657400	-3.63901600	-0.14335300
H	2.66829100	-3.09678100	1.01767300
H	2.18056300	-3.94146400	-0.46357800
C	3.04282900	-2.08510600	-2.28028300
H	2.30664800	-2.77705600	-2.69349800
H	2.94722800	-1.12871400	-2.79689500
H	4.04611200	-2.48316300	-2.44255500
O	1.44798800	-1.38797400	-0.60589900
H	0.80068800	-2.07640600	-1.05859500
F	3.53614300	0.33081600	-0.79305000
F	4.96249500	-1.22382300	-0.33057400
F	3.45539000	-0.67494600	1.11188400
Br	-3.71965400	-1.45926100	-0.29750000
C	-1.65625500	-2.10328600	-1.37506700
H	-2.07135800	-2.08648900	-2.37053100
H	-1.16256700	-1.21229600	-1.02085700
C	-1.13011600	-3.37460700	-0.86433700
H	-1.69447500	-4.24285000	-1.21866500
C	-0.83280400	-3.47385000	0.61625200
H	-1.76086200	-3.51963200	1.19016700
H	-0.24043900	-4.36992100	0.81690400
H	-0.25277300	-2.60505700	0.93723500
O	-0.04732500	-3.05946000	-1.69208600

N	-0.43985700	1.77316900	0.50538500
C	-1.69041400	2.60964200	0.32237600
C	-2.64157900	2.14015800	-0.76977900
H	-1.35690400	3.63057300	0.12749400
H	-2.19349100	2.61036300	1.28992200
C	-4.03559300	2.73547900	-0.56331600
H	-2.26058600	2.43464600	-1.75327900
H	-2.75200200	1.05230900	-0.76827300
C	-4.98449600	2.31128700	-1.68057600
H	-4.42555300	2.38128500	0.39660400
H	-3.97744700	3.82859200	-0.50510900
H	-5.98565200	2.71517700	-1.52270400
H	-4.62753400	2.66601100	-2.65102000
H	-5.05486200	1.22157900	-1.71791800
C	0.50968600	2.56155400	1.37013200
C	1.82699200	1.86502400	1.65977000
H	-0.03005300	2.79024600	2.29096700
H	0.68583000	3.50643100	0.85415100
C	2.69251600	2.71375300	2.59186000
H	1.66207400	0.88342600	2.11190700
H	2.37340100	1.68737200	0.73104200
C	4.05198000	2.06390600	2.83733100
H	2.83274900	3.70839900	2.15416200
H	2.17196300	2.86150100	3.54440400
H	4.67047100	2.67757100	3.49394400
H	3.93526400	1.07994400	3.29646500
H	4.58693200	1.92227700	1.89549200
C	0.19275400	1.44509500	-0.83169100
C	0.72242100	2.63340200	-1.61542000

H	-0.57779900	0.92571100	-1.40274500
H	0.97964600	0.71327200	-0.64674700
C	1.20696100	2.15457100	-2.98680900
H	-0.04401700	3.40521400	-1.75142100
H	1.56604700	3.09667400	-1.09341200
C	1.78518800	3.29373800	-3.82011400
H	1.96095600	1.37560900	-2.83948900
H	0.37364100	1.68698600	-3.52095200
H	2.12709800	2.93613000	-4.79224800
H	1.03688200	4.07156100	-3.99298100
H	2.63767100	3.75422600	-3.31464200
C	-0.79083200	0.44138700	1.15915900
C	-1.19971600	0.50181900	2.62343300
H	0.07849200	-0.20537000	1.01541900
H	-1.61948000	0.02446500	0.58374200
C	-1.56284800	-0.90802500	3.10230200
H	-0.39473800	0.89355000	3.25359000
H	-2.07248500	1.14821600	2.76213700
C	-2.10959200	-0.89715000	4.52633400
H	-2.29952800	-1.33852600	2.41689500
H	-0.67290400	-1.54302300	3.05045400
H	-2.34572500	-1.90792700	4.86165500
H	-1.38558300	-0.47136900	5.22657000
H	-3.02603500	-0.30471900	4.58540900

TS2

C	0.88276800	4.18489600	0.41683100
C	-1.28829500	3.37079900	-0.46734900
F	-1.83537000	3.11197900	0.74107100
F	-1.62463000	4.63164400	-0.77920200

F	-1.92640600	2.57178400	-1.34291200
O	0.40891000	1.86641200	0.07111400
H	0.94967400	1.20821700	-0.55088200
C	3.19846400	-0.32439300	0.33241700
H	2.60735400	-1.18092300	0.65120100
H	2.95350100	0.54806600	0.93802600
C	2.94068500	-0.02663300	-1.14468500
H	3.25826700	-0.90273500	-1.73487600
C	3.73303800	1.18318600	-1.63067200
H	4.80976600	1.00460700	-1.60915200
H	3.43297700	1.40985500	-2.65579000
H	3.51085300	2.05021500	-0.99940000
O	1.56927100	0.15562200	-1.25653100
Br	5.05801500	-0.79608800	0.76254500
C	0.67145300	-0.38943000	-3.10165300
O	1.59289500	-0.83599900	-3.65815700
O	-0.42110500	-0.05054000	-2.85339200
N	-1.76399400	-1.38128500	0.75179300
C	-1.21728100	-1.17441300	2.14511700
C	-0.14849600	-0.10203100	2.26215900
H	-0.84112300	-2.14761100	2.46848100
H	-2.07383300	-0.92579800	2.77512400
C	0.48877600	-0.14751300	3.65138900
H	0.62359200	-0.22462400	1.49800800
H	-0.57163200	0.88823700	2.07760300
C	1.53994500	0.94574500	3.82476000
H	-0.28841900	-0.03742600	4.41639100
H	0.94928700	-1.12938200	3.81169100
H	1.96092900	0.93298500	4.83130800

H	2.35885600	0.80980000	3.11572600
H	1.10585600	1.93185500	3.64564100
C	-2.78862000	-2.48835400	0.83377600
C	-3.73269300	-2.61437500	-0.35352300
H	-3.36523900	-2.32665100	1.74533200
H	-2.22537400	-3.41230300	0.97038400
C	-4.58152100	-3.88028300	-0.21784800
H	-4.39366500	-1.74427800	-0.40333300
H	-3.17977700	-2.65278400	-1.29627500
C	-5.58832600	-4.01362400	-1.35703200
H	-3.92619300	-4.75698300	-0.19889000
H	-5.10965500	-3.86330600	0.74148600
H	-6.18422900	-4.92126300	-1.25294000
H	-6.27193600	-3.16171800	-1.37436700
H	-5.07970300	-4.05459000	-2.32303000
C	-0.65614000	-1.76800900	-0.21364200
C	0.29637700	-2.85687400	0.25648800
H	-0.08123700	-0.86574100	-0.43430800
H	-1.15403300	-2.06078400	-1.13912300
C	1.24398200	-3.20866200	-0.89628000
H	0.88988000	-2.49893400	1.10451600
H	-0.22066900	-3.76399100	0.58797800
C	2.41044600	-4.08002900	-0.44020600
H	0.67836300	-3.71849300	-1.68347100
H	1.62097400	-2.28035900	-1.33311700
H	3.05061100	-4.34448600	-1.28292000
H	3.03063000	-3.55195000	0.28970700
H	2.05900000	-5.00727100	0.02136300
C	-2.36687400	-0.09224800	0.22432600

C	-3.49298800	0.46879100	1.08826400
H	-2.70280400	-0.31082600	-0.79072600
H	-1.53830600	0.61383300	0.13898500
C	-4.45654900	1.32692400	0.26444700
H	-4.07174400	-0.32951300	1.56610500
H	-3.06517500	1.07763800	1.89041200
C	-5.43859900	2.08373700	1.15249500
H	-3.88784600	2.03250100	-0.34065600
H	-4.99988700	0.68158900	-0.43510700
H	-6.14031000	2.66845200	0.55597200
H	-6.01775200	1.40063600	1.78006700
H	-4.90177600	2.77308800	1.80876500
C	0.22084900	3.13455400	-0.47641300
C	0.69750000	3.24564600	-1.92522300
H	0.40724300	4.20723600	-2.35408500
H	1.78295800	3.16060400	-1.95626100
H	0.26849600	2.43862400	-2.51935700
H	0.73584000	5.19820000	0.03925200
H	0.48414800	4.11602900	1.43065400
H	1.95116600	3.96747300	0.45370800

TS3

C	-3.93966500	-0.70620100	-1.00903000
C	-3.71339000	-2.16635000	-0.61855900
C	-3.41920300	-2.96936100	-1.88320100
H	-4.26359300	-2.93565300	-2.57329600
H	-2.52363000	-2.58755400	-2.37516300
H	-3.23769900	-4.00543900	-1.59408500
C	-4.94968600	-2.67555200	0.11073300
H	-4.78496800	-3.72165000	0.36905300

H	-5.10340900	-2.11157800	1.03160600
H	-5.84075400	-2.59717500	-0.51403100
O	-2.64050700	-2.19234900	0.28780500
H	-1.79703000	-2.20708100	-0.21259300
F	-4.22561600	0.06818800	0.06240600
F	-4.94920300	-0.54929900	-1.87425500
F	-2.84427900	-0.16317400	-1.57231300
Br	5.09812500	0.06317100	-0.39956000
C	3.13397500	-1.01442100	-1.33137900
H	3.73562800	-1.33242800	-2.16587600
H	2.72572800	-0.01980500	-1.36372500
C	2.82173400	-1.96002000	-0.17988500
H	3.18305200	-1.54966200	0.75853600
C	3.40741300	-3.33785100	-0.41999300
H	4.49611400	-3.26500100	-0.45195200
H	3.11723400	-4.01143700	0.38645200
H	3.04543800	-3.73771500	-1.36922800
O	1.39230900	-2.02366000	-0.03950800
C	0.75691100	-1.92297700	-1.25888200
O	-0.46471500	-2.01850400	-1.26484900
O	1.53858800	-1.66748100	-2.21633000
N	-0.21597100	1.50939900	0.86314200
C	0.94594600	1.78814400	1.78786700
C	1.94164300	0.64836400	1.93760600
H	0.50531400	2.05668400	2.75001100
H	1.44691900	2.67468900	1.39536500
C	2.85101500	0.89727400	3.14358800
H	1.43237100	-0.31290600	2.05717200
H	2.56805600	0.57665200	1.04256200

C	3.86108100	-0.23132900	3.33176800
H	3.38190700	1.84500700	3.00533900
H	2.23556300	1.00456500	4.04489200
H	4.48800400	-0.05212700	4.20672600
H	3.35023300	-1.18788200	3.47513500
H	4.51039800	-0.31280100	2.45728400
C	-1.07796500	2.75140300	0.83562400
C	-2.12239300	2.80079800	-0.26923300
H	-0.39966900	3.60206900	0.75294900
H	-1.55617400	2.81068400	1.81442400
C	-3.10108400	3.95286500	-0.03630900
H	-1.64040300	2.92875100	-1.24351100
H	-2.68832900	1.87016800	-0.31279600
C	-4.16343400	4.00384600	-1.13105800
H	-3.58348600	3.82378300	0.93810100
H	-2.55741600	4.90278400	0.00394700
H	-4.87598800	4.81095400	-0.95631600
H	-3.70673100	4.16334900	-2.11064100
H	-4.71863500	3.06329800	-1.17063300
C	-1.02577600	0.31051900	1.34375200
C	-1.34968400	0.29276400	2.82997600
H	-0.45951800	-0.57896800	1.06223600
H	-1.93678200	0.29794700	0.74913100
C	-2.36056600	-0.81700400	3.13291800
H	-0.44131600	0.11895200	3.41658400
H	-1.77015800	1.24762000	3.16362800
C	-2.66197700	-0.91051900	4.62515500
H	-3.27748900	-0.62684200	2.56814200
H	-1.98036600	-1.76960300	2.75692800

H	-3.39517900	-1.69269200	4.82744400
H	-1.75905700	-1.14502100	5.19477700
H	-3.06403200	0.03175200	5.00767800
C	0.27907200	1.15690300	-0.52112000
C	1.17190100	2.18617900	-1.19543400
H	-0.60523100	0.92107700	-1.11560300
H	0.82836800	0.23055200	-0.38859000
C	1.28694600	1.84906300	-2.69002000
H	0.78628000	3.20479200	-1.08331600
H	2.17139100	2.16715900	-0.74309200
C	2.50161300	2.51696900	-3.32699600
H	1.34717600	0.76321000	-2.82033400
H	0.36644600	2.16157600	-3.19381600
H	2.54879000	2.30738100	-4.39638500
H	2.46944400	3.60215800	-3.19653200
H	3.42451000	2.15011800	-2.86879100

TBABR PLUS HFB

TS1

C	-3.22980600	0.46541800	-0.81028300
C	-4.12795400	-1.32591900	0.71113000
F	-3.98402000	-0.52234300	1.77413700
F	-5.39877700	-1.20814600	0.29957500
F	-3.95371500	-2.57900400	1.12860700
F	-2.86653300	1.29897200	0.18346600
F	-4.45746700	0.82151600	-1.19387200
F	-2.40145100	0.72662800	-1.83730400
O	-1.84022900	-1.17205300	0.08715400

H	-1.45225100	-2.17112000	-0.14717500
C	0.85279200	-2.94254700	0.12727800
H	1.03287200	-3.77559600	0.78702400
H	0.63479600	-1.98113000	0.57017200
C	0.27453000	-3.20723000	-1.19093300
H	0.60080900	-4.15628200	-1.62308300
C	0.28396100	-2.09293300	-2.21455700
H	1.30182100	-1.92257600	-2.57290000
H	-0.34907200	-2.36128800	-3.06352200
H	-0.10956700	-1.17440800	-1.77131100
O	-0.89782500	-3.34658500	-0.42972600
Br	3.23592400	-2.44218800	-0.06032700
N	1.47523300	1.72353900	0.34856500
C	0.39796000	0.92944800	1.06585300
C	-0.41106400	1.69072000	2.10155500
H	0.91709900	0.08594800	1.52329600
H	-0.26937400	0.51263000	0.30862700
C	-1.25439200	0.68687400	2.89649400
H	0.22939700	2.25914100	2.78523100
H	-1.07971000	2.40196800	1.60618600
C	-2.38454600	1.36432400	3.66273900
H	-1.67067800	-0.04665300	2.20266100
H	-0.60083000	0.14047700	3.58466900
H	-2.95332700	0.63471900	4.24058800
H	-2.00583600	2.12473000	4.35183800
H	-3.07647700	1.84341600	2.96573300
C	1.91837200	0.86334700	-0.82106800
C	3.20254800	1.28583000	-1.51318500
H	1.07858900	0.86080800	-1.51616600

H	2.03732900	-0.15430500	-0.44396300
C	3.39997200	0.44397900	-2.77713300
H	3.19334400	2.34868200	-1.78283600
H	4.05711600	1.11431200	-0.85004600
C	4.71592600	0.77326300	-3.47457700
H	3.38259800	-0.61278700	-2.49432100
H	2.56060300	0.61296600	-3.46062600
H	4.83885700	0.17870000	-4.38075700
H	4.76211000	1.82902200	-3.75587800
H	5.56317400	0.55942200	-2.81884700
C	2.62815300	2.02291600	1.28094400
C	3.26651000	0.80877000	1.93848700
H	2.24556000	2.71751000	2.03051500
H	3.36185300	2.56360100	0.68112300
C	4.66582600	1.14704600	2.45565100
H	2.65035400	0.46453600	2.77484900
H	3.34834800	-0.02925900	1.23960400
C	5.29577800	-0.05096600	3.16105200
H	5.29373800	1.44819300	1.60967500
H	4.62056000	2.00558100	3.13539600
H	6.31402700	0.17048300	3.48417700
H	4.71526500	-0.33048900	4.04355400
H	5.32364400	-0.91537600	2.49359300
C	0.94942500	3.05539200	-0.13332900
C	-0.23319600	2.97720900	-1.08573700
H	1.79281100	3.57343400	-0.59282200
H	0.67318100	3.61034800	0.76461300
C	-0.95777600	4.32147800	-1.17138400
H	0.09284100	2.68019300	-2.08653700

H	-0.94419100	2.22521700	-0.74490600
C	-2.16963900	4.24057400	-2.09622800
H	-1.28183000	4.61728100	-0.16771200
H	-0.26706400	5.09628000	-1.52115800
H	-2.68416700	5.20031200	-2.15932400
H	-1.87164400	3.94963600	-3.10627400
H	-2.88106700	3.49614400	-1.73221000
C	-3.11558600	-1.00860500	-0.40540700
C	-3.43075200	-1.88996300	-1.61653300
H	-4.44637300	-1.72269300	-1.97563000
H	-2.71937200	-1.66653600	-2.41061400
H	-3.30401100	-2.93347100	-1.32892100

TS2

C	1.51298400	3.36865200	0.21247000
C	-0.82791500	3.23924700	-0.68226900
F	-1.44712300	3.03109900	0.49405700
F	-0.81267200	4.55821800	-0.89474200
F	-1.61364300	2.68944500	-1.62093000
F	1.00852000	3.48166200	1.44972000
F	1.79427100	4.60465900	-0.21698300
F	2.67429700	2.71008100	0.31854100
O	0.43576300	1.32700700	-0.23516900
H	0.98972300	0.57174000	-0.81449900
C	2.95258100	-1.04674100	0.25838800
H	2.17455800	-1.70445100	0.64133700
H	2.90712300	-0.07866600	0.75781300
C	2.80062800	-0.87900300	-1.25268000
H	2.93694400	-1.86049300	-1.73161400
C	3.82340900	0.08961900	-1.83477800

H	4.83944900	-0.30137700	-1.75557000
H	3.59181100	0.25436800	-2.88888200
H	3.77834600	1.04592300	-1.30547200
O	1.48851700	-0.45122700	-1.45374700
Br	4.64375000	-1.88023500	0.80281800
C	0.47622500	-1.02217400	-3.08768600
O	1.23200100	-1.74353400	-3.61460400
O	-0.52620400	-0.43434000	-2.90681600
N	-2.13415600	-1.27513500	0.79262100
C	-1.57726500	-1.02797800	2.17711300
C	-0.35538500	-0.12947900	2.23513200
H	-1.35878700	-2.01489000	2.59165000
H	-2.39350400	-0.59827900	2.76138700
C	0.21258400	-0.09673200	3.65450000
H	0.41844400	-0.47362500	1.54449400
H	-0.59838500	0.88420300	1.90898300
C	1.47829100	0.75459300	3.72413700
H	-0.54123400	0.29980700	4.34373900
H	0.43638700	-1.11709600	3.98716400
H	1.85494700	0.82080500	4.74593300
H	2.26685200	0.32205100	3.10344200
H	1.28759900	1.76584100	3.35989300
C	-3.30313400	-2.22049600	0.95187900
C	-4.24028500	-2.33960000	-0.24190600
H	-3.86463500	-1.89092300	1.82684200
H	-2.87461900	-3.19337400	1.19497900
C	-5.26522800	-3.44844900	0.00728700
H	-4.76895000	-1.39583900	-0.40472800
H	-3.68790600	-2.56238600	-1.15931800

C	-6.26091600	-3.57002400	-1.14293500
H	-4.74430000	-4.40089800	0.14775600
H	-5.80169300	-3.24442200	0.94006400
H	-6.98767900	-4.36120500	-0.95458000
H	-6.80946000	-2.63579500	-1.28349900
H	-5.74775300	-3.80059600	-2.07932400
C	-1.08175400	-1.89090400	-0.11330200
C	-0.31038100	-3.07277700	0.45528900
H	-0.38500700	-1.09514800	-0.38022800
H	-1.60179500	-2.17025300	-1.03078800
C	0.57497100	-3.66484100	-0.64789900
H	0.32554300	-2.74612300	1.28497500
H	-0.96523600	-3.85780200	0.84765600
C	1.60223300	-4.64710600	-0.09395700
H	-0.05974400	-4.15894200	-1.39079100
H	1.08323400	-2.85076100	-1.17012100
H	2.19650900	-5.08297700	-0.89810300
H	2.29335500	-4.14533700	0.58943900
H	1.11887600	-5.46336700	0.45054600
C	-2.55501800	0.02876600	0.13945700
C	-3.58159100	0.82249800	0.93733300
H	-2.93075100	-0.24170800	-0.84859100
H	-1.63751600	0.60007500	-0.01446100
C	-4.36266700	1.77777500	0.03091600
H	-4.30012900	0.16567800	1.44017100
H	-3.07233400	1.39929500	1.71577400
C	-5.22758000	2.74008700	0.83804300
H	-3.66672300	2.33991300	-0.59275800
H	-4.98794400	1.18953600	-0.65022200

H	-5.81985900	3.38271000	0.18515300
H	-5.91626900	2.19852200	1.49250200
H	-4.60233800	3.38199100	1.46332600
C	0.56806800	2.60171500	-0.72798300
C	1.09550500	2.67685600	-2.16140500
H	1.07641100	3.70070600	-2.53662000
H	2.11710600	2.30082600	-2.18943800
H	0.47554300	2.03618000	-2.78751700

TS3

C	-3.56392800	0.06346100	-1.09472400
C	-3.46676300	-1.43491600	-0.75969000
C	-3.33929600	-2.23003000	-2.05557700
H	-4.22485200	-2.10624000	-2.67901200
H	-2.45048100	-1.89916500	-2.59253000
H	-3.21749100	-3.28199000	-1.80105100
C	-4.71574500	-1.88306900	0.00966300
O	-2.40275700	-1.61240600	0.11598000
H	-1.57276600	-1.74783000	-0.40684500
F	-3.77849500	0.82194700	-0.00407100
F	-4.52065600	0.35272700	-1.97425200
F	-2.39757300	0.47990100	-1.61739100
Br	5.43448700	-0.49941700	-0.30250800
C	3.37440500	-1.26964600	-1.35260000
H	3.96739500	-1.64826800	-2.16783100
H	3.12251500	-0.22406000	-1.36359800
C	2.88229500	-2.18925900	-0.24441000
H	3.25934100	-1.86316000	0.72016300
C	3.26447000	-3.63278200	-0.50541400
H	4.35209200	-3.72537300	-0.48691000

H	2.83875000	-4.27598900	0.26479200
H	2.89420600	-3.95038300	-1.48208100
O	1.45279600	-2.03916400	-0.16064000
C	0.89884800	-1.81198900	-1.39752100
O	-0.32498900	-1.72496500	-1.46125100
O	1.74773000	-1.65125300	-2.31546200
N	0.41382000	1.68028400	0.88609700
C	1.58789100	1.74688100	1.83558500
C	2.38421700	0.45963400	1.97466100
H	1.17589900	2.06001700	2.79711400
H	2.23266600	2.54997400	1.47395100
C	3.34760500	0.56210700	3.15992100
H	1.72330100	-0.40096800	2.11759700
H	2.97177700	0.27786900	1.06914800
C	4.10822000	-0.74216500	3.38425700
H	4.05959400	1.37338800	2.97653800
H	2.78448200	0.82605300	4.06290000
H	4.77285500	-0.66378400	4.24605500
H	3.41423200	-1.56704600	3.56995500
H	4.71532300	-0.98629900	2.50976700
C	-0.24199800	3.04284400	0.88860500
C	-1.26936000	3.28112400	-0.20745800
H	0.56151200	3.77732800	0.81833500
H	-0.69996400	3.15659700	1.87171100
C	-2.03031300	4.58426000	0.04439800
H	-0.77808200	3.33421700	-1.18410700
H	-1.98877100	2.46265600	-0.25369300
C	-3.07029600	4.83993000	-1.04333500
H	-2.52499300	4.52947100	1.01963600

H	-1.32686700	5.42209800	0.09403600
H	-3.62671700	5.75790500	-0.85001200
H	-2.59597700	4.93364700	-2.02301400
H	-3.78508100	4.01490500	-1.09437800
C	-0.57970900	0.60839700	1.31790200
C	-0.96535200	0.61470000	2.78889000
H	-0.13635900	-0.35016900	1.04204400
H	-1.45751100	0.73691400	0.68899000
C	-2.10524600	-0.38039000	3.02773000
H	-0.10879400	0.33643700	3.41187100
H	-1.29463700	1.60681400	3.11557600
C	-2.50016200	-0.44272100	4.49943600
H	-2.96432800	-0.09789900	2.41481100
H	-1.80563200	-1.36938300	2.67195400
H	-3.31100100	-1.15594600	4.65305800
H	-1.65693000	-0.75478600	5.12131900
H	-2.83973300	0.53222300	4.85943100
C	0.86919000	1.29401500	-0.50188300
C	1.92597200	2.18612400	-1.13277700
H	-0.03072800	1.22022400	-1.11492200
H	1.26028100	0.28717600	-0.39313200
C	2.01926000	1.87540500	-2.63482300
H	1.70199600	3.24943200	-0.99890800
H	2.89967300	1.99948600	-0.66316800
C	3.34237600	2.35131200	-3.22677300
H	1.90374100	0.79872400	-2.79936800
H	1.17549300	2.34993500	-3.14637100
H	3.38454000	2.15890500	-4.29950500
H	3.48127600	3.42450700	-3.06992700

H	4.18141800	1.83179200	-2.75492400
F	-4.79705000	-1.31524600	1.21496200
F	-4.69969000	-3.20349900	0.18893700
F	-5.83566500	-1.57576300	-0.65860200

TBABR PLUS PFB

TS1

C	2.88567600	0.76876300	-1.24634900
C	3.69434800	-1.44445300	-0.37342300
F	3.22276200	-1.89007100	-1.54925300
F	5.01639100	-1.31066800	-0.49549500
F	3.45375000	-2.38559600	0.53196100
F	1.80207300	0.45189200	-1.96873800
F	3.94957000	0.66417700	-2.04052200
F	2.75803800	2.06371500	-0.92001600
O	1.75108800	-0.35819400	0.51510200
H	1.66677000	-1.14370600	1.61400600
C	-0.22240000	-2.26852300	1.94610300
H	-0.24775500	-3.33120900	2.12265700
H	-0.20401200	-1.90320700	0.93247800
C	0.16661000	-1.36864700	3.02050700
H	0.05379600	-1.78831600	4.01724200
C	-0.13072100	0.10447600	2.95380700
H	-1.18526900	0.25970900	3.19271500
H	0.48825600	0.64216600	3.67427200
H	0.09347200	0.49104300	1.95832200
O	1.41469800	-1.79959400	2.45087300
Br	-2.79172600	-2.24947700	1.79489400
N	-2.09762500	0.92059800	-0.99327600
C	-1.18969000	-0.29906700	-0.91673800

C	-0.84617900	-0.97922500	-2.23261200
H	-1.70072800	-1.00293000	-0.25713100
H	-0.26852600	0.02461000	-0.42476300
C	0.04486500	-2.18559700	-1.91167700
H	-1.74240300	-1.33204200	-2.75216200
H	-0.30977800	-0.30679500	-2.90863400
C	0.66424500	-2.79503000	-3.16383100
H	0.83544400	-1.86461100	-1.22981200
H	-0.55627800	-2.93313800	-1.38172400
H	1.26744400	-3.66900100	-2.91410800
H	-0.10415800	-3.10507800	-3.87737700
H	1.31818500	-2.07097800	-3.65600000
C	-2.60289100	1.16625600	0.41005700
C	-3.56093100	2.33444000	0.56799700
H	-1.71459700	1.30685300	1.02371400
H	-3.06083400	0.23424600	0.74594900
C	-3.80363300	2.58518000	2.05900400
H	-3.16883800	3.24827700	0.10807400
H	-4.51876800	2.11383100	0.08578400
C	-4.83280100	3.68573500	2.29765100
H	-4.13352600	1.65270600	2.52850400
H	-2.85430700	2.85423000	2.53462000
H	-4.98724100	3.85646800	3.36380900
H	-4.50865000	4.62893000	1.85021000
H	-5.79734500	3.41939300	1.85862700
C	-3.25441400	0.67136600	-1.92671200
C	-4.14465600	-0.49866500	-1.53218600
H	-2.82012900	0.52136700	-2.91658700
H	-3.83221500	1.59666000	-1.96155800

C	-5.10137000	-0.84773000	-2.67295900
H	-3.55259800	-1.37983400	-1.26957300
H	-4.72229200	-0.25084100	-0.63639700
C	-6.05308200	-1.97560600	-2.28396200
H	-5.67538300	0.04054900	-2.95986700
H	-4.51958000	-1.14117800	-3.55377500
H	-6.71492400	-2.23709900	-3.11081900
H	-5.49566600	-2.86984800	-1.99667500
H	-6.67231500	-1.68580500	-1.43211300
C	-1.31592900	2.10659100	-1.51560900
C	-0.34020100	2.73956300	-0.53244900
H	-2.04817300	2.84821800	-1.84155400
H	-0.78398600	1.75214100	-2.40062200
C	0.42670400	3.87393900	-1.21683300
H	-0.88075400	3.15767000	0.32223900
H	0.37094100	2.00304100	-0.14241800
C	1.29471400	4.64091800	-0.22240200
H	1.04938100	3.46063200	-2.01436800
H	-0.28466600	4.56098800	-1.68940100
H	1.87433900	5.41739000	-0.72367900
H	0.67612700	5.12221100	0.53945100
H	1.99117400	3.96940300	0.28213400
C	2.97897400	-0.11977900	0.02410200
C	3.85152500	0.62338200	1.07195100
F	3.14460400	1.59009200	1.66044300
F	4.24148700	-0.22388000	2.02671800
F	4.94413500	1.18177900	0.54151900

TS2

C	1.11727400	-3.23243800	0.80700700
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H	1.57892000	-2.35605100	1.25884500
H	1.63093400	-4.13735200	1.12304800
C	1.07482700	-3.10588000	-0.70644900
H	0.38711400	-3.85194900	-1.11795000
C	2.46955700	-3.37766000	-1.26751900
H	2.75773500	-4.41820800	-1.10052100
H	2.45052600	-3.18863400	-2.34090200
H	3.21190000	-2.72507000	-0.80582600
O	0.59852100	-1.83143100	-1.06339100
Br	-0.67365000	-3.37382000	1.61592600
N	-2.46284500	0.85678600	0.56377000
C	-2.25403600	-0.31853300	-0.38139500
C	-3.22759800	-1.47756400	-0.24771500
H	-1.23024200	-0.66191000	-0.23255500
H	-2.28262400	0.08851200	-1.39064000
C	-2.83705900	-2.56644200	-1.25225100
H	-3.20229300	-1.90399900	0.76033200
H	-4.25816400	-1.16682600	-0.45357700
C	-3.71605400	-3.80418100	-1.11979000
H	-2.89473700	-2.16183500	-2.26759200
H	-1.79312700	-2.84117500	-1.08898800
H	-3.43722300	-4.55693600	-1.85835400
H	-3.60463100	-4.25088400	-0.12785700
H	-4.77242000	-3.56206500	-1.26711100
C	-1.59527800	1.98015000	0.03252400
C	-1.55560900	3.23512000	0.89417800
H	-1.97996900	2.20566900	-0.96278100
H	-0.59721500	1.55365600	-0.09814500
C	-1.04273000	4.42220800	0.07256600

H	-2.54481400	3.49402500	1.28511400
H	-0.90018300	3.07896600	1.75580300
C	-0.70357000	5.61889900	0.95524900
H	-0.15988000	4.12170400	-0.49458900
H	-1.80563000	4.69956600	-0.66270700
H	-0.39229000	6.47632200	0.35692300
H	-1.56452500	5.92292100	1.55681700
H	0.11346500	5.36984600	1.63667100
C	-2.07068200	0.49101000	1.97893600
C	-0.59976100	0.20210100	2.22299600
H	-2.67219400	-0.38247500	2.23958400
H	-2.39864400	1.32225500	2.60806900
C	-0.40869200	-0.22969300	3.67823200
H	-0.24622300	-0.59171700	1.56514900
H	0.02060900	1.07538800	2.00936100
C	1.04218500	-0.59873900	3.97033000
H	-0.72930900	0.57643800	4.34806700
H	-1.05031500	-1.09248300	3.88607200
H	1.17097900	-0.89928300	5.01133700
H	1.35555100	-1.43495200	3.34013000
H	1.71028700	0.24068100	3.77028500
C	-3.91545800	1.25451100	0.60698400
C	-4.51774100	1.70151300	-0.71652500
H	-4.00944200	2.04883200	1.34733900
H	-4.45075400	0.38830700	0.99796800
C	-6.03953800	1.80428700	-0.59182900
H	-4.11578300	2.67736100	-1.00560000
H	-4.27001500	0.99998600	-1.51809000
C	-6.68245500	2.33949200	-1.86799800

H	-6.44732300	0.81509300	-0.35840800
H	-6.29432900	2.45430000	0.25214600
H	-7.76787700	2.38908700	-1.77198200
H	-6.31865900	3.34400300	-2.09626700
H	-6.44856500	1.69740500	-2.72034300
C	3.52071100	0.42397200	0.72027900
C	2.29881700	2.41236900	-0.21830200
F	1.71591200	2.90426900	-1.31432600
F	1.48592700	2.68489600	0.81120000
F	3.43610800	3.07349700	-0.01736800
F	3.21856600	0.97748500	1.89982700
F	4.77833500	0.74666800	0.42610200
F	3.45869500	-0.90034600	0.87541400
O	1.30587100	0.29231500	-0.15378100
H	1.10834300	-0.68512500	-0.60082800
C	2.50935800	0.88477800	-0.35940700
C	-0.09882700	-1.69119600	-2.64826300
O	-0.47786000	-0.56089200	-2.72506600
O	-0.02525800	-2.75307100	-3.18215200
C	3.09909100	0.59870100	-1.76728300
F	3.67740300	-0.60675400	-1.78786200
F	4.02898400	1.49830900	-2.10243700
F	2.15008500	0.61516500	-2.68426500

TS3

C	-3.38954800	0.26508700	-0.81378700
C	-3.34105200	-1.06823500	-0.03017100
C	-3.48520500	-2.24977800	-1.03573100
C	-4.51622500	-1.12198900	0.97584700
O	-2.19018400	-1.13599900	0.70924600

H	-1.39998500	-1.41874900	0.14103400
F	-3.56087000	1.29830700	0.02861200
F	-4.36212200	0.30742100	-1.71590400
F	-2.22830400	0.47676400	-1.44071700
Br	5.61556300	-1.04332200	-0.21001700
C	3.40172000	-1.75643200	-0.96204000
H	3.89302600	-2.43107600	-1.64229100
H	3.30045200	-0.72874300	-1.26621900
C	2.86696000	-2.24600900	0.37681800
H	3.33136800	-1.70535500	1.19578700
C	3.06008200	-3.74012500	0.54096800
H	4.12857200	-3.96260200	0.55742700
H	2.61051500	-4.07470300	1.47587000
H	2.59456500	-4.27290600	-0.29068900
O	1.46833000	-1.89879400	0.43899100
C	0.88710500	-1.94486300	-0.80049200
O	-0.31877200	-1.70905100	-0.87402200
O	1.69653200	-2.15357400	-1.74160300
N	0.90448600	2.03216000	0.40981700
C	2.14522600	2.24851600	1.24650700
C	2.83568300	0.98069500	1.72337100
H	1.83005100	2.86264700	2.09228300
H	2.82672000	2.84663100	0.63907600
C	3.85388800	1.31217400	2.81758200
H	2.10926900	0.26097300	2.11305900
H	3.36567600	0.49860100	0.89561900
C	4.51028600	0.05271300	3.37691900
H	4.62167400	1.97540300	2.40625200
H	3.35342000	1.86206100	3.62370800

H	5.21867500	0.30042500	4.16885800
H	3.75766700	-0.61985700	3.79865300
H	5.05002700	-0.47922200	2.59064100
C	0.36370500	3.39745300	0.04853100
C	-0.73706100	3.41611800	-1.00085600
H	1.21539100	3.99025500	-0.28848000
H	0.00893300	3.84082500	0.97976800
C	-1.29103300	4.83295300	-1.16625700
H	-0.35369900	3.06704200	-1.96448400
H	-1.55657400	2.75119500	-0.72163800
C	-2.41487900	4.87477700	-2.19801700
H	-1.66367900	5.19190100	-0.20139700
H	-0.48521500	5.51160300	-1.46491800
H	-2.81267200	5.88421600	-2.30877700
H	-2.05919600	4.54356500	-3.17632200
H	-3.23701900	4.21881300	-1.90143100
C	-0.13836600	1.23218300	1.17803400
C	-0.40616600	1.68900300	2.60406900
H	0.19629200	0.19372000	1.16555400
H	-1.04881900	1.27085200	0.58339600
C	-1.65060800	0.97757800	3.14118300
H	0.44979400	1.45944100	3.24732200
H	-0.57159300	2.77008100	2.66031900
C	-1.91789700	1.31943200	4.60289600
H	-2.51042700	1.25541600	2.52656600
H	-1.53779200	-0.10259900	3.01718700
H	-2.81808600	0.81663700	4.95898700
H	-1.08572800	1.00720800	5.23898500
H	-2.05900000	2.39518800	4.73870000

C	1.22718300	1.22630400	-0.82808500
C	2.28680000	1.80784900	-1.74976400
H	0.27990100	1.05556600	-1.34233100
H	1.56121000	0.26470000	-0.45171200
C	2.23734900	1.07726200	-3.09940400
H	2.14352800	2.87993800	-1.91982100
H	3.28061200	1.68000600	-1.30324800
C	3.50024000	1.31748000	-3.92017400
H	2.09574800	0.00358700	-2.93633900
H	1.35306900	1.41524800	-3.64988600
H	3.43078600	0.83315300	-4.89497800
H	3.66698100	2.38540200	-4.08536500
H	4.37640000	0.91500800	-3.40493600
F	-4.26557600	-0.36132800	2.03789000
F	-4.70201800	-2.36767800	1.40169400
F	-5.65150500	-0.68906900	0.42544400
F	-2.99158600	-3.35820400	-0.50703900
F	-4.76800800	-2.46086500	-1.34466600
F	-2.83705000	-1.99444600	-2.16825800

TBABr PLUS HFTI

TS1

C	-2.59695400	0.63855400	0.06542600
C	-2.38434400	1.23501500	-1.34282100
C	-2.78140000	1.77811000	1.09261700
F	-2.84216100	1.26675200	2.31862500
F	-1.73159500	2.62244900	1.06401700
F	-3.87529800	2.52339400	0.90335100
F	-1.18727400	1.84597500	-1.45201200

F	-3.30638500	2.14229700	-1.68143500
F	-2.39928000	0.27510100	-2.27052300
O	-1.43058000	-0.01024600	0.36715900
H	-1.39931000	-0.60690500	1.34179900
C	0.31564000	-2.31421200	1.67038100
H	0.12947300	-2.18832300	0.61436200
H	0.12223200	-3.27715100	2.11841000
C	0.27372900	-1.14024600	2.53514700
H	0.64253500	-0.22275900	2.06304700
C	0.72755000	-1.28655000	3.96314400
H	1.81705000	-1.34454800	4.00633900
H	0.38018400	-0.43733300	4.55409700
H	0.30758000	-2.20014200	4.38779000
O	-1.10945400	-1.33226400	2.33162000
Br	2.68635300	-2.89456400	1.23704000
N	2.53499500	0.80816900	-0.91865700
C	3.03130700	0.80735500	0.51084100
C	4.27325200	1.64369200	0.77195500
H	3.20006000	-0.23643100	0.78419700
H	2.19380800	1.16227200	1.11172600
C	4.50333600	1.75622900	2.28105900
H	5.15110700	1.17453300	0.31652400
H	4.18127700	2.64806800	0.34297900
C	5.78378700	2.51694200	2.61177200
H	3.64421700	2.25734800	2.73924700
H	4.54359900	0.75004300	2.71067900
H	5.93114500	2.59022600	3.69004500
H	6.65658500	2.01438300	2.18821200
H	5.75126800	3.53191400	2.20759000

C	1.37238400	-0.17409000	-0.96141000
C	0.83658900	-0.54267100	-2.33840300
H	0.56826200	0.25741300	-0.36081900
H	1.73969000	-1.06786000	-0.45343900
C	-0.08357500	-1.76151400	-2.19300900
H	0.27018200	0.28194600	-2.78038000
H	1.63955300	-0.80840700	-3.03294800
C	-0.71677200	-2.15705500	-3.52263600
H	0.50441600	-2.59656200	-1.79334300
H	-0.86327000	-1.53079400	-1.46211600
H	-1.36098200	-3.02960200	-3.40429300
H	-1.32831800	-1.34198000	-3.91529500
H	0.04656100	-2.40101000	-4.26688800
C	3.63565500	0.38643700	-1.86070900
C	4.15793800	-1.02427500	-1.64733500
H	4.43835700	1.11523800	-1.73950000
H	3.23867200	0.51035900	-2.86938600
C	5.25991700	-1.34128700	-2.65929900
H	4.54948400	-1.14525100	-0.63337000
H	3.35432800	-1.75983000	-1.74130200
C	5.80884600	-2.75221100	-2.46371200
H	4.86519400	-1.23444600	-3.67580300
H	6.07049400	-0.61073400	-2.56013200
H	6.59549600	-2.97362800	-3.18664700
H	6.22329600	-2.87170700	-1.46038300
H	5.01767800	-3.49569600	-2.58154700
C	2.07731800	2.18682800	-1.34511800
C	1.29649600	2.98809400	-0.31243300
H	1.47265700	2.03435900	-2.24128100

H	2.97299700	2.73886500	-1.63755900
C	0.74929100	4.25988000	-0.96725700
H	0.46645300	2.40795600	0.09862400
H	1.94972100	3.27311900	0.51848200
C	0.10593700	5.19823400	0.04985100
H	1.56293900	4.78165800	-1.48462900
H	0.01618700	3.98016800	-1.72837300
H	-0.28814800	6.09165800	-0.43683600
H	-0.71698100	4.70251800	0.56617400
H	0.83360300	5.51882000	0.79986600
C	-3.84182900	-0.25754700	0.04407600
C	-3.70135800	-1.60511000	0.36404900
C	-5.10301800	0.22324300	-0.31337000
C	-4.80224400	-2.45173700	0.33407400
H	-2.73359900	-1.99571400	0.64996500
C	-6.19522100	-0.63336700	-0.34379900
H	-5.24204700	1.26398100	-0.57343100
C	-6.06545900	-1.98280900	-0.01902100
H	-4.67359700	-3.49800400	0.59080600
H	-7.16702400	-0.24410800	-0.62849400
C	-7.25951300	-2.90101900	-0.02105100
H	-7.69399600	-2.96799200	0.98023300
H	-8.03487900	-2.53854300	-0.69741000
H	-6.97903800	-3.90990500	-0.32787500

TS2

C	1.16566500	-2.73850600	1.54986700
H	1.31039000	-1.73854500	1.95646500
H	1.76904200	-3.46197100	2.09366600

C	1.43866600	-2.76917700	0.05269700
H	1.08980900	-3.72805000	-0.35023200
C	2.95009100	-2.67057500	-0.17497300
H	3.46950400	-3.54291800	0.22944700
H	3.13595000	-2.61694700	-1.24867900
H	3.35868200	-1.76914300	0.28681300
O	0.74436600	-1.74179400	-0.59204600
Br	-0.69773300	-3.21982900	1.98381400
N	-2.87972700	0.58667600	0.09675800
C	-2.27076500	-0.62662900	-0.59300700
C	-3.08603500	-1.90857200	-0.52634400
H	-1.28627400	-0.78206300	-0.15218400
H	-2.09451700	-0.33560800	-1.62786400
C	-2.35542600	-3.01634400	-1.29271100
H	-3.21887000	-2.23316600	0.51063900
H	-4.08150800	-1.78186200	-0.96642800
C	-3.05362800	-4.36269600	-1.14026000
H	-2.29093100	-2.73917400	-2.35005600
H	-1.33162800	-3.08619700	-0.91884800
H	-2.53768000	-5.13531300	-1.71198800
H	-3.06247300	-4.67324300	-0.09190600
H	-4.08899800	-4.31779800	-1.49033700
C	-2.03758800	1.77836200	-0.31350500
C	-2.39542200	3.09756700	0.36128700
H	-2.14493200	1.85561700	-1.39640700
H	-1.00175400	1.49415100	-0.10925500
C	-1.90946600	4.27536900	-0.48953100
H	-3.47431100	3.20928600	0.50821100
H	-1.93028600	3.14724600	1.34981900

C	-1.99184500	5.59613500	0.26765100
H	-0.88098600	4.09526500	-0.80586600
H	-2.51400200	4.32399200	-1.40200900
H	-1.69186200	6.43387200	-0.36350000
H	-3.00907700	5.78776200	0.62030700
H	-1.33093700	5.57827300	1.13755700
C	-2.87364900	0.41184300	1.59988600
C	-1.51702500	0.36006200	2.28424300
H	-3.42223500	-0.51258600	1.79092000
H	-3.46548800	1.23784700	2.00277400
C	-1.73075900	-0.04760200	3.74448700
H	-0.85762200	-0.36301400	1.80419200
H	-1.00258400	1.32256700	2.22489400
C	-0.42124800	-0.15037500	4.51911000
H	-2.39869200	0.66883300	4.23720800
H	-2.23507400	-1.01966800	3.76581600
H	-0.59880900	-0.49818000	5.53827800
H	0.25275000	-0.86053900	4.03318300
H	0.08773500	0.81309700	4.56820200
C	-4.32043300	0.76453500	-0.30893800
C	-4.57734600	0.92033000	-1.80035000
H	-4.69843900	1.63415700	0.22789200
H	-4.85219100	-0.10546300	0.07859200
C	-6.08201100	0.88676800	-2.07815600
H	-4.16795500	1.86770700	-2.16332100
H	-4.09242200	0.11962200	-2.36568200
C	-6.39246000	1.07321500	-3.56044000
H	-6.48930600	-0.06932600	-1.73248100
H	-6.57988700	1.66838200	-1.49445500

H	-7.46660200	1.03688100	-3.74652600
H	-6.02155900	2.03613100	-3.91942000
H	-5.92044800	0.28955000	-4.15753600
C	2.51512600	1.18158000	1.80137400
C	1.60895400	2.69658600	0.02382300
F	1.04951500	2.76555800	-1.19096300
F	0.68228400	3.15129700	0.89260500
F	2.62831400	3.55306800	0.04836400
F	1.51266700	1.38270900	2.66242500
F	3.46070700	2.08662400	2.09203600
F	3.02110700	-0.02912800	2.07751000
O	0.87296200	0.49049400	0.26499400
H	0.92900400	-0.57180900	-0.16285100
C	2.01794600	1.24044100	0.33869100
C	0.43077700	-2.00687300	-2.47191200
O	-0.12196400	-1.00622800	-2.77245600
O	0.87287700	-3.07364500	-2.68895600
C	3.10187200	0.81556300	-0.65570100
C	2.66459200	0.40103100	-1.91459600
C	4.46554900	0.79922400	-0.37817000
C	3.56992900	-0.05002500	-2.86125100
H	1.60705900	0.41821700	-2.14239500
C	5.36610600	0.33288700	-1.33138500
H	4.84624700	1.12748900	0.57976000
C	4.93652500	-0.10572300	-2.58066600
H	3.20592200	-0.37962000	-3.82950700
H	6.42411300	0.31015200	-1.09283700
C	5.90622800	-0.63904800	-3.60215100
H	5.76199700	-1.71329400	-3.74422900

H	5.75736800	-0.15699800	-4.57075600
H	6.93870500	-0.47419400	-3.29237300

TS3

C	2.92093200	-2.23608000	-1.79723200
C	2.64069900	-1.26213100	-0.63041500
C	2.00502500	-2.03235400	0.54828200
F	1.91003600	-1.23197500	1.62829000
F	2.68234500	-3.12089400	0.91674600
F	0.76585100	-2.40969200	0.24118600
O	1.72676800	-0.30203200	-1.03625600
H	0.90922300	-0.67799000	-1.48214700
C	-3.62101600	-1.80112300	-0.32274500
H	-3.15679100	-1.42967600	0.57118800
H	-3.86574100	-2.84944100	-0.35466500
C	-3.91615600	-0.89239000	-1.50707000
H	-4.54950000	-0.06634600	-1.19648500
C	-4.55032900	-1.65830600	-2.65111800
H	-5.51607400	-2.05030600	-2.32737000
H	-4.69785000	-0.99864000	-3.50624400
H	-3.90649000	-2.48893600	-2.94876100
O	-2.68199300	-0.28506100	-1.92350200
Br	-5.70604800	-1.40774100	0.87925000
C	-1.60498700	-1.10816400	-1.70954500
O	-1.87347100	-2.14786600	-1.05327500
O	-0.52289400	-0.69978700	-2.13072000
N	-0.88368200	1.93705300	0.77541700
C	-0.55145600	2.09536900	-0.69554800
C	-0.59119500	3.51463100	-1.23267900

H	-1.24572700	1.45943400	-1.24336800
H	0.43748900	1.65364000	-0.82413600
C	-0.09852300	3.51111900	-2.68340300
H	-1.61104400	3.91316800	-1.20608600
H	0.04100000	4.18811200	-0.64331200
C	-0.19229900	4.89204500	-3.32431800
H	0.93663900	3.15610900	-2.70776800
H	-0.68403600	2.78686000	-3.25791500
H	0.17150100	4.87376500	-4.35243800
H	-1.22631500	5.24520400	-3.34171200
H	0.40242700	5.62332700	-2.77078700
C	-0.93216900	0.44232700	1.03882100
C	-0.91048900	0.02057600	2.50040300
H	-0.08951500	0.00233100	0.50552500
H	-1.83674300	0.10126100	0.54167800
C	-1.37033100	-1.43867400	2.62395100
H	0.10780600	0.11633800	2.89173500
H	-1.56026000	0.64764600	3.11917200
C	-0.88686100	-2.07739900	3.92173800
H	-2.46408700	-1.47006100	2.58291800
H	-1.00609100	-2.01270900	1.76681700
H	-1.27673600	-3.09018800	4.02904200
H	0.20476100	-2.12998700	3.93882500
H	-1.21241400	-1.49879100	4.79049800
C	-2.21492100	2.57377300	1.11376200
C	-3.42454500	2.05145800	0.35129600
H	-2.08647300	3.64257300	0.93324600
H	-2.35721100	2.43936800	2.18758900
C	-4.62720900	2.96865800	0.58948700

H	-3.21898900	1.99621400	-0.72207500
H	-3.69609000	1.04347500	0.68346800
C	-5.85896800	2.48110400	-0.16862700
H	-4.84666500	3.00736900	1.66162700
H	-4.37385200	3.98941700	0.28005400
H	-6.71307400	3.13636300	0.00933400
H	-5.66754400	2.46492100	-1.24531700
H	-6.13042500	1.47021800	0.14503800
C	0.15601900	2.60549500	1.63923000
C	1.59309600	2.16258800	1.40258000
H	-0.13667300	2.40193200	2.67030700
H	0.05121900	3.67980500	1.48038300
C	2.45049900	2.54766300	2.61074400
H	1.65654200	1.08316700	1.24564800
H	1.99520600	2.62920500	0.49738800
C	3.92377800	2.21769900	2.39850200
H	2.33327300	3.61690800	2.82126300
H	2.07526600	2.01417400	3.49124200
H	4.50853800	2.43872200	3.29334400
H	4.05430000	1.15983000	2.15480200
H	4.33749200	2.79732200	1.57035500
C	3.94534300	-0.57602900	-0.24533100
C	4.87744000	-1.14395900	0.62052300
C	4.24235400	0.63963500	-0.85945100
C	6.06931400	-0.48110200	0.89146800
H	4.68910000	-2.10293900	1.08524900
C	5.44297600	1.28236900	-0.59615700
H	3.52760500	1.06402400	-1.55236700
C	6.37088700	0.74053800	0.29337000

H	6.78138600	-0.92971900	1.57578900
H	5.66357700	2.22388400	-1.08897000
C	7.64733000	1.47124000	0.61538800
H	8.05127100	1.96578700	-0.26948600
H	7.46750200	2.24001600	1.37280300
H	8.40496000	0.79037100	1.00483500
F	3.83984500	-3.14867400	-1.47138000
F	3.36950500	-1.55783700	-2.85155100
F	1.81342400	-2.87986600	-2.16627500

TBABr PLUS 2 MOLECULES OF TFE

TS1

C	-2.49996600	-1.64728100	2.30067700
C	-0.66460800	-1.34929800	3.94495700
F	-2.43651200	-0.35271900	1.93191300
F	-3.43008200	-1.73862300	3.25836800
F	-2.97168600	-2.31484900	1.22832900
O	-0.30125200	-2.03774400	1.63662700
H	0.49366200	-1.48803000	1.85951100
C	0.86414900	1.02605200	1.52447300
H	-0.14478500	0.66987100	1.66709100
H	1.24457600	1.18645700	0.52760700
C	1.85388800	0.77504800	2.56527100
H	1.45579800	0.76002400	3.58332500
C	3.17177800	1.49803800	2.46644900
H	3.06007300	2.51410400	2.84923900
H	3.93550000	0.97099500	3.04081600
H	3.49736600	1.54940100	1.42527000
O	1.79538700	-0.49470200	1.94003800
Br	0.04753800	3.36938900	1.48412900

N	-1.64629800	0.39682300	-1.78021800
C	-2.15025500	1.28865800	-0.65650300
C	-2.59632000	2.68978100	-1.04485900
H	-1.34341100	1.38044500	0.06925000
H	-2.95778400	0.73749800	-0.17695100
C	-3.39314800	3.29478300	0.11599300
H	-1.71643300	3.31506800	-1.22630300
H	-3.21391700	2.70203800	-1.94971400
C	-3.56890300	4.80017100	-0.04801400
H	-4.36725300	2.79734200	0.18145300
H	-2.85773300	3.09805000	1.04872700
H	-4.18700900	5.21328900	0.75038500
H	-2.59468200	5.29282100	-0.00711100
H	-4.04202400	5.04524500	-1.00342600
C	-0.92487700	-0.76887600	-1.13281800
C	-0.37922500	-1.80511900	-2.10203300
H	-1.62563700	-1.21101600	-0.42675800
H	-0.10626700	-0.35374800	-0.54717700
C	0.05223300	-3.04961700	-1.32369000
H	-1.12548600	-2.09357200	-2.85092100
H	0.48715000	-1.39556700	-2.63254800
C	0.57574700	-4.14977400	-2.24095700
H	0.80905200	-2.75352200	-0.59475300
H	-0.79474500	-3.41869000	-0.73663700
H	0.89477900	-5.02116400	-1.66566200
H	-0.19500900	-4.47931000	-2.94325800
H	1.43259200	-3.80871200	-2.82866500
C	-0.71690000	1.16014500	-2.69848700
C	0.53306500	1.68843000	-2.01815400

H	-1.31023400	1.97318700	-3.12168300
H	-0.45815100	0.47763700	-3.51047600
C	1.31704800	2.62341800	-2.93865500
H	0.27292000	2.24882000	-1.11364900
H	1.18547600	0.85932000	-1.72443200
C	2.56573000	3.13519000	-2.22379400
H	1.59572400	2.09667200	-3.85876300
H	0.68329500	3.46716100	-3.23369400
H	3.14393100	3.80811800	-2.85905500
H	2.28690800	3.67321100	-1.31385500
H	3.20907300	2.30145100	-1.93257600
C	-2.81561900	-0.08212900	-2.60773000
C	-3.71645200	-1.12115900	-1.95234500
H	-2.40337400	-0.48404400	-3.53431000
H	-3.38954700	0.80906100	-2.86654500
C	-4.91213800	-1.42172800	-2.85896300
H	-3.16530300	-2.04778100	-1.76950000
H	-4.08100400	-0.77733100	-0.98089300
C	-5.83185400	-2.47641300	-2.25014400
H	-5.47449000	-0.49988100	-3.03958500
H	-4.55148200	-1.76465100	-3.83465200
H	-6.67683100	-2.69015700	-2.90605200
H	-5.29283100	-3.41098000	-2.07886800
H	-6.22717900	-2.13893900	-1.28931300
C	4.85077500	-0.58059500	-0.42723400
C	3.70960200	-1.46113200	-2.44557000
F	4.82288200	0.68390000	-0.86881200
F	6.01398100	-1.11580900	-0.83765800
F	4.89077200	-0.53128800	0.91061100

O	2.47612900	-0.70892500	-0.58057700
H	2.35220200	-0.68508500	0.40761400
C	-1.14064500	-2.17584700	2.75167600
C	-1.28059300	-3.65376000	3.10805300
C	3.65377200	-1.39309100	-0.92562400
C	3.70948700	-2.77648600	-0.27881400
H	-1.57167700	-4.22100300	2.22320900
H	-0.31023200	-4.01760600	3.44725100
H	-2.01768700	-3.81199400	3.89736300
H	-1.30042000	-1.51996400	4.81462700
H	0.35827800	-1.64425100	4.18610900
H	-0.67046200	-0.28173400	3.71392800
H	2.83966000	-2.01850100	-2.79552600
H	3.67449000	-0.45489200	-2.86805800
H	4.61506300	-1.96327300	-2.78761000
H	4.68227100	-3.24745900	-0.43273600
H	3.52299900	-2.68922900	0.79355800
H	2.93959800	-3.41058200	-0.72003300

TS2

C	-3.04282500	1.25293900	-3.20442100
C	-4.45151700	0.56143000	-1.27122300
F	-4.52641900	1.81866700	-0.82045600
F	-5.52529500	0.35030700	-2.04636400
F	-4.57495300	-0.24486500	-0.19887700
O	-2.17250800	0.53990700	-1.04675200
H	-1.28608600	0.76089600	-1.39645200
C	4.11979700	-0.57350000	-0.41530200
H	3.86036400	0.23865400	0.26252100
H	5.19948500	-0.64701900	-0.53227100

C	3.38692200	-0.43220700	-1.74689500
H	3.56885900	-1.36202500	-2.31216500
C	4.07619600	0.70256000	-2.52239300
H	5.12107900	0.46668900	-2.74164500
H	3.55400700	0.84336300	-3.47116800
H	4.04077300	1.63791800	-1.95790900
O	2.03205200	-0.24741500	-1.59060600
Br	3.61755800	-2.23590900	0.52175700
N	-0.47694500	-0.96800500	1.87719200
C	-0.14078500	-1.43521900	0.46021500
C	0.08261100	-2.92977700	0.28873900
H	0.75080900	-0.89125600	0.14348900
H	-0.95935200	-1.09831300	-0.17443900
C	0.50107600	-3.19366300	-1.16109800
H	0.87203200	-3.29517300	0.95361500
H	-0.82550800	-3.50283300	0.50757400
C	0.88294700	-4.65071800	-1.39299600
H	-0.32775200	-2.91066700	-1.82135300
H	1.34064500	-2.53708500	-1.40402900
H	1.15080800	-4.82135500	-2.43704300
H	1.74679900	-4.92084400	-0.77973000
H	0.06097800	-5.32649400	-1.13939600
C	-1.12331900	0.39678700	1.76060800
C	-1.52551400	1.03462000	3.08071300
H	-1.98997300	0.27280100	1.11482100
H	-0.42236200	1.01442500	1.19708300
C	-1.94973500	2.48397200	2.82843600
H	-2.36333400	0.49405300	3.53501800
H	-0.70604700	1.02590300	3.80679200

C	-2.50132400	3.15091500	4.08467200
H	-1.08553400	3.04273700	2.45583900
H	-2.70296900	2.50264200	2.03272400
H	-2.77522800	4.18930700	3.89237600
H	-3.39215000	2.63016300	4.44475300
H	-1.76029900	3.14309700	4.88823800
C	0.79491900	-0.89799000	2.69685400
C	1.68371200	0.30041700	2.39487500
H	1.33239900	-1.82980100	2.51027600
H	0.49476700	-0.88368900	3.74712700
C	2.96514900	0.24963300	3.22726500
H	1.92548600	0.34431500	1.32756900
H	1.16037100	1.22859200	2.63236800
C	3.77849000	1.53312300	3.06951200
H	2.70731100	0.11049900	4.28376100
H	3.56355100	-0.61555800	2.93097000
H	4.71041600	1.48367700	3.63489100
H	4.02444400	1.71570800	2.02129200
H	3.21121300	2.39822800	3.42244400
C	-1.42258000	-1.92582600	2.55007100
C	-2.77183500	-2.05160200	1.85398800
H	-1.55437500	-1.57376500	3.57436100
H	-0.90872300	-2.88703500	2.59837300
C	-3.52399800	-3.29681500	2.32072900
H	-3.38248800	-1.16637000	2.05251800
H	-2.64372800	-2.09322000	0.76857500
C	-4.89845300	-3.39462600	1.66396300
H	-2.93267600	-4.18768100	2.08231200
H	-3.63277900	-3.27571900	3.41059700

H	-5.43264300	-4.28882700	1.98828100
H	-5.51003500	-2.52392800	1.91153500
H	-4.80444200	-3.43134700	0.57582400
C	1.62678600	3.25826900	-0.04985400
C	-0.69820400	3.51115100	-0.86779600
F	1.15167500	3.15118900	1.20886800
F	1.96673100	4.54359000	-0.22427300
F	2.76532600	2.54058900	-0.08382600
O	0.41636800	1.40555100	-0.85099200
H	1.23727800	0.78999800	-1.18576400
C	-3.15116500	0.29240200	-2.02516700
C	-3.13717900	-1.16760900	-2.47706500
C	0.61650700	2.76534900	-1.08596800
C	1.16535600	3.02088600	-2.48978000
C	0.90068400	-0.87044500	-3.43963400
O	-0.10479000	-0.34732300	-3.16081600
O	1.74705400	-1.47177700	-3.95514400
H	-1.38572800	3.25149900	-1.67296500
H	-1.15352700	3.20582600	0.07492900
H	-0.54707300	4.59240100	-0.86867400
H	-3.12907500	2.28514600	-2.86272200
H	-3.82571200	1.05911200	-3.93925700
H	-2.07114900	1.10902800	-3.68039700
H	1.28702200	4.08704200	-2.68865700
H	2.12106700	2.51647600	-2.62793500
H	0.45463300	2.60107900	-3.20399200
H	-3.98089700	-1.38612100	-3.13414400
H	-3.18775300	-1.82695500	-1.60778600
H	-2.20843300	-1.35891600	-3.01226800

TS3

C	4.21621800	0.11898300	-1.59535000
C	3.29029400	-1.28689900	-3.42319100
F	3.24358700	1.02625300	-1.74032900
F	5.25485200	0.52704300	-2.34010000
F	4.60971900	0.18310300	-0.30664600
O	2.74240200	-1.65139900	-1.08111400
H	1.89267700	-1.74429100	-1.56080000
C	-1.37347600	1.49543500	-1.63676800
H	-1.45663900	1.09383700	-0.63887500
C	-0.02391800	1.52393400	-2.32497700
H	0.63098800	2.28857400	-1.92194300
O	0.62932300	0.27628700	-2.13096200
Br	-0.99041800	3.63403500	-0.20757000
N	0.77763500	-0.26619500	1.99941700
C	1.30660500	0.84329000	1.10673900
C	1.82110400	2.07266000	1.83504900
H	0.48575600	1.14082500	0.45401300
H	2.06920800	0.37998500	0.47706700
C	2.61008600	2.94929700	0.85895100
H	0.97519300	2.65201300	2.22033800
H	2.46751800	1.80805600	2.67952800
C	2.92818000	4.31319000	1.46068400
H	3.52633200	2.42676700	0.56821600
H	2.01339600	3.08785900	-0.04720200
H	3.53150600	4.91413400	0.77871400
H	2.00385100	4.85967700	1.66228000
H	3.48033700	4.21327400	2.39966900
C	0.25063500	-1.33912500	1.06534300

C	-0.48940900	-2.50255900	1.70496900
H	1.11098100	-1.68178900	0.49202300
H	-0.42771300	-0.83273200	0.37912800
C	-0.67306500	-3.60708100	0.65938600
H	0.05123600	-2.91669200	2.56185400
H	-1.47299300	-2.17178000	2.05422700
C	-1.47222400	-4.78343100	1.20983700
H	-1.16346100	-3.18504200	-0.22080900
H	0.31093400	-3.94808100	0.32190900
H	-1.61782300	-5.55205800	0.44842700
H	-0.96340100	-5.24713500	2.05936400
H	-2.45963900	-4.46211900	1.55337400
C	-0.30990100	0.23327900	2.92251600
C	-1.52429900	0.82976400	2.23706500
H	0.16087700	0.97838800	3.56630500
H	-0.58703200	-0.61891100	3.54845700
C	-2.53996100	1.30178300	3.28122700
H	-1.23368900	1.69669600	1.63609200
H	-2.00345600	0.10411200	1.57213300
C	-3.69157300	2.05665100	2.62163500
H	-2.91985100	0.44175000	3.84572900
H	-2.04233500	1.95767900	4.00434700
H	-4.41047800	2.40996600	3.36298900
H	-3.31008900	2.91804000	2.06803100
H	-4.21994400	1.41944000	1.90975000
C	1.87972200	-0.81545300	2.87952400
C	3.20132800	-1.10795700	2.18819600
H	1.47859300	-1.71739500	3.34168400
H	2.02911000	-0.08524600	3.67605300

C	4.14947700	-1.83004600	3.14709700
H	3.06023000	-1.70737700	1.28421200
H	3.67072200	-0.17446600	1.86832600
C	5.47696200	-2.16164800	2.47032900
H	4.32865500	-1.20375600	4.02794200
H	3.68106700	-2.75194300	3.50829700
H	6.18069600	-2.61222100	3.17190500
H	5.32184000	-2.86491400	1.64892800
H	5.93734300	-1.26113800	2.05633700
C	-4.99886900	-0.65336600	-0.82616900
C	-4.59119700	-1.88864000	1.29171500
F	-4.95396800	0.52426500	-0.18843000
F	-6.28490300	-1.03016700	-0.87718100
F	-4.59586100	-0.43064100	-2.08580300
O	-2.81125000	-1.20895300	-0.10068200
H	-2.46078000	-1.08895200	-1.00756200
C	3.77191800	-1.29416000	-1.97649600
C	-4.12704700	-1.70886200	-0.14573700
C	-0.24776600	-0.76949600	-2.18720900
O	-1.46547900	-0.40136400	-2.26465600
O	0.21497900	-1.89772200	-2.10922000
C	-2.59341700	2.02087300	-2.32702200
H	-3.42230700	2.11983800	-1.63016400
H	-2.86393000	1.32137400	-3.12050200
H	-2.38243700	2.99608200	-2.76454900
H	-0.18342600	1.69548900	-3.39434500
C	4.94690100	-2.24456400	-1.76987700
H	5.80126400	-1.96598800	-2.38832200
H	5.24852200	-2.23994900	-0.72142800

H	4.62433000	-3.25157700	-2.03539300
C	-4.19505300	-3.00483800	-0.94940400
H	-3.79847600	-2.84617500	-1.95449600
H	-3.58379600	-3.75836400	-0.45065600
H	-5.21968700	-3.37175200	-1.02705800
H	4.10139300	-1.00937800	-4.09758400
H	2.94001700	-2.28738200	-3.68219500
H	2.46422300	-0.58512400	-3.54208900
H	-4.49264000	-0.94799700	1.83702400
H	-5.62960000	-2.21946100	1.33056300
H	-3.96212500	-2.64009500	1.77086400

TBABr PLUS 2 MOLECULES OF HFB

TS1

C	2.63771400	-0.92118300	-2.45686000
C	1.41608300	-2.93121900	-3.31669400
F	1.89393800	-0.17909600	-3.28724500
F	3.78791000	-1.19348400	-3.07370800
F	2.91580200	-0.15154000	-1.39359900
O	0.80086700	-1.81585900	-1.24284700
H	0.05009300	-1.39492300	-1.76331200
C	-0.57603000	1.04683300	-1.76578700
H	0.46310600	0.82289400	-1.59213800
H	-1.22904000	1.30068500	-0.94511000
C	-1.18465200	0.60853100	-3.01096800
H	-0.49539900	0.52206100	-3.85144400
C	-2.52856800	1.16802300	-3.38835600
H	-2.39223100	2.14496300	-3.85563000
H	-3.03667100	0.49752500	-4.08366100
H	-3.15160300	1.29168900	-2.50075500

O	-1.20789800	-0.57374100	-2.21000600
Br	0.05560400	3.49988200	-1.80102900
N	1.38602600	0.98333600	1.99947800
C	2.01982600	1.79445400	0.88036600
C	2.26961500	3.26767700	1.16240200
H	1.35903200	1.72640000	0.01809900
H	2.94536600	1.27932600	0.62658300
C	3.20240300	3.82612200	0.08200600
H	1.32173700	3.81259000	1.11769300
H	2.71499500	3.43872700	2.14849100
C	3.20899600	5.35052600	0.08106600
H	4.21321300	3.43438300	0.24135000
H	2.85838700	3.47222100	-0.89370600
H	3.91897500	5.74073300	-0.64969600
H	2.21650300	5.72270200	-0.18318900
H	3.48032500	5.74928500	1.06298300
C	0.89377200	-0.31451300	1.38884600
C	0.27554700	-1.29131200	2.37756000
H	1.74250700	-0.75174000	0.86406700
H	0.16059500	-0.04570600	0.62992400
C	0.04449700	-2.64208200	1.69607500
H	0.92393600	-1.44390700	3.24743800
H	-0.68209900	-0.90802400	2.74047400
C	-0.54105000	-3.67589100	2.65339300
H	-0.61257100	-2.48979500	0.83690600
H	0.99165300	-3.00667800	1.28898100
H	-0.70451400	-4.62891800	2.14617200
H	0.13519400	-3.86123600	3.49252700
H	-1.49676300	-3.34043900	3.06141800

C	0.23867100	1.74131300	2.63244900
C	-0.89615100	2.06432100	1.67549300
H	0.67146800	2.65236200	3.05080000
H	-0.11298900	1.12664700	3.46279400
C	-1.90171800	3.02905200	2.30373300
H	-0.50956300	2.53302000	0.76400000
H	-1.42328700	1.14981500	1.38599000
C	-2.99054100	3.38535900	1.29327800
H	-2.34677800	2.57768100	3.19740900
H	-1.38274000	3.93896500	2.62572900
H	-3.71255700	4.08565800	1.71665400
H	-2.54680500	3.84089900	0.40392500
H	-3.52973000	2.48862000	0.98053600
C	2.41543000	0.71918200	3.07294600
C	3.49577800	-0.29658500	2.72187300
H	1.87080300	0.38883200	3.95851000
H	2.86400000	1.68581900	3.30816300
C	4.53344200	-0.37036200	3.84431400
H	3.05821500	-1.28806000	2.57679000
H	3.99945800	-0.03658500	1.78683400
C	5.60985100	-1.41077400	3.54856400
H	4.99517600	0.61289800	3.98094300
H	4.03224700	-0.61488400	4.78698800
H	6.34023000	-1.46471500	4.35689800
H	5.16832300	-2.40246900	3.42559900
H	6.14386600	-1.16730200	2.62720600
C	-4.63581200	-0.64960400	-0.60940400
C	-3.91967600	-1.03119000	1.77414200
F	-2.95454700	-1.52947900	2.56332200

F	-4.02733400	0.26639000	2.06396000
F	-5.06177800	-1.62663800	2.12060700
F	-4.67951500	0.67805100	-0.49712300
F	-5.85911600	-1.12335900	-0.35615600
F	-4.34672000	-0.93319700	-1.88518600
O	-2.35686200	-0.62821100	0.10483400
H	-2.04925600	-0.69287200	-0.84627800
C	1.85439200	-2.18512300	-2.06016000
C	2.73100200	-3.09857600	-1.19427900
C	-3.56778000	-1.27958900	0.30267000
C	-3.49290600	-2.78053500	0.03464900
F	2.02665500	-4.15085600	-0.77582000
F	3.18718100	-2.46622700	-0.09931500
F	3.79117200	-3.55990700	-1.86023800
H	-4.46906000	-3.25446300	0.14295900
H	-2.78999700	-3.23183300	0.73503100
H	-3.12690700	-2.93320500	-0.98102800
H	0.91042300	-3.84881100	-3.01836400
H	2.26556100	-3.17335300	-3.95606300
H	0.71237200	-2.30726200	-3.86804600

TS2

C	2.81409700	-1.99193900	-2.46868800
C	4.02809700	-2.00772100	-0.27676600
F	3.59761800	-3.26556100	-0.13576300
F	5.26292800	-2.05554100	-0.78783500
F	4.11339700	-1.48077500	0.94709300
O	1.94767100	-0.98886100	-0.39366700
H	1.09825600	-1.07858100	-0.86679900

C	-4.21921700	0.80543100	-0.71335900
H	-4.05640700	0.35863300	0.26701200
H	-5.28334400	0.86551300	-0.93160700
C	-3.44670500	0.07415000	-1.80391600
H	-3.49319000	0.69605000	-2.70921800
C	-4.17822700	-1.23393400	-2.12025000
H	-5.18365200	-1.03177700	-2.49829800
H	-3.62224100	-1.76778400	-2.89111400
H	-4.25011200	-1.87535800	-1.24131100
O	-2.10761900	-0.09169300	-1.46848200
Br	-3.64341000	2.68413000	-0.55992100
N	0.35467200	2.01712700	1.38468300
C	0.12663500	1.83223200	-0.11623200
C	-0.06856900	3.12102300	-0.90223900
H	-0.74821100	1.18882500	-0.22744800
H	0.98268100	1.27544000	-0.49547900
C	-0.43342900	2.79640100	-2.35302100
H	-0.87144300	3.72591000	-0.46913800
H	0.83975000	3.73330900	-0.90060100
C	-0.73838300	4.05917800	-3.15112000
H	0.39339600	2.24496200	-2.81197900
H	-1.30528900	2.13720900	-2.35585100
H	-0.97435200	3.81786600	-4.18867500
H	-1.59920700	4.58207800	-2.72560600
H	0.11222000	4.74663900	-3.14925000
C	0.98771300	0.74550500	1.90702600
C	1.28802400	0.75763900	3.39972800
H	1.90133800	0.59233200	1.33496900
H	0.31565300	-0.06428900	1.61461200

C	1.57877900	-0.66339600	3.88699800
H	2.15773800	1.39073500	3.60712700
H	0.45275000	1.16272600	3.98005700
C	2.09254500	-0.68538300	5.32317400
H	0.65864900	-1.25245200	3.81391400
H	2.30950800	-1.13206600	3.21914100
H	2.27110900	-1.70639400	5.66323400
H	3.03214800	-0.13417900	5.40938000
H	1.37030800	-0.22716800	6.00390400
C	-0.97396100	2.28146400	2.06696800
C	-1.86609800	1.06292200	2.25938600
H	-1.48479000	3.03116900	1.46120000
H	-0.74593100	2.73112600	3.03533400
C	-3.17850100	1.47312400	2.93135000
H	-2.06232500	0.56794300	1.30249200
H	-1.37295300	0.32443300	2.89651400
C	-4.02302400	0.25880100	3.31328300
H	-2.95620000	2.05505500	3.83358100
H	-3.74350000	2.13035800	2.26490900
H	-4.96672200	0.56546600	3.76729400
H	-4.25024100	-0.35615100	2.43999100
H	-3.49185800	-0.37657100	4.02580100
C	1.25376000	3.19513700	1.65674000
C	2.64207300	3.07387200	1.04770400
H	1.32004500	3.29705900	2.74121500
H	0.73266400	4.07551600	1.27768900
C	3.37226900	4.41648700	1.06597600
H	3.23312400	2.33543400	1.59721900
H	2.58283900	2.71458800	0.01759100

C	4.78390200	4.28964700	0.49961600
H	2.80135600	5.14562700	0.48085000
H	3.41434200	4.80135300	2.09067400
H	5.29726300	5.25209700	0.49189000
H	5.37993500	3.59260200	1.09329600
H	4.75584400	3.91066200	-0.52468800
C	-2.14615800	-2.70299700	1.36872400
C	0.29865900	-3.16202600	1.20897300
F	-1.86435200	-2.12671400	2.55114300
F	-2.55115400	-3.95052300	1.62250500
F	-3.19126000	-2.03381700	0.85972100
O	-0.74629000	-1.33044400	0.05034000
H	-1.53994400	-0.86050300	-0.63289100
C	3.07043100	-1.21704300	-1.18322000
C	3.69141400	0.15175900	-1.51786400
C	-0.91825300	-2.63371900	0.44728100
C	-1.12132900	-3.53690200	-0.78197900
F	-2.26674700	-3.28573500	-1.42036800
F	-1.10797500	-4.83945800	-0.47741100
F	-0.12431600	-3.32412100	-1.65564600
F	4.13216500	0.78449600	-0.41885700
F	2.77165800	0.94737100	-2.07898600
F	4.71546100	0.05982100	-2.36604500
C	-0.86361000	-0.25749500	-3.12322600
O	0.15901800	-0.42108600	-2.56789700
O	-1.61639200	-0.11259500	-3.99990300
H	1.14026300	-3.26078500	0.52626400
H	0.56898500	-2.44180500	1.97692100
H	0.08982700	-4.12919200	1.66810400

H	2.25295400	-2.89454900	-2.23134100
H	3.75686400	-2.26267500	-2.94428000
H	2.22121900	-1.38174100	-3.14750600

TS3

C	4.26997300	0.10455300	-1.42590300
C	3.24202900	-1.64007000	-2.88940600
F	3.36388000	0.99579200	-1.83893400
F	5.34326500	0.22349900	-2.21005700
F	4.63224000	0.46684000	-0.18646000
O	2.63259700	-1.33742600	-0.54109300
H	1.78786700	-1.59976900	-0.98415400
C	-1.44300500	1.49587500	-1.92157900
H	-1.56231400	1.32866000	-0.86229800
C	-0.06858100	1.41764600	-2.55468700
H	0.55037500	2.27241300	-2.30613200
O	0.60790400	0.26018200	-2.07849800
Br	-1.16557600	3.89981800	-0.95286900
N	0.67045000	0.61858900	2.11250400
C	1.18089500	1.48474900	0.97426300
C	1.69131500	2.85818600	1.37484400
H	0.34921700	1.61037800	0.28104600
H	1.94156000	0.89018700	0.46366700
C	2.43673100	3.48946800	0.19631500
H	0.84642700	3.50294100	1.63970900
H	2.36807900	2.80891600	2.23445500
C	2.77576800	4.95143100	0.46457000
H	3.34309700	2.91154700	-0.00803000
H	1.80207000	3.42912600	-0.69218500

H	3.34604200	5.38091800	-0.36029100
H	1.85949300	5.53540400	0.57878500
H	3.36934100	5.05907300	1.37690500
C	0.18947300	-0.67271100	1.47829600
C	-0.52432500	-1.65562800	2.39170800
H	1.07132600	-1.12409200	1.02828800
H	-0.48511900	-0.38113100	0.67346700
C	-0.62787900	-3.01572100	1.69436500
H	0.00435600	-1.79040800	3.34055700
H	-1.53106300	-1.29075900	2.62059800
C	-1.36605000	-4.03635100	2.55393700
H	-1.13340800	-2.88909300	0.73487900
H	0.38100300	-3.37756300	1.46989000
H	-1.45059500	-4.99400400	2.03850600
H	-0.84648200	-4.20550800	3.50109000
H	-2.37970000	-3.69778400	2.78175000
C	-0.44541300	1.30001800	2.86795800
C	-1.67169300	1.67014900	2.05243200
H	-0.00835600	2.19960800	3.30469800
H	-0.70715700	0.62678000	3.68787100
C	-2.69139100	2.36797400	2.95824900
H	-1.40176300	2.36561500	1.25166400
H	-2.12677400	0.78593100	1.59227400
C	-3.86454400	2.93336200	2.16188800
H	-3.05091800	1.66821600	3.72227500
H	-2.19365400	3.18496700	3.49232800
H	-4.56019000	3.46559200	2.81287400
H	-3.50535900	3.62582900	1.39679900
H	-4.41586700	2.14028000	1.65363100

C	1.77044200	0.34755300	3.11589500
C	3.09448900	-0.14643000	2.55559000
H	1.36375400	-0.37075900	3.82813900
H	1.92461600	1.28190300	3.65722700
C	4.06728100	-0.40632000	3.70906600
H	2.97095600	-1.05449700	1.95888200
H	3.53172200	0.60305800	1.89234800
C	5.41503700	-0.92036200	3.21027500
H	4.21086800	0.52139000	4.27401800
H	3.63112700	-1.13125500	4.40495500
H	6.12390600	-1.02716300	4.03273000
H	5.30410700	-1.89169300	2.72613000
H	5.84381200	-0.23505200	2.47528100
C	-4.89256000	-0.42042500	-0.69066800
C	-4.57755300	-1.28442700	1.63169800
F	-4.60989100	0.83827800	-0.33074700
F	-6.20967700	-0.58655500	-0.57320700
F	-4.57043300	-0.54587300	-1.98021600
O	-2.74793500	-1.05466300	0.14114000
H	-2.41436300	-1.03776800	-0.78706100
C	3.67442900	-1.31160200	-1.46525100
C	-4.09666000	-1.39438900	0.19371700
C	-0.24780600	-0.78573500	-1.90160800
O	-1.46987500	-0.48056300	-2.09821400
O	0.22587900	-1.85270800	-1.53563200
C	-2.62853700	1.84217700	-2.76728500
H	-3.47583700	2.13390300	-2.15331700
H	-2.88790400	0.96664400	-3.36662100
H	-2.37671900	2.66894000	-3.43105600

H	-0.19233100	1.34875200	-3.64002000
C	4.70518000	-2.34554700	-0.98789300
C	-4.26090800	-2.83657100	-0.31453600
H	4.09966300	-1.63276400	-3.56200700
H	2.77965800	-2.62703300	-2.90114700
H	2.51059800	-0.90191800	-3.21581100
H	-4.49057100	-0.24716100	1.95827500
H	-5.61420000	-1.60764700	1.72428600
H	-3.94452400	-1.91055400	2.25921800
F	5.78912200	-2.37680100	-1.76953000
F	5.11310500	-2.10332500	0.26202000
F	4.15916700	-3.56315800	-1.00213200
F	-3.70067800	-3.69057200	0.54943600
F	-5.54657200	-3.17594700	-0.44436500
F	-3.66166300	-3.00873600	-1.49087400

TBABR PLUS 2 MOLECULES OF PFB

TS1

C	2.84616600	-1.59109700	-1.50406000
C	1.19719500	-3.44326200	-2.03074800
F	0.99435400	-2.74415600	-3.15331500
F	2.04658700	-4.42961100	-2.30781700
F	0.03973400	-3.97106500	-1.66523000
F	2.30186900	-0.60098400	-2.20938100
F	3.69773100	-2.24481000	-2.28470000
F	3.54800900	-1.02426100	-0.50926200
O	0.73839100	-1.73963400	-0.38412600
H	0.03755100	-1.42160700	-1.07205500
C	-0.37869300	0.88347200	-1.94722800

H	0.55610000	0.74159800	-1.43997200
H	-1.15491100	1.49776800	-1.51509900
C	-0.71972500	-0.02818600	-3.02380000
H	0.12883800	-0.47015700	-3.54263200
C	-1.88440600	0.28987000	-3.91648700
H	-1.55809600	0.98421200	-4.69270400
H	-2.26187000	-0.62263100	-4.38044800
H	-2.68778900	0.75625700	-3.34541200
O	-1.04277700	-0.75078500	-1.82503100
Br	0.70376500	3.04941900	-2.79224200
N	1.65321800	1.77368600	1.76658300
C	2.43108900	1.97306800	0.47432300
C	2.92086000	3.38165300	0.17663000
H	1.77868100	1.67366200	-0.34294400
H	3.25956600	1.26692600	0.50958300
C	3.91080100	3.31732100	-0.99169500
H	2.07490400	4.00689700	-0.12473400
H	3.40633500	3.85063300	1.03915400
C	4.18482100	4.70026900	-1.57147100
H	4.84108100	2.84822300	-0.65208700
H	3.48441900	2.68451600	-1.77534600
H	4.92551300	4.64976700	-2.37081700
H	3.26406900	5.11113000	-1.99178200
H	4.55791200	5.38750700	-0.80658600
C	0.96979600	0.42325600	1.67918700
C	0.14750100	0.03906000	2.89883700
H	1.75365400	-0.30510700	1.47497000
H	0.33085500	0.45129900	0.79839000
C	-0.30019700	-1.42232500	2.79754500

H	0.72004400	0.16838800	3.82422100
H	-0.73980300	0.67475200	2.96632700
C	-1.10749600	-1.85101100	4.01922100
H	-0.89057000	-1.54882200	1.88769600
H	0.57950800	-2.06272600	2.68751800
H	-1.43756900	-2.88635400	3.92296700
H	-0.51130300	-1.77092400	4.93263800
H	-1.99734000	-1.22990800	4.13716700
C	0.63385500	2.87591600	1.95679700
C	-0.41688800	2.94927400	0.86287500
H	1.20225200	3.80620800	2.01404500
H	0.17405000	2.70484000	2.93165300
C	-1.26403200	4.21639100	0.99239100
H	0.05599700	2.96753200	-0.12483700
H	-1.07501500	2.07490100	0.90554100
C	-2.24945100	4.32172100	-0.16985100
H	-1.80063100	4.21316600	1.94779400
H	-0.60687600	5.09307200	0.99534600
H	-2.85081400	5.22943800	-0.09852300
H	-1.71114400	4.33697800	-1.12135500
H	-2.92900500	3.46698700	-0.17628900
C	2.60673700	1.82019100	2.93821700
C	3.51924700	0.61100400	3.10568600
H	1.99871800	1.94908400	3.83461000
H	3.19744200	2.72867800	2.81132000
C	4.53768400	0.87555200	4.21719300
H	2.93410600	-0.27730600	3.36106200
H	4.05473900	0.38093900	2.18027700
C	5.44419300	-0.32916400	4.45266200

H	5.14332000	1.74885100	3.95441700
H	4.00937100	1.12732300	5.14285300
H	6.16770500	-0.13002500	5.24421900
H	4.86047900	-1.20584900	4.74262700
H	5.99866900	-0.58210000	3.54603200
C	-4.35796700	0.15329400	-0.73862800
C	-3.99855800	0.55367300	1.72776400
F	-3.11158100	0.45774100	2.71720200
F	-4.08881100	1.84267300	1.39751600
F	-5.18005200	0.15459600	2.18785200
F	-3.87384400	1.29933000	-1.21556500
F	-5.64667800	0.32581900	-0.46111900
F	-4.25152100	-0.76104400	-1.70112400
O	-2.20893400	-0.03837900	0.33957200
H	-1.88571500	-0.37123100	-0.55147200
C	1.73660000	-2.50476300	-0.92074900
C	2.32795300	-3.35309900	0.22874800
C	-3.54941900	-0.28323500	0.51141500
C	-3.78773700	-1.79015800	0.78372900
F	-3.04553500	-2.51556400	-0.04352400
F	-5.06473300	-2.12972500	0.62189200
F	-3.43084300	-2.09856400	2.03271300
F	1.50006600	-4.33757700	0.55878900
F	2.51736800	-2.60138700	1.31806000
F	3.50402200	-3.88185600	-0.10512900

TS2

C	3.85834900	0.54403300	-0.82354100
C	3.21804100	-1.37980600	-2.32576600

F	3.09247100	-0.39966200	-3.21795600
F	4.39595300	-1.97041100	-2.53268300
F	2.25854800	-2.26449600	-2.53690600
F	3.08928000	1.49797400	-1.35518400
F	5.01872500	0.53578800	-1.46770100
F	4.09324200	0.89686300	0.44822900
O	1.84130700	-0.66533300	-0.42288200
H	1.18849100	-0.54903600	-1.14559400
C	-4.20464800	0.77459000	-1.26144100
H	-4.05122100	0.21382500	-0.34235500
H	-5.25027700	0.73930100	-1.55797100
C	-3.29329700	0.27548100	-2.36975200
H	-3.24112300	1.02950200	-3.16041400
C	-3.84836300	-1.01348300	-2.96997600
H	-4.79661500	-0.81680800	-3.47512600
H	-3.13811200	-1.39181900	-3.70568100
H	-4.00378400	-1.77571300	-2.20760100
O	-1.97557900	0.11770500	-1.87997500
Br	-3.87223500	2.65879500	-0.80717400
N	0.12470300	2.24945000	1.55243600
C	-0.02103400	2.16000600	0.03739300
C	-0.30171100	3.47381800	-0.67616600
H	-0.80918900	1.43076500	-0.15335800
H	0.90618100	1.72199400	-0.33148400
C	-0.49713100	3.22104300	-2.17289000
H	-1.20319700	3.95188300	-0.28029600
H	0.52963300	4.17563400	-0.55009400
C	-0.83419100	4.50354100	-2.92480900
H	0.41048000	2.76582900	-2.58236600

H	-1.30598100	2.49892300	-2.30310100
H	-0.95272100	4.30801100	-3.99139800
H	-1.77087200	4.93047700	-2.55607500
H	-0.04822000	5.25411600	-2.80423400
C	0.74798600	0.93947300	1.99402100
C	0.88403500	0.75467100	3.49759900
H	1.72293400	0.89190600	1.51116600
H	0.13874400	0.15529000	1.54099200
C	1.88082100	-0.37062300	3.79070400
H	1.24411100	1.66553200	3.98774900
H	-0.08512900	0.50989000	3.94306200
C	1.90288200	-0.74095700	5.26966400
H	1.62759000	-1.24610000	3.18952400
H	2.87706700	-0.05438700	3.46432500
H	2.64094900	-1.51916500	5.46902800
H	2.15114300	0.12465100	5.89016200
H	0.92686400	-1.11505100	5.58853800
C	-1.21781600	2.46528600	2.21585900
C	-2.22255500	1.32822800	2.13572400
H	-1.63808100	3.36513700	1.76059200
H	-1.00075300	2.69162000	3.26254700
C	-3.50902800	1.76511700	2.84055800
H	-2.44003300	1.07207100	1.09935900
H	-1.83597100	0.41659400	2.59660000
C	-4.59234000	0.69333500	2.77420600
H	-3.29037500	2.00131400	3.88838200
H	-3.87957800	2.68563300	2.37753900
H	-5.50604200	1.02736000	3.26845800
H	-4.84082900	0.45870700	1.73593300

H	-4.26192800	-0.23077600	3.25134200
C	0.99198500	3.42152700	1.94013600
C	2.41818600	3.36688200	1.41792700
H	0.99210000	3.47010400	3.02872100
H	0.47744000	4.31328300	1.58005100
C	3.12151900	4.71031200	1.60978600
H	2.98141500	2.59077200	1.94298700
H	2.43712400	3.10480200	0.35677800
C	4.56988600	4.65247600	1.13100400
H	2.57921800	5.48642400	1.05905400
H	3.08974500	4.99598200	2.66678000
H	5.06946100	5.61364700	1.25907800
H	5.13383600	3.90044200	1.68783800
H	4.61662300	4.38539300	0.07225700
C	-2.98713500	-2.66000700	0.88180600
C	-0.60963900	-2.63778700	1.66487300
F	0.66928600	-2.65551900	1.29198100
F	-0.72375300	-1.72024800	2.63729700
F	-0.89977300	-3.82215500	2.20625000
F	-3.24773300	-2.24946600	2.12810000
F	-3.22580400	-3.97002100	0.82498100
F	-3.87127100	-2.05239700	0.08195100
O	-1.43648800	-0.96754900	0.19282900
H	-1.78560900	-0.49001600	-0.93539500
C	3.12955000	-0.82071700	-0.87833700
C	3.80244200	-1.81455500	0.09941700
C	-1.53601400	-2.28124500	0.47080800
C	-1.12568800	-3.16000800	-0.74296900
F	-2.12198300	-3.20033900	-1.63871700

F	-0.83585700	-4.41633000	-0.40214100
F	-0.06613500	-2.64237500	-1.35353300
F	3.41588100	-3.05610800	-0.16945800
F	3.45280300	-1.53551600	1.35214000
F	5.13234600	-1.75559000	0.02243900
C	-0.64148900	0.18721500	-3.12106800
O	0.34958000	0.03934300	-2.47661700
O	-1.16479900	0.38971800	-4.15244300

TS3

C	4.45488100	0.18900300	-0.68903600
C	3.86209700	-1.84331600	-2.07914300
F	3.17472100	-2.97611300	-2.07396600
F	3.20368700	-0.96275700	-2.83514400
F	5.04778200	-2.07122000	-2.63952200
F	3.40275700	0.97927700	-0.89605300
F	5.34617700	0.42123100	-1.64757400
F	4.99991900	0.55517600	0.47749400
O	2.84408700	-1.40675300	0.07810500
H	2.03055700	-1.51790900	-0.50609700
C	-1.45694100	1.25896900	-2.27561600
H	-1.72992200	1.25037900	-1.23059400
C	0.00573800	1.36044200	-2.66699700
H	0.42262600	2.33889300	-2.45901400
O	0.76585300	0.41584700	-1.91397200
Br	-1.77400200	3.79425700	-1.77981700
N	0.34771600	1.53780300	1.93505500
C	0.73945500	2.37236700	0.73165300
C	0.81885500	3.87428700	0.95099400

H	-0.00270300	2.17079500	-0.04026600
H	1.68778300	1.96598400	0.38053400
C	1.56103500	4.51810000	-0.22381100
H	-0.19093200	4.29486600	1.00088900
H	1.34242900	4.13022100	1.87770700
C	1.48553500	6.03982400	-0.17173200
H	2.60387600	4.18183300	-0.21806600
H	1.10794200	4.17401300	-1.15721800
H	2.04929600	6.49042900	-0.98970200
H	0.44691900	6.36640800	-0.26058100
H	1.88888900	6.42544400	0.76885400
C	0.21714100	0.10900300	1.43880600
C	-0.08391400	-0.94105800	2.49661700
H	1.15173100	-0.11177600	0.92537200
H	-0.58227800	0.12473800	0.69861000
C	-0.01690900	-2.34393200	1.88187700
H	0.64242400	-0.89622300	3.31422000
H	-1.08004800	-0.78325500	2.92158300
C	-0.39399200	-3.42038300	2.89443900
H	-0.68283500	-2.39423000	1.01954200
H	0.99497700	-2.51710000	1.50373500
H	-0.32209700	-4.41307100	2.44751900
H	0.26714800	-3.39598600	3.76516200
H	-1.42062400	-3.28553900	3.24237600
C	-0.95108600	2.03062400	2.53605700
C	-2.14435100	2.06268800	1.59530700
H	-0.74187500	3.03628500	2.90618200
H	-1.14907900	1.39333000	3.40018900
C	-3.34299200	2.71512300	2.29204300

H	-1.91659500	2.65233800	0.70198000
H	-2.41861800	1.05350600	1.27235500
C	-4.49066800	2.95980500	1.31483700
H	-3.67768000	2.08498500	3.12312100
H	-3.02804700	3.67148700	2.72481500
H	-5.32654300	3.45664100	1.81037000
H	-4.15628200	3.58624200	0.48430200
H	-4.85485100	2.01971600	0.89859700
C	1.39648200	1.63662900	3.01722700
C	2.80329900	1.20389100	2.63237600
H	1.02842800	1.04089900	3.85242500
H	1.40192300	2.67568600	3.34652400
C	3.69273300	1.22524300	3.87962100
H	2.81470600	0.19943600	2.19543400
H	3.22184200	1.88502900	1.88554800
C	5.15120600	0.91409300	3.55711500
H	3.62230100	2.20836800	4.35824300
H	3.31055500	0.49770800	4.60362100
H	5.76055900	0.92083600	4.46205100
H	5.24596600	-0.06616900	3.08736500
H	5.56263300	1.65248800	2.86528900
C	-4.66484500	-1.06340000	-0.94109600
C	-4.24923200	-1.54242600	1.51091900
F	-3.29557700	-1.77331300	2.40919600
F	-4.68160000	-0.29393600	1.70044000
F	-5.25936600	-2.37352800	1.74368100
F	-4.55546200	0.26268300	-0.89075600
F	-5.93160600	-1.39118500	-0.71431300
F	-4.33824300	-1.44584900	-2.17664900

O	-2.47978700	-1.08007900	0.04608300
H	-2.06489500	-1.12182200	-0.85900800
C	4.01205600	-1.29773100	-0.63665200
C	5.08679500	-2.12243000	0.11197600
C	-3.69874400	-1.71497100	0.07937100
C	-3.52752800	-3.22304900	-0.23956000
F	-2.68261200	-3.36820100	-1.25269900
F	-4.68585400	-3.79213200	-0.56322800
F	-3.02369900	-3.86699400	0.81315800
F	4.92430500	-3.42180400	-0.11876000
F	4.99084000	-1.92606900	1.42435000
F	6.31692600	-1.77932500	-0.27117800
C	0.08292600	-0.73726700	-1.73642500
O	-1.13652500	-0.67549000	-2.11875600
O	0.64354100	-1.68155900	-1.19782700
C	-2.52315200	1.22354300	-3.32904900
H	-3.50044400	1.42400300	-2.89827100
H	-2.51750200	0.23487800	-3.79298900
H	-2.31916300	1.97612300	-4.08981500
H	0.10304300	1.13423800	-3.73276100

TBABr PLUS 2 MOLECULES OF HFTI

TS1

C	-0.47878100	3.33193700	-0.90924900
F	-0.40814300	2.83135900	-2.14563000
F	-0.59724100	4.65536100	-1.00262500
F	-1.61684800	2.86667500	-0.36617100
O	0.64668000	1.49829400	0.05371500
H	0.75853200	0.98785700	-0.81077400

C	-0.87348300	-0.32458700	-2.16984800
H	-1.26322800	0.57410500	-1.71923100
H	-1.06258600	-1.29060500	-1.72949200
C	0.22856300	-0.21472300	-3.11283900
H	0.28919900	0.73401500	-3.64606900
C	0.56484100	-1.41335600	-3.95659800
H	-0.11854300	-1.45706000	-4.80638000
H	1.59318300	-1.34910300	-4.31611200
H	0.45327800	-2.33079800	-3.37404100
O	0.88055700	-0.15927000	-1.84352800
Br	-3.10627800	-0.61082100	-3.33545800
N	-3.15784200	-0.36689500	1.43803700
C	-3.64870500	0.41459800	0.23431300
C	-5.05486600	0.10029800	-0.24843300
H	-2.95469900	0.21185600	-0.57987900
H	-3.54294000	1.46659800	0.49987500
C	-5.50850000	1.20289500	-1.21106600
H	-5.04993600	-0.85251500	-0.78710500
H	-5.77234500	0.02391300	0.57606500
C	-6.74509400	0.78645100	-1.99919900
H	-5.70221900	2.11963100	-0.64253100
H	-4.69557400	1.41090400	-1.91186900
H	-7.09084200	1.59548600	-2.64422000
H	-6.50463000	-0.06953500	-2.63389700
H	-7.56825300	0.50714100	-1.33508500
C	-1.67857000	-0.04753700	1.58906500
C	-1.04416700	-0.49232800	2.89816700
H	-1.57302900	1.02755500	1.45077000
H	-1.17199900	-0.51871100	0.74603000

C	0.46948600	-0.29880200	2.81081200
H	-1.44216700	0.08129600	3.74277100
H	-1.24485600	-1.55212600	3.09102100
C	1.19973900	-0.74573800	4.07118500
H	0.82370600	-0.87563500	1.95857200
H	0.69607600	0.74652700	2.58959800
H	2.28020100	-0.66536100	3.92992600
H	0.92288400	-0.13240900	4.93319200
H	0.97362300	-1.78844400	4.30682800
C	-3.37610300	-1.85655400	1.24442000
C	-2.68008800	-2.45248200	0.03492800
H	-4.45712600	-1.98895800	1.16707700
H	-3.04524000	-2.33832600	2.16641900
C	-3.08828300	-3.90897100	-0.19124500
H	-2.94333500	-1.89332200	-0.86874200
H	-1.59377700	-2.42230200	0.15695300
C	-2.42698600	-4.43912700	-1.46248700
H	-2.79482600	-4.51779500	0.67067200
H	-4.17817000	-3.97749800	-0.28230900
H	-2.69804900	-5.47965200	-1.64876600
H	-2.73202600	-3.84129100	-2.32567100
H	-1.33940300	-4.38116600	-1.37716400
C	-3.92088700	0.03212400	2.67484900
C	-3.85932600	1.50894400	3.04231200
H	-3.52158800	-0.57797900	3.48589200
H	-4.95522400	-0.27522800	2.51747700
C	-4.37036300	1.71397600	4.46992100
H	-2.83701400	1.89240600	2.96962300
H	-4.47354300	2.09747800	2.35485000

C	-4.39856000	3.18865900	4.86021400
H	-5.37431700	1.28611800	4.56393300
H	-3.72863200	1.15936400	5.16286500
H	-4.75429800	3.31945300	5.88300700
H	-3.40059700	3.62810200	4.79113900
H	-5.05929100	3.75480500	4.19957800
C	2.25551900	-3.75773600	-1.11440000
C	1.16964900	-3.94004600	1.16547800
F	0.88074500	-3.28663900	2.29699700
F	0.02776300	-4.46863800	0.72096500
F	1.98286700	-4.95308200	1.47793700
F	1.25492200	-4.45876000	-1.65335100
F	3.25278400	-4.60921000	-0.86607100
F	2.67827600	-2.88630100	-2.03389300
O	0.74266900	-2.15568000	-0.23228700
H	0.98735200	-1.46782700	-0.91904500
C	0.75519400	2.86817100	-0.10511500
C	0.70522300	3.41658000	1.33354800
C	1.79779100	-2.97749500	0.13718400
F	1.77381000	3.00925600	2.01457200
F	-0.37830400	2.97557300	1.99615300
F	0.66848700	4.75012400	1.37817900
C	2.04149400	3.32684900	-0.79488600
C	2.95211700	2.36980600	-1.23052100
C	2.33435100	4.67986900	-0.99268200
C	4.13685300	2.75740400	-1.84795300
H	2.74458200	1.31459100	-1.11233400
C	3.51868400	5.05269400	-1.60917200
H	1.64433000	5.44607400	-0.66618200

C	4.44147400	4.10013700	-2.04595000
H	4.83099600	1.99406400	-2.18261600
H	3.73106500	6.10667300	-1.75534000
C	2.98961400	-2.23209700	0.74496900
C	2.99614400	-0.84053700	0.72045300
C	4.07635200	-2.89828600	1.31474100
C	4.05586500	-0.12490700	1.26191200
H	2.16025100	-0.29568500	0.30523900
C	5.13137700	-2.17492800	1.85533300
H	4.11100900	-3.97900700	1.33626400
C	5.14018900	-0.78015400	1.84219000
H	4.02638000	0.96030500	1.23265700
H	5.96755800	-2.70831100	2.29492200
C	6.27378800	-0.00585400	2.46094700
H	6.06967400	0.19407100	3.51658400
H	7.21011500	-0.56282800	2.40355500
H	6.41113300	0.95477800	1.96262500
C	5.71954900	4.52719700	-2.71791500
H	6.30875100	5.17120100	-2.06084100
H	6.33039400	3.66558200	-2.98806700
H	5.50680300	5.09226600	-3.62851100

TS2

C	-4.73773200	0.04309700	-1.61883600
F	-4.23310000	0.64186600	-2.69838700
F	-5.98780000	0.48738100	-1.43995500
F	-4.81422100	-1.26024200	-1.88733200
O	-2.69704700	-0.49091800	-0.54731700
H	-2.06224700	-0.03921700	-1.13266500

C	4.01484400	-0.77466600	-1.92813500
H	4.05099300	-0.56246900	-0.86121200
H	4.99923600	-0.65624100	-2.37479000
C	2.96905500	0.08082400	-2.62949900
H	2.78704600	-0.32658900	-3.62953400
C	3.47818900	1.51603200	-2.76753200
H	4.37114000	1.55448800	-3.39597700
H	2.69843400	2.12116000	-3.23300200
H	3.71193400	1.94718700	-1.79252500
O	1.74966100	0.02872400	-1.92766100
Br	3.61997700	-2.69758400	-2.07093500
N	-0.04232200	-2.90041000	0.93727200
C	0.02388100	-2.37146200	-0.48756100
C	0.02505100	-3.41489300	-1.59346500
H	0.91256600	-1.74378500	-0.54676400
H	-0.83761000	-1.71718900	-0.59367700
C	0.04267500	-2.71049600	-2.95322700
H	0.90275900	-4.06560600	-1.52295500
H	-0.86688600	-4.04807100	-1.54948900
C	0.17254800	-3.70023800	-4.10529000
H	-0.87829100	-2.12645900	-3.06091800
H	0.87787400	-2.00726600	-2.97505200
H	0.14865200	-3.18366400	-5.06586700
H	1.11962800	-4.24237800	-4.03969900
H	-0.64021700	-4.43166800	-4.09444900
C	-0.35008600	-1.70551000	1.81980600
C	-0.35406200	-1.99281000	3.31523300
H	-1.32489000	-1.33864800	1.48923200
H	0.39683600	-0.94935000	1.55995100

C	-1.07613000	-0.87150300	4.06879500
H	-0.86034900	-2.93556000	3.54604600
H	0.67191400	-2.07783500	3.68581000
C	-0.88621600	-0.98942700	5.57744300
H	-0.70444100	0.09517700	3.72541400
H	-2.14016900	-0.90346200	3.81665200
H	-1.43470100	-0.20842400	6.10610600
H	-1.23929700	-1.95635300	5.94645900
H	0.17032300	-0.89334900	5.83998000
C	1.26589200	-3.55125200	1.32661700
C	2.48929900	-2.65514000	1.44407800
H	1.44222700	-4.32370300	0.57508100
H	1.08202600	-4.05396300	2.27923300
C	3.71802900	-3.55753900	1.59740300
H	2.60969000	-2.01774200	0.56758200
H	2.40527600	-1.97608900	2.29691500
C	5.02136100	-2.77425400	1.70527600
H	3.59810400	-4.19745500	2.47973300
H	3.77275700	-4.22295800	0.72920800
H	5.87510900	-3.45093200	1.77194400
H	5.15972900	-2.13862100	0.82727300
H	5.02435400	-2.12923000	2.58537500
C	-1.10379600	-3.96520100	1.06277700
C	-2.52658000	-3.53835500	0.73119400
H	-1.05476600	-4.34037400	2.08465600
H	-0.78577100	-4.78109500	0.41254100
C	-3.39851800	-4.78669900	0.56951700
H	-2.92979800	-2.90761500	1.52962100
H	-2.57141400	-2.94148000	-0.18410700

C	-4.86894100	-4.45193400	0.33749200
H	-3.01818600	-5.37487900	-0.27328600
H	-3.30123800	-5.42063600	1.45837100
H	-5.45125300	-5.35822300	0.16369300
H	-5.29240200	-3.93531300	1.20076200
H	-4.98768500	-3.79580700	-0.52757100
C	3.83830800	1.27084100	1.44659900
C	1.55016800	1.55468300	2.41887400
F	0.23224600	1.59594200	2.15644300
F	1.74798400	0.47654000	3.19996300
F	1.83500700	2.63253400	3.15087500
F	4.07508600	0.03386000	1.89186700
F	4.29216600	2.11381000	2.38724900
F	4.60863100	1.44121100	0.36016200
O	1.90543000	0.34781900	0.44405400
H	1.84238300	0.28151700	-0.82402100
C	-3.83241900	0.30935400	-0.39542300
C	-4.51993400	-0.20867200	0.88203400
C	2.34183200	1.46097800	1.09379000
F	-3.65143000	-0.21457200	1.90015600
F	-4.96122000	-1.46436800	0.73941400
F	-5.55539100	0.54894200	1.22776900
C	0.16902700	0.47479600	-2.91724000
O	-0.65144100	0.48782000	-2.06153200
O	0.54144600	0.57051500	-4.02071700
C	2.11176000	2.77175800	0.32644200
C	1.01635100	2.80688200	-0.52806900
C	2.90178100	3.91593000	0.45336500
C	0.71904400	3.95041200	-1.26043400

H	0.38504200	1.93300600	-0.60965500
C	2.60705600	5.05086200	-0.29016400
H	3.75226500	3.93309700	1.12248600
C	1.51460800	5.08846700	-1.16052900
H	-0.15305300	3.95083500	-1.90808300
H	3.23656900	5.92927500	-0.19009600
C	-3.48334400	1.78104500	-0.21526600
C	-2.30488600	2.07687500	0.47087500
C	-4.28317700	2.82500700	-0.67270800
C	-1.93046300	3.39352800	0.68490400
H	-1.66958000	1.27618300	0.83076100
C	-3.88273300	4.14202100	-0.47711400
H	-5.20964300	2.62945300	-1.19608800
C	-2.70212100	4.44774900	0.19633800
H	-1.00784500	3.60243300	1.21495900
H	-4.50170200	4.94484000	-0.86247500
C	1.21904700	6.32655700	-1.96674000
H	0.24257300	6.25802900	-2.44825400
H	1.23017500	7.21832400	-1.33577600
H	1.97017100	6.46741800	-2.74828800
C	-2.24360000	5.86808700	0.39191900
H	-2.28698500	6.14762300	1.44761500
H	-1.20516900	5.97783300	0.06636200
H	-2.86155500	6.56790500	-0.17159900

TS3

C	3.98997200	0.43338600	-1.87687700
C	3.77015900	-2.06915100	-2.24334100
F	3.48734800	-3.22907900	-1.65583700

F	2.86503500	-1.86940400	-3.20529800
F	4.96698000	-2.17913500	-2.82532700
F	2.98338800	0.76104900	-2.68380100
F	5.11480400	0.46774400	-2.59756900
F	4.07844400	1.39119300	-0.94255500
O	2.46285100	-0.87523700	-0.64268400
H	1.71949600	-0.90172100	-1.30041900
C	-2.18733900	1.95179700	-2.10470700
H	-2.19295200	1.82967400	-1.03184700
C	-0.85886500	2.11021300	-2.81713700
H	-0.41476800	3.08578900	-2.65788200
O	0.06163400	1.14569000	-2.30963200
Br	-2.39005900	4.42498700	-1.35700800
N	0.38594500	1.89992300	1.70131600
C	0.54835300	2.83337000	0.51756800
C	0.63117600	4.31427800	0.84765700
H	-0.30586200	2.65899900	-0.13670800
H	1.43733600	2.49144000	-0.01556500
C	1.13587300	5.08063200	-0.37808400
H	-0.36113700	4.69164000	1.11460400
H	1.30725100	4.50873000	1.68689400
C	0.99044300	6.58764500	-0.19992500
H	2.18152400	4.81224300	-0.56551000
H	0.55406600	4.77175500	-1.25028000
H	1.40026500	7.12623100	-1.05556600
H	-0.06590700	6.85154900	-0.11082600
H	1.51089400	6.93320000	0.69780000
C	0.22899500	0.50102400	1.12586900
C	0.35961400	-0.64645300	2.11640000

H	0.98273200	0.40447400	0.34774800
H	-0.75342700	0.47366100	0.65216500
C	0.06744700	-1.97101400	1.40672100
H	1.37272800	-0.68279600	2.53314100
H	-0.34345000	-0.53215200	2.94907900
C	0.11970400	-3.15970500	2.35990000
H	-0.92154900	-1.90679200	0.95458300
H	0.77846400	-2.10770700	0.58835100
H	-0.13485000	-4.08203600	1.83422100
H	1.11778000	-3.28177300	2.79169900
H	-0.59253600	-3.03616700	3.17912900
C	-0.81885300	2.28332000	2.53587200
C	-2.14171300	2.36551700	1.79465000
H	-0.57922800	3.25460400	2.97374100
H	-0.86945500	1.55518000	3.34813300
C	-3.24724500	2.85161100	2.73593400
H	-2.07649000	3.07578900	0.96554600
H	-2.43543300	1.39307400	1.39067300
C	-4.55856900	3.03838700	1.97641300
H	-3.38203100	2.13382800	3.55192200
H	-2.94622100	3.80255800	3.18999400
H	-5.34877800	3.39958600	2.63687700
H	-4.42805800	3.75829300	1.16470200
H	-4.88584700	2.09241900	1.54105100
C	1.59107200	1.97346200	2.60706700
C	2.92809300	1.73898300	1.92285500
H	1.42203300	1.24147600	3.39728600
H	1.57249700	2.95832700	3.07382000
C	4.02903500	1.52718200	2.96503000

H	2.89071100	0.86963400	1.25860500
H	3.18541500	2.60203300	1.30086800
C	5.41669400	1.59785600	2.33453400
H	3.94131900	2.28118600	3.75581500
H	3.88505100	0.55088100	3.44108800
H	6.19549600	1.34903800	3.05823800
H	5.49606700	0.90265200	1.49688000
H	5.61530300	2.60331000	1.95456300
C	-5.14177500	-1.12659600	-0.24249600
C	-3.93455200	-1.43499900	1.96801900
F	-2.82523600	-1.89883700	2.55096100
F	-4.07870500	-0.16558100	2.35954300
F	-4.97225400	-2.11934600	2.45412000
F	-5.52894000	0.09079700	0.14599100
F	-6.14874100	-1.96559500	-0.00024500
F	-4.94662000	-1.08183000	-1.56392000
O	-2.85930300	-0.59975100	0.10859200
H	-2.65230400	-0.58977600	-0.85219900
C	3.72959600	-0.93170800	-1.20259200
C	-3.82047800	-1.55220400	0.43516700
C	-0.55249900	-0.04701600	-2.09929700
O	-1.82228700	0.00724300	-2.22436600
O	0.12758600	-1.01366300	-1.78408600
C	-3.48387100	1.96286700	-2.85805800
H	-4.32289900	2.08291800	-2.17623400
H	-3.57771100	1.01869300	-3.39782800
H	-3.49612900	2.78630200	-3.57082400
H	-1.01113500	1.94105500	-3.88739600
C	4.74492500	-1.21523100	-0.10200200

C	4.28088700	-1.63894500	1.14121800
C	6.11963100	-1.10445500	-0.31208900
C	5.17709100	-1.91550700	2.16621800
H	3.21529500	-1.75938700	1.29321200
C	7.00522800	-1.38030500	0.72137900
H	6.50638100	-0.80667700	-1.27749400
C	6.55159200	-1.78001200	1.97834600
H	4.80023700	-2.25017200	3.12754900
H	8.07114400	-1.28423900	0.54474400
C	-3.45508100	-2.97756100	0.01787900
C	-2.34194300	-3.19224800	-0.79226100
C	-4.21926600	-4.07474000	0.42166000
C	-1.99654500	-4.48132000	-1.17863400
H	-1.71458400	-2.37491900	-1.12731500
C	-3.86076000	-5.35734700	0.03124100
H	-5.09616200	-3.93840700	1.03954600
C	-2.74591800	-5.58410900	-0.77458000
H	-1.12240600	-4.62339900	-1.80531000
H	-4.46251700	-6.19808300	0.35954100
C	-2.38178800	-6.97440200	-1.22394300
H	-1.30055500	-7.08738000	-1.31662200
H	-2.74951800	-7.72522800	-0.52329300
H	-2.82238600	-7.18583800	-2.20218100
C	7.51879700	-2.03212800	3.10414500
H	7.73586700	-1.10135000	3.63634100
H	7.10976000	-2.74093200	3.82537600
H	8.46434000	-2.42760200	2.73036100

CO₂/PO COUPLING USING FLUORINATED HBDS: THE KEY ROLE OF THE CF₃ GROUPS

TBABr PLUS 2 MOLECULES OF TERT-BUTANOL

TS1

C	-1.96441500	1.18483000	4.18328600
C	-3.09919400	2.54465500	2.40687700
O	-0.99896700	1.44393700	1.99388800
H	-1.53778800	0.66344800	1.74369000
C	-0.91873800	-1.67925200	1.17308200
H	-0.26389500	-1.04370100	1.75120500
H	-0.87338900	-1.66780000	0.09573000
C	-2.20747400	-2.04048300	1.75981200
H	-2.18780200	-2.14835100	2.84861000
C	-2.98763500	-3.14337400	1.08813400
H	-2.58907900	-4.11562400	1.38420900
H	-4.04179500	-3.08293700	1.36818700
H	-2.90539800	-3.05065800	0.00233500
O	-2.51121400	-0.72895200	1.34737300
Br	0.73539600	-3.49198300	1.15497700
N	1.95585200	0.61588600	-0.94508800
C	2.40798300	-0.26105100	0.21106000
C	3.47494800	-1.29968900	-0.10088600
H	1.52461300	-0.78019100	0.58066500
H	2.74059700	0.42326000	0.99249400
C	4.05033900	-1.84126600	1.21191500
H	3.02250200	-2.13111100	-0.64974700
H	4.29010300	-0.89483100	-0.71019100
C	4.86442900	-3.10985400	0.98440100
H	4.66567100	-1.06670500	1.68322100
H	3.22404200	-2.06908200	1.89051500

H	5.31642900	-3.45943700	1.91374700
H	4.21313600	-3.90268000	0.60930500
H	5.66579700	-2.94610600	0.25798100
C	0.68075900	1.30817200	-0.49845600
C	0.07417600	2.25836300	-1.51690500
H	0.91129200	1.80962100	0.44145700
H	-0.04095100	0.52795700	-0.26071000
C	-0.99238500	3.11811000	-0.83626600
H	0.82910700	2.91226500	-1.96959300
H	-0.40080700	1.68192900	-2.31727000
C	-1.65164600	4.09175700	-1.80692500
H	-1.73110900	2.44716000	-0.39395500
H	-0.53739100	3.66612800	-0.00380900
H	-2.43696800	4.66714100	-1.31197800
H	-0.92578800	4.79998500	-2.21676200
H	-2.10946300	3.56199600	-2.64661200
C	1.71383700	-0.21284200	-2.18958500
C	0.64921700	-1.28057000	-2.02948400
H	2.67905100	-0.65107500	-2.45398800
H	1.43910600	0.49281400	-2.97585200
C	0.58573800	-2.20025800	-3.24899800
H	0.85799600	-1.90357100	-1.15364900
H	-0.33219400	-0.81507900	-1.89288800
C	-0.49962600	-3.25569000	-3.04561000
H	0.37949700	-1.61478800	-4.15244800
H	1.55555900	-2.68792600	-3.39814800
H	-0.56339700	-3.93674200	-3.89571700
H	-0.29493700	-3.84102900	-2.14509600
H	-1.47406200	-2.77626400	-2.91693000

C	3.03521100	1.61896500	-1.27850400
C	3.22219400	2.76237200	-0.29068700
H	2.79700100	2.02138900	-2.26367300
H	3.96027400	1.04878400	-1.37584400
C	4.42881000	3.60999100	-0.70036700
H	2.33097600	3.39555300	-0.26686900
H	3.37787000	2.38902500	0.72508000
C	4.63643600	4.79584800	0.23763400
H	5.32699900	2.98406400	-0.70918400
H	4.28837500	3.97043100	-1.72492000
H	5.50020300	5.39058000	-0.06254600
H	3.76137800	5.44993700	0.23900500
H	4.80193500	4.45685300	1.26299500
C	-4.28390200	-1.11557200	-1.76527900
C	-3.12441800	0.44487600	-3.35450300
O	-2.26999900	0.08054300	-1.19030700
H	-2.46515900	-0.22279700	-0.27142600
C	-1.75130400	2.12426100	2.99523000
C	-0.92559900	3.33762400	3.39980900
C	-3.50011200	0.18918300	-1.90062700
C	-4.31644600	1.35067700	-1.33168000
H	0.04818700	3.01482400	3.77568600
H	-0.99909600	0.85253900	4.57255500
H	-1.43069800	3.91102500	4.18042500
H	-0.76740200	3.98766400	2.53546400
H	-2.51748700	1.67726300	4.98746500
H	-2.52877600	0.30738300	3.85550600
H	-3.71574800	3.05799200	3.14948600
H	-2.94635800	3.21290400	1.55490100

H	-3.63352300	1.65506200	2.06139100
H	-3.76806500	2.28981200	-1.43541200
H	-4.50900900	1.17973000	-0.26906500
H	-5.27613600	1.44954300	-1.84583600
H	-4.01459000	0.53535400	-3.98121700
H	-4.50285600	-1.30870500	-0.71184700
H	-5.22689600	-1.06885800	-2.31585900
H	-3.69459500	-1.95066000	-2.15252500
H	-2.51252700	-0.37961300	-3.73139300
H	-2.54804800	1.37017300	-3.43547300

TS2

C	3.36782000	-0.44515700	-2.62643100
C	2.86722500	-2.91038700	-2.58060600
O	2.83767600	-1.57654600	-0.56262700
H	1.87516000	-1.72480600	-0.63008600
C	-3.99890000	-0.39523900	0.26070600
H	-3.58398600	-0.77061000	1.19663200
H	-5.07990000	-0.52123600	0.24126600
C	-3.29749000	-1.01485900	-0.94882400
H	-3.65783400	-0.45661500	-1.83409500
C	-3.83866800	-2.44864600	-1.09850600
H	-4.92273300	-2.46470200	-1.24359200
H	-3.37236300	-2.90205300	-1.97468400
H	-3.59425000	-3.05795100	-0.22337500
O	-1.93199000	-0.95311900	-0.85369300
Br	-3.74449300	1.56212400	0.32781300
N	0.74409900	1.63964700	0.92286600
C	0.11149900	1.34445500	-0.43529700

C	-0.57446900	2.52831600	-1.10325000
H	-0.61641900	0.53850500	-0.29267100
H	0.90740800	0.94847600	-1.06858800
C	-1.29428100	2.05185100	-2.36786600
H	-1.31610100	2.97401900	-0.43320600
H	0.13886900	3.31477000	-1.37422300
C	-2.11473600	3.16544600	-3.00860500
H	-0.55174700	1.67467300	-3.07980500
H	-1.94277700	1.21221700	-2.10193600
H	-2.59812000	2.81719100	-3.92269900
H	-2.89799400	3.50491100	-2.32570000
H	-1.48992900	4.02615900	-3.26454000
C	1.74185200	0.53733000	1.19050200
C	2.50310000	0.65025100	2.50145200
H	2.43479900	0.53005300	0.35193800
H	1.18696900	-0.39987500	1.12194700
C	3.24946000	-0.66193900	2.75794600
H	3.22561100	1.47365700	2.46225100
H	1.83395100	0.85081300	3.34558300
C	4.17691300	-0.57228000	3.96504900
H	2.51031700	-1.45433800	2.91059400
H	3.80383100	-0.94317200	1.85770300
H	4.67738400	-1.52417800	4.14905900
H	4.94894100	0.18636400	3.81132600
H	3.62210900	-0.30523800	4.86868200
C	-0.33324800	1.66729200	1.98852500
C	-0.89515500	0.31072200	2.39455300
H	-1.13273100	2.30133000	1.60123900
H	0.10172300	2.16563400	2.85731400

C	-1.98023400	0.50623600	3.45786300
H	-1.30037100	-0.22048900	1.52561500
H	-0.10506200	-0.32112400	2.81323100
C	-2.45976100	-0.82267800	4.03675400
H	-1.58839700	1.13101200	4.26919500
H	-2.82238800	1.04973800	3.02055000
H	-3.25208000	-0.66961300	4.77142000
H	-2.84693100	-1.47847100	3.25352300
H	-1.64034900	-1.35257000	4.53006800
C	1.43057400	2.97714700	0.92935200
C	2.56978500	3.11286500	-0.07204100
H	1.80151100	3.13627400	1.94322500
H	0.65705000	3.72399000	0.74264400
C	2.99074400	4.57685100	-0.20757900
H	3.42946200	2.51819500	0.25132800
H	2.27297700	2.73084000	-1.05300400
C	4.16319500	4.74545900	-1.16957800
H	2.13590500	5.16527500	-0.55786800
H	3.25957500	4.97281900	0.77771700
H	4.45067100	5.79347200	-1.26449700
H	5.03605000	4.18716600	-0.82277400
H	3.90447900	4.37545000	-2.16456500
C	-1.12752700	-3.39816100	1.66373600
C	1.26728100	-3.92485000	1.14305700
O	0.18255000	-2.04977900	0.17243000
H	-0.67490900	-1.69547800	-0.21660700
C	3.48661200	-1.74054200	-1.81876400
C	4.94820600	-2.02601600	-1.49077700
C	-0.04636000	-3.39476200	0.58233500

C	-0.48127800	-4.21433500	-0.63314000
C	-1.02952700	-1.08731500	-2.92398500
O	0.08344600	-0.98715800	-2.58903100
O	-2.01151500	-1.19513300	-3.53339300
H	5.36891300	-1.20089700	-0.91038600
H	5.02313900	-2.93831800	-0.89530600
H	5.53786200	-2.14753100	-2.40238000
H	-0.77856000	-2.84121500	2.53769200
H	-1.38383300	-4.41427200	1.97504800
H	-2.02705300	-2.90723600	1.28360600
H	2.31913600	-0.23047200	-2.84195700
H	3.79336600	0.38372000	-2.05177400
H	3.90762500	-0.51729200	-3.57467100
H	-1.37864000	-3.77497700	-1.07413700
H	-0.69351300	-5.25183100	-0.36133600
H	0.31225400	-4.20427000	-1.38460100
H	1.15689200	-4.96364100	1.46372100
H	2.05623400	-3.86143600	0.39163700
H	1.57595400	-3.32500900	2.00272800
H	2.94918400	-3.82755400	-1.99116300
H	1.81138400	-2.71139500	-2.77845300
H	3.37368900	-3.06720000	-3.53629800

TS3

C	-3.57252500	2.02579800	0.40873700
C	-3.88234300	1.47920700	-0.98465800
C	-3.36316800	2.42781500	-2.06101200
C	-5.37871100	1.23476200	-1.14723000
O	-3.23483100	0.20730300	-1.12141100

H	-2.49594600	0.29536000	-1.74614500
Br	4.15962100	0.43414900	0.36101200
C	2.40186000	1.01140600	-1.25642800
H	2.96421100	1.88226000	-1.55346800
H	1.79497000	1.10349400	-0.37399300
C	2.46682700	-0.25362200	-2.09682900
H	2.91699300	-1.06543800	-1.53428600
C	3.22520400	-0.02049900	-3.39002300
H	4.26443600	0.22292000	-3.15956000
H	3.19931800	-0.92113700	-4.00383400
H	2.77587700	0.80500000	-3.94524000
O	1.11949600	-0.67164300	-2.35373400
C	0.26081800	0.39428600	-2.47130000
O	-0.91351800	0.15865000	-2.68820300
O	0.83438500	1.52088300	-2.27624600
N	-0.45621500	-1.92161000	1.08681600
C	0.59891800	-2.99401700	1.22131600
C	1.79449600	-2.84531400	0.29338200
H	0.09406400	-3.94765000	1.05632800
H	0.92674300	-2.96869200	2.26252700
C	2.86721500	-3.88595500	0.61768000
H	1.48981000	-2.95399000	-0.75190500
H	2.24929400	-1.85626400	0.40410300
C	4.07232600	-3.72724000	-0.30656700
H	3.18596600	-3.76199300	1.65813300
H	2.45004500	-4.89511200	0.52901400
H	4.84979200	-4.45664100	-0.07461400
H	3.78006400	-3.86898000	-1.35073800
H	4.50004600	-2.72610800	-0.20466800

C	-1.52095600	-2.19712300	2.11720600
C	-2.67989200	-1.20979600	2.13297600
H	-1.02364500	-2.22104600	3.08779000
H	-1.88212100	-3.20664500	1.91271100
C	-3.80474600	-1.73878400	3.02549200
H	-2.34733800	-0.24090000	2.51814900
H	-3.06672800	-1.03046600	1.12406100
C	-4.97569200	-0.76298100	3.09815000
H	-4.15290400	-2.70188500	2.63644500
H	-3.41768000	-1.92897000	4.03260900
H	-5.76831300	-1.14350800	3.74403000
H	-4.65375200	0.20386500	3.49306100
H	-5.39986200	-0.59357200	2.10540000
C	-1.05364000	-1.91281000	-0.30901200
C	-1.91926300	-3.10241800	-0.68376500
H	-0.21756000	-1.81624200	-0.99758000
H	-1.63705600	-0.99716500	-0.37787100
C	-2.34806500	-2.95360100	-2.14775500
H	-1.38253200	-4.05001300	-0.55899500
H	-2.81901600	-3.14464000	-0.06060300
C	-3.22466900	-4.11638000	-2.60193700
H	-2.88608100	-2.00862300	-2.25601100
H	-1.45796200	-2.87578000	-2.77916100
H	-3.52528400	-3.99644800	-3.64374400
H	-2.69676100	-5.06991300	-2.51333400
H	-4.13384100	-4.17844600	-1.99805700
C	0.15406700	-0.54747800	1.28651600
C	1.00459400	-0.37738400	2.53575300
H	-0.66657700	0.17061800	1.25095900

H	0.75985900	-0.37345100	0.39864300
C	1.27025500	1.10891800	2.78008200
H	0.51268400	-0.79741400	3.42025200
H	1.96678800	-0.88527100	2.41172600
C	2.30208500	1.32583600	3.88007400
H	1.62833000	1.56518500	1.85352200
H	0.32364200	1.60216900	3.02334800
H	2.44730300	2.38989300	4.07663100
H	1.99497200	0.84945400	4.81574500
H	3.26448900	0.90849300	3.57452200
C	-0.78655300	4.70585400	-0.66814200
C	1.59579500	4.14606200	-0.10759300
O	-0.17193600	2.51521500	0.13801000
H	-0.01480100	2.27119300	-0.78936200
C	0.13081800	3.91080500	0.25991600
C	-0.13036200	4.28029600	1.71370200
H	2.24984200	3.51598400	0.50303100
H	1.76053000	3.90336400	-1.16120700
H	1.87352400	5.19116300	0.05025600
H	-0.01850300	5.35707600	1.85860600
H	-0.57731700	5.77631800	-0.60048400
H	-1.83248000	4.53315100	-0.40285300
H	-0.63677100	4.39175000	-1.70538700
H	-1.14701500	3.99301400	1.99412500
H	0.57380700	3.76886800	2.37229500
H	-3.56955600	2.02369100	-3.05526100
H	-2.28169000	2.55140900	-1.96229800
H	-3.83612400	3.40898900	-1.97451800
H	-4.05444000	2.99567400	0.56522500

H	-5.58657700	0.83264600	-2.14082700
H	-5.94381700	2.16053800	-1.01365200
H	-5.72012500	0.50831300	-0.40533600
H	-3.94518500	1.33390500	1.16948200
H	-2.49220000	2.14560400	0.52942100

CO₂/PO COUPLING USING FLUORINATED DIOLS AS HBDS

TBABR PLUS 1,3-BIS-HFAB

TS1

H	0.58025100	0.57060000	-0.92477400
C	-0.04068400	-1.91991700	-1.13798800
H	-0.29305200	-1.52598800	-0.16757200
H	0.63842300	-2.75986600	-1.18403000
C	-0.18738600	-1.07594400	-2.31490500
H	-1.02910700	-0.37492600	-2.26810000
C	-0.02349400	-1.70395700	-3.67274900
H	-0.91876400	-2.27307000	-3.92935700
H	0.14849700	-0.93141800	-4.42404700
H	0.83417800	-2.37954100	-3.66336800
O	0.99450800	-0.53784200	-1.75047300
Br	-2.04876100	-3.40761600	-1.04376700
N	-3.77426300	0.08807800	0.74432200
C	-3.98929400	-0.17278400	-0.73276500
C	-5.41066800	0.00196800	-1.23905600
H	-3.62505200	-1.18469800	-0.92686900
H	-3.31325200	0.51217600	-1.24727800
C	-5.41504300	-0.08966000	-2.76754400
H	-6.06075000	-0.78195700	-0.83808800
H	-5.83019100	0.96729300	-0.93403700
C	-6.82556400	-0.01430000	-3.34372900
H	-4.80256200	0.72062100	-3.17647000
H	-4.93628100	-1.02673000	-3.06882900
H	-6.80839300	-0.06800500	-4.43296100
H	-7.44072400	-0.83998300	-2.97838100
H	-7.31562100	0.92099600	-3.06143600

C	-2.31959400	-0.26046300	1.00220700
C	-1.80817300	-0.07009300	2.42150600
H	-1.72914700	0.35142700	0.31860600
H	-2.22495000	-1.30300800	0.69172300
C	-0.43807200	-0.74874600	2.54409000
H	-1.69829000	0.99310000	2.65941200
H	-2.48752300	-0.51229900	3.15857500
C	0.17129700	-0.57525400	3.93104000
H	-0.54397600	-1.81452600	2.31176200
H	0.23103900	-0.31800400	1.79405100
H	1.15263300	-1.04852200	3.98297500
H	0.29608800	0.48338100	4.16813700
H	-0.46362500	-1.02505100	4.69907200
C	-4.69419100	-0.76233300	1.59073300
C	-4.46805800	-2.26146600	1.50286600
H	-5.70881100	-0.50722300	1.28069300
H	-4.57418900	-0.41212600	2.61757100
C	-5.58200200	-3.00995900	2.23660000
H	-4.42751000	-2.59772100	0.46351100
H	-3.50235000	-2.53207500	1.94033100
C	-5.34298900	-4.51755100	2.21737000
H	-5.64831600	-2.65667300	3.27179000
H	-6.54456200	-2.78146400	1.76562000
H	-6.15299100	-5.05261700	2.71542800
H	-5.26745100	-4.88435600	1.19151100
H	-4.40836100	-4.76783700	2.72378000
C	-4.06419600	1.52616600	1.10138600
C	-3.43050400	2.58444200	0.21168300
H	-3.72653100	1.64729800	2.13190800

H	-5.15070000	1.63441600	1.10023500
C	-3.61990200	3.95810200	0.86348700
H	-2.36450600	2.39403300	0.05988500
H	-3.90832500	2.58799300	-0.77363400
C	-3.11674200	5.09921200	-0.01510500
H	-4.68243800	4.10757300	1.08755400
H	-3.09031800	3.97207400	1.82088400
H	-3.29299500	6.06413900	0.46273700
H	-2.04740000	5.00108600	-0.20088600
H	-3.62844700	5.10384400	-0.98085600
C	1.01629800	2.35634500	-0.06730000
C	0.63606500	2.98037800	1.28536100
C	0.71299600	3.34388100	-1.21795000
F	1.19632600	2.87213800	-2.36368100
F	-0.60717200	3.49988300	-1.37541000
F	1.22684900	4.56548700	-1.01987300
F	-0.64747300	3.38052400	1.31300300
F	1.38694100	4.03932900	1.58570200
F	0.78317700	2.08112900	2.26000200
O	0.18399700	1.26545200	-0.23937100
C	2.50069500	1.98412000	-0.04689100
C	3.53611300	2.90179200	-0.21425300
C	2.80572300	0.63977400	0.09562000
C	4.84700500	2.44623900	-0.28167200
H	3.33052200	3.96015900	-0.30412000
C	4.10347700	0.17250500	-0.06082700
H	2.01588200	-0.07135000	0.27934900
C	5.13923500	1.08719300	-0.23126200
H	5.65192800	3.15901800	-0.41032600

H	6.16361100	0.75812800	-0.34081100
C	4.25511900	-1.34594700	-0.08816500
C	5.48354600	-1.79383200	-0.90681400
C	4.36110900	-1.86728100	1.35917500
F	5.45907000	-1.22023600	-2.11244300
F	6.64148100	-1.45770000	-0.31743300
F	5.49532300	-3.10830800	-1.08310200
F	5.36524500	-1.28109600	2.01596800
F	3.23060300	-1.59708100	2.02014700
F	4.55246700	-3.18265000	1.40583600
O	3.14839100	-1.99152300	-0.64004300
H	2.61747100	-1.39554000	-1.20351900

TS2

H	0.14114000	-0.13174100	-0.43625400
C	-2.15795400	2.57205600	-1.03648100
H	-2.31936100	2.97741800	-0.04086700
C	-0.76863500	1.94609000	-1.15112500
H	-0.03847500	2.76093300	-1.03125100
C	-0.55994500	1.25978000	-2.49505800
H	-0.68794100	1.96102800	-3.32143700
H	0.44227400	0.83269000	-2.55156400
O	-0.62565600	1.02322000	-0.09627900
Br	-2.38091100	4.08134000	-2.26619200
N	3.68206300	0.72480900	0.85259700
C	2.90253000	1.26538000	-0.33230900
C	3.64819400	2.29370900	-1.16971400
H	1.97735800	1.68739400	0.06671900
H	2.60861200	0.39772000	-0.92146900

C	2.90312000	2.53245700	-2.48534500
H	3.73542800	3.24381700	-0.63226000
H	4.66527600	1.95789300	-1.39947800
C	3.58257000	3.59550300	-3.34246800
H	2.84122000	1.58778200	-3.03653000
H	1.87349100	2.83317100	-2.26970200
H	3.04440000	3.74724700	-4.27873300
H	3.61813400	4.55381100	-2.81874000
H	4.60836600	3.30710000	-3.58700500
C	2.78053300	-0.26075200	1.58788500
C	3.20001000	-0.63149800	3.00168400
H	2.72178600	-1.14464700	0.95768000
H	1.78111300	0.16634700	1.59783600
C	2.23523100	-1.69478500	3.53733200
H	4.22194700	-1.02482000	3.03859800
H	3.16104100	0.23786300	3.66542100
C	2.55234100	-2.07387000	4.98031100
H	1.21293800	-1.31142700	3.46467000
H	2.28105900	-2.57986000	2.89655500
H	1.85319500	-2.82505900	5.34981600
H	3.56227300	-2.48326200	5.06838600
H	2.48365400	-1.20331700	5.63747100
C	4.10908500	1.85045900	1.76066900
C	2.96057800	2.67756900	2.31454200
H	4.78658000	2.47773100	1.17906400
H	4.69129300	1.39436900	2.56377600
C	3.45552900	3.66866000	3.36778000
H	2.46344900	3.22976500	1.51293500
H	2.20169800	2.03217700	2.76659300

C	2.30488400	4.50796000	3.91771700
H	3.94201400	3.12243200	4.18362400
H	4.21752100	4.32215500	2.92915400
H	2.65776800	5.22356700	4.66165300
H	1.80996200	5.06072700	3.11647500
H	1.55208500	3.87059900	4.38734800
C	4.92755900	-0.00268100	0.39061300
C	4.71457800	-0.94497900	-0.78686800
H	5.28862900	-0.55166300	1.26191100
H	5.67424300	0.75577700	0.15046700
C	5.85919500	-1.95186600	-0.90284600
H	3.77618400	-1.49292000	-0.68602400
H	4.63806200	-0.37494900	-1.71833700
C	5.64555900	-2.89486700	-2.08394600
H	6.81387700	-1.42515300	-1.00869100
H	5.92008000	-2.53213500	0.02393100
H	6.45338600	-3.62377900	-2.16070400
H	4.70362400	-3.43663900	-1.97433000
H	5.60091900	-2.33890400	-3.02346000
C	0.37729900	-2.11428100	-1.11782400
C	0.90627100	-3.22157200	-0.17792700
C	1.01774500	-2.30004300	-2.51393700
F	0.42716300	-1.52803200	-3.42584600
F	2.31430300	-1.95958000	-2.49824100
F	0.95213000	-3.56560400	-2.94920600
F	2.25662300	-3.26019900	-0.17152000
F	0.47768200	-4.43635700	-0.50800100
F	0.52540200	-2.97511300	1.07581200
O	0.84412300	-0.91661900	-0.61465000

C	-1.14533200	-2.20192600	-1.17254500
C	-1.87096800	-2.79837200	-2.20031000
C	-1.82357900	-1.57807500	-0.13356500
C	-3.25842800	-2.71728700	-2.19333300
H	-1.37271900	-3.30780800	-3.01465300
C	-3.20334800	-1.42242900	-0.16768900
H	-1.26274800	-1.16599000	0.69431000
C	-3.92862500	-2.01500200	-1.19886800
H	-3.82349300	-3.18078200	-2.99232900
H	-5.00535000	-1.92543500	-1.24509500
C	-3.80263100	-0.54303000	0.92531700
C	-5.16133300	0.05897000	0.51072000
C	-3.97562500	-1.38440500	2.20812500
F	-5.06368600	0.63423600	-0.69433900
F	-6.12931000	-0.86766600	0.43702500
F	-5.56234000	0.98874300	1.36592000
F	-4.68770600	-2.49199000	1.97610900
F	-2.78129100	-1.75912400	2.66872900
F	-4.58818000	-0.70024400	3.17238500
O	-2.99079100	0.53757900	1.25682700
H	-2.19555600	0.59853900	0.68099500
C	-0.19551900	1.87574900	1.66996900
O	-0.10270300	3.01381400	1.39679900
O	-0.14915200	0.92603600	2.36138100
H	-1.28025700	0.44285500	-2.60869200
H	-2.94176000	1.85724000	-1.28434000

TS3

C	-0.28539500	2.93113700	0.23109600
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C	-0.41495500	3.50870200	1.65502000
C	-0.84352100	3.92502400	-0.80963200
F	-0.90797200	3.30615800	-1.99268600
F	-2.06880200	4.33654000	-0.49729500
F	-0.07025700	5.00301600	-0.94654400
F	-1.68125900	3.61527200	2.03342300
F	0.14682800	4.71472400	1.77053900
F	0.19307300	2.68974300	2.52991900
O	-1.11445600	1.81831600	0.27083800
C	1.17322200	2.59808400	-0.10247900
C	2.21167500	3.50481800	0.11048900
C	1.46535100	1.34267000	-0.62881000
C	3.51986600	3.13188400	-0.17078600
H	2.01244700	4.49646600	0.49279200
C	2.77532400	0.96560900	-0.90558300
H	0.67266600	0.63362700	-0.82171000
C	3.81101300	1.86988900	-0.67266600
H	4.32326600	3.83770400	-0.00034800
H	4.83674800	1.60506600	-0.89114600
C	3.01266700	-0.44128800	-1.47059000
C	3.47702300	-0.33438900	-2.94105600
C	4.08100400	-1.19040500	-0.64619400
F	2.50065200	0.19538500	-3.67086600
F	4.55794600	0.44216100	-3.07071800
F	3.77438000	-1.52953900	-3.44576500
F	5.29920100	-0.66188300	-0.78187600
F	3.76909400	-1.13989600	0.66132900
F	4.15705400	-2.47407600	-0.97727100
O	1.89459700	-1.25868900	-1.39063900

H	1.20179700	-1.02757900	-2.06858300
C	-3.27464600	-0.44641100	-1.23469000
H	-2.91258900	-1.25189600	-0.62481800
H	-3.51737000	0.49455400	-0.76720400
C	-3.53881600	-0.69098600	-2.71227800
H	-4.18875800	-1.55325100	-2.83289800
C	-4.10117200	0.53634500	-3.39772900
H	-3.43323500	1.38851600	-3.24995700
H	-4.21016000	0.35172000	-4.46605000
H	-5.07860800	0.76644000	-2.97035600
O	-2.28365900	-1.07785600	-3.31872800
H	-1.15390600	1.35146100	-0.59118500
Br	-5.44974300	-1.22702600	-0.34400800
N	-0.17575600	-1.83865200	2.01552800
C	0.57017400	-2.99999500	2.63757900
C	1.99397900	-3.19426600	2.13317800
H	-0.03165300	-3.88862900	2.44419100
H	0.57218300	-2.83731400	3.71602500
C	2.56287500	-4.53280200	2.60430500
H	2.04254400	-3.15379200	1.04048500
H	2.63467100	-2.38722900	2.49846900
C	4.02243000	-4.68868200	2.18463400
H	2.47872700	-4.60768900	3.69402600
H	1.96586300	-5.34967800	2.18616200
H	4.42255500	-5.65492700	2.49429800
H	4.12479300	-4.60831600	1.09994300
H	4.63979600	-3.90734600	2.63438100
C	-1.38455900	-1.53180600	2.87173900
C	-2.22671400	-0.36037800	2.38901600

H	-1.00434100	-1.33682100	3.87636700
H	-1.97456900	-2.44934300	2.91082100
C	-3.56280200	-0.30888700	3.13281900
H	-1.69049600	0.58166000	2.53378300
H	-2.43248300	-0.43311600	1.31766100
C	-4.35981800	0.93431800	2.74895600
H	-4.14567100	-1.20232700	2.88558600
H	-3.38241400	-0.32204800	4.21408400
H	-5.30154500	0.97744100	3.29784400
H	-3.79393700	1.84440500	2.96234700
H	-4.60290600	0.91213500	1.68439100
C	-0.59068800	-2.21364100	0.60120400
C	-1.74707800	-3.20089100	0.49216800
H	0.30528400	-2.60110400	0.11483600
H	-0.83579600	-1.27878600	0.09441600
C	-1.84541600	-3.72541100	-0.94564500
H	-1.61581200	-4.05744000	1.16034600
H	-2.69707100	-2.73032100	0.77385500
C	-3.14436400	-4.49106300	-1.17981600
H	-1.78099500	-2.89608500	-1.65662100
H	-0.97910800	-4.36148400	-1.15355000
H	-3.19247400	-4.87050600	-2.20143400
H	-3.22311800	-5.34364000	-0.49967600
H	-4.00928800	-3.84336100	-1.01142600
C	0.71678100	-0.62054500	1.90633800
C	1.26176400	-0.09057300	3.22628500
H	0.11961100	0.14960000	1.41842600
H	1.51688400	-0.89582700	1.21895100
C	2.48748800	0.79361200	2.96362400

H	0.49055600	0.49801100	3.73278000
H	1.55029500	-0.89869400	3.90628900
C	2.85991700	1.63248700	4.18118600
H	3.32746200	0.15844300	2.66864200
H	2.28652000	1.45141400	2.11358100
H	3.75543600	2.22532400	3.98810000
H	2.04945800	2.31934900	4.43574800
H	3.05657100	1.00154600	5.05231600
C	-1.21715700	-0.58655000	-2.67084900
O	-1.53738500	0.10391700	-1.62627900
O	-0.09018700	-0.84968400	-3.04995400

KEY ROLE OF TRIFLUOROMETHYL GROUPS

TBABR PLUS α, α' -DIHYDROXY-1,3-DIISOPROPYLBENZENE TS1

H	1.41628400	0.84474000	-1.09034300
C	0.04732000	-2.09376200	-1.41638900
H	0.06196500	-1.92541000	-0.35634200
H	0.47595000	-3.02254400	-1.77060200
C	0.04880400	-0.96308200	-2.33968500
H	-0.62615000	-0.14208600	-2.05883600
C	-0.06668300	-1.27884900	-3.81278700
H	-1.08884600	-1.57259900	-4.06152100
H	0.21429700	-0.40432000	-4.40335000
H	0.61258100	-2.09624200	-4.06317400
O	1.35096000	-0.81590600	-1.85559000
Br	-2.25627100	-2.94542600	-1.20289500
N	-2.38781000	0.85799100	0.96914200
C	-3.12033200	0.55686400	-0.32341600
C	-4.56288100	1.02406200	-0.39797400
H	-3.05255300	-0.52129500	-0.48331500
H	-2.52629600	1.02144900	-1.11065500
C	-5.08143800	0.81885300	-1.82494900
H	-5.19039000	0.44483200	0.28666900
H	-4.66260200	2.08102800	-0.12478400
C	-6.55929300	1.17336700	-1.95482900
H	-4.48967500	1.43228200	-2.51235900
H	-4.91583100	-0.22326700	-2.11554100
H	-6.90889400	1.03198100	-2.97829600
H	-7.17011200	0.54315300	-1.30395200
H	-6.73931500	2.21581800	-1.67935200

C	-1.04030000	0.17254400	0.83797300
C	-0.05294000	0.35609300	1.97634400
H	-0.58985400	0.55099100	-0.07752100
H	-1.28591200	-0.87857900	0.68587000
C	1.05440400	-0.69144700	1.81190700
H	0.39706600	1.35226700	1.92096500
H	-0.52232300	0.23692100	2.95934000
C	2.19767000	-0.50545100	2.79892100
H	0.62197300	-1.69256200	1.92807600
H	1.44941100	-0.63654500	0.79382300
H	2.93957400	-1.29368600	2.66300200
H	2.70005100	0.45145400	2.63272300
H	1.84329700	-0.53879100	3.83370400
C	-3.14366800	0.31328500	2.15846100
C	-3.24820000	-1.20340600	2.21957600
H	-4.13429000	0.76902900	2.12241500
H	-2.64173500	0.70109200	3.04654400
C	-4.30532400	-1.62489900	3.24124300
H	-3.49989900	-1.62907100	1.24324000
H	-2.28238400	-1.63501900	2.50027300
C	-4.36323000	-3.14307200	3.38783500
H	-4.09144400	-1.16404600	4.21221800
H	-5.28283900	-1.24582500	2.92321600
H	-5.15006300	-3.44472300	4.08069900
H	-4.55489400	-3.61651700	2.42233800
H	-3.41413500	-3.53242400	3.76308600
C	-2.23231300	2.34494600	1.18158300
C	-1.70549300	3.12996200	-0.00972000
H	-1.56607700	2.45837200	2.03893200

H	-3.21527100	2.71906100	1.47702400
C	-1.42730700	4.57857000	0.40086900
H	-0.78215600	2.68545600	-0.39918800
H	-2.44886500	3.13408100	-0.81349800
C	-1.14532300	5.45884200	-0.81445400
H	-2.28453800	4.98288800	0.95119200
H	-0.57479100	4.59929700	1.08705800
H	-0.85880700	6.46888900	-0.51793700
H	-0.33824500	5.04102700	-1.42119600
H	-2.03055700	5.53215900	-1.45099500
C	2.53365800	2.42647600	-0.58485500
C	2.22774500	3.69799500	0.19382900
C	2.95594200	2.76255300	-2.01766800
O	1.30062400	1.70144300	-0.62061100
C	3.61440200	1.57859500	0.09028600
C	4.45531600	2.02702800	1.10943700
C	3.74237400	0.26153100	-0.33396000
C	5.36879800	1.15065600	1.68937100
H	4.40037100	3.04768100	1.46923000
C	4.59538100	-0.64734000	0.28013700
H	3.11784300	-0.08628500	-1.14720500
C	5.42896400	-0.18362600	1.29651800
H	6.02157900	1.50548200	2.47880900
H	6.11464500	-0.85490100	1.79962700
C	4.50118600	-2.10370700	-0.18584500
C	5.06438300	-2.23094100	-1.60452100
C	5.21257300	-3.06435400	0.75660000
O	3.13607600	-2.51467300	-0.17457000
H	2.62869500	-2.00380500	-0.82603000

H	4.82394000	-2.96095900	1.77190000
H	6.29049700	-2.89075600	0.76593100
H	5.02393300	-4.08404000	0.41888300
H	4.99457300	-3.27095800	-1.93079700
H	6.10815900	-1.91026500	-1.64258400
H	4.48754600	-1.61244700	-2.29714300
H	1.94642100	3.45707500	1.22250500
H	1.39634200	4.21502700	-0.28798000
H	2.17992200	3.36487000	-2.49699400
H	3.08581700	4.37218800	0.21010000
H	3.08565700	1.84316400	-2.59373200
H	3.89903700	3.31356100	-2.02968500

TS2

H	0.16459700	1.05574800	-0.35887800
C	2.69957300	-1.63744000	-0.63497700
H	2.73891900	-2.22934400	0.27610800
C	1.25703700	-1.26172500	-0.97928800
H	0.72076800	-2.20037800	-1.20692700
C	1.22023900	-0.37303600	-2.22534900
H	1.55829800	-0.91736700	-3.10979300
H	0.20538900	-0.01115100	-2.40424700
O	0.71678800	-0.63978500	0.14603100
Br	3.57917900	-2.73804300	-2.00933600
N	-3.15833200	-0.19164800	0.18954000
C	-2.31393700	-0.59323500	-1.00445500
C	-3.07256000	-1.30027900	-2.11451800
H	-1.49868100	-1.20805500	-0.61848400
H	-1.84578700	0.32769700	-1.35371000
C	-2.15879700	-1.47740200	-3.32960700

H	-3.41367200	-2.28651800	-1.78309700
H	-3.96245900	-0.73491100	-2.41478800
C	-2.83882700	-2.25575400	-4.45150200
H	-1.84921100	-0.49152700	-3.69215000
H	-1.24278400	-1.99012200	-3.01805100
H	-2.17439800	-2.36828900	-5.30910700
H	-3.12377800	-3.25583000	-4.11590900
H	-3.74354700	-1.74479700	-4.79144900
C	-2.20690700	0.43976500	1.20398600
C	-2.68699000	0.53055500	2.64165300
H	-1.97775200	1.42785200	0.81302200
H	-1.27456900	-0.12055200	1.14972300
C	-1.63843600	1.31508900	3.44011800
H	-3.65714500	1.03509200	2.72557700
H	-2.79147000	-0.46157700	3.09106800
C	-1.97344900	1.36250800	4.92741500
H	-0.66118300	0.84550000	3.29252300
H	-1.57023600	2.33188600	3.03885900
H	-1.22426400	1.93142500	5.47972200
H	-2.94728900	1.82927400	5.10062100
H	-2.00168400	0.35440900	5.34782800
C	-3.87452300	-1.38589700	0.76871200
C	-2.95948500	-2.51917000	1.19627200
H	-4.58253600	-1.72668200	0.01112200
H	-4.45312600	-1.01316700	1.61643000
C	-3.74509700	-3.64289800	1.87232200
H	-2.41994700	-2.92783500	0.33686300
H	-2.21111300	-2.14662400	1.89685100
C	-2.81171300	-4.76016200	2.33261000

H	-4.29180200	-3.23933300	2.73179000
H	-4.49498300	-4.04109600	1.18005300
H	-3.36486400	-5.56521900	2.81854100
H	-2.26390700	-5.18259800	1.48751000
H	-2.07415000	-4.37670000	3.04169400
C	-4.20723500	0.82413000	-0.20324300
C	-3.72610300	1.94107200	-1.12324100
H	-4.58570100	1.23666600	0.73449500
H	-5.02588700	0.27830800	-0.67624000
C	-4.76603400	3.05990200	-1.19193800
H	-2.76673500	2.34608800	-0.78851500
H	-3.55953700	1.54698500	-2.13101400
C	-4.34401800	4.15677500	-2.16604100
H	-5.73472800	2.64816600	-1.49604000
H	-4.90625000	3.48672300	-0.19344600
H	-5.08530200	4.95580200	-2.21182900
H	-3.39095900	4.59752400	-1.86338600
H	-4.21966900	3.75433700	-3.17431600
C	0.45483400	2.98746200	-0.94432300
C	-0.06531700	4.18143700	-0.13878200
C	0.24869500	3.23788900	-2.43855700
O	-0.35480800	1.86893200	-0.57651700
C	1.91129700	2.71841000	-0.58271000
C	2.98562500	3.07026500	-1.39791300
C	2.16668200	2.03435800	0.60107900
C	4.27811900	2.70421800	-1.03537800
H	2.82385700	3.59887700	-2.32954400
C	3.44411300	1.60438100	0.94526500
H	1.33791000	1.75593100	1.24147500

C	4.50843700	1.95875300	0.11594600
H	5.11055900	2.97150900	-1.67590800
H	5.51666700	1.63789200	0.34894500
C	3.59358500	0.73524900	2.19183700
C	4.80777400	-0.19507600	2.11354500
C	3.70859100	1.63305900	3.42671100
O	2.42413200	-0.04635600	2.38613600
H	1.96360600	-0.22452000	1.54193000
C	0.22405900	-2.15097000	1.59269300
O	0.36984000	-3.12071400	0.95640000
O	-0.06248000	-1.47051400	2.50155500
H	1.87087200	0.49594600	-2.08355000
H	3.30776200	-0.73759000	-0.53948900
H	4.77287900	-0.86545800	2.97366700
H	4.78583900	-0.80063900	1.20513500
H	5.75060000	0.35591200	2.14487700
H	3.74655800	1.00843800	4.32209600
H	4.60636300	2.25368500	3.38040700
H	2.83220700	2.28081300	3.49076900
H	0.67099400	2.42313000	-3.03002400
H	-0.82603700	3.28807400	-2.63201200
H	0.69744700	4.18019900	-2.76060000
H	0.49175000	5.08867600	-0.38232900
H	-1.12412200	4.34551300	-0.36290600
H	0.04128400	3.98093800	0.92909900

TS3

C	-0.95556700	-3.37118200	0.72031700
C	-1.19129000	-4.21037900	1.97014900
C	-0.23326800	-4.19656900	-0.34902500

O	-0.11549300	-2.29171500	1.13641000
C	-2.25268900	-2.81298900	0.12507000
C	-3.50993800	-3.34339500	0.40041900
C	-2.16358200	-1.72184800	-0.74103400
C	-4.64573300	-2.78524500	-0.18171200
H	-3.61976000	-4.18484400	1.07357200
C	-3.28855300	-1.13942500	-1.31631700
H	-1.18727200	-1.30880300	-0.96484300
C	-4.54042200	-1.69296500	-1.03237600
H	-5.62156600	-3.20450300	0.03562400
H	-5.43912900	-1.27537700	-1.47165300
C	-3.13870100	0.05740100	-2.26242700
C	-3.16957600	-0.43522700	-3.71143300
C	-4.22501800	1.10293700	-2.01652400
O	-1.91272600	0.73944100	-2.02110600
H	-1.17748500	0.21643500	-2.39319600
C	3.08931900	-0.72567400	-0.52879600
H	2.75640300	0.27150300	-0.30832500
H	3.11099200	-1.45709500	0.26212800
C	3.56188500	-1.05756700	-1.93526900
H	4.33450800	-0.35510100	-2.23649000
C	4.03979600	-2.49069100	-2.04736800
H	3.24907900	-3.17342500	-1.72646800
H	4.30553700	-2.71613000	-3.08000000
H	4.91532000	-2.62831200	-1.41056600
O	2.46410500	-0.81908300	-2.83849200
H	0.37563700	-1.97099400	0.36233900
Br	5.21711300	0.08440100	0.38265700
N	-0.38195100	1.93354400	1.18472000

C	-1.06586600	3.27713100	1.25151400
C	-2.26453300	3.44669800	0.32421900
H	-0.29964400	4.02249200	1.03074300
H	-1.37416200	3.42086700	2.28876100
C	-2.65577600	4.92183000	0.22378600
H	-2.06357000	3.05295900	-0.67636200
H	-3.11551400	2.87822700	0.71041400
C	-3.91940500	5.11157200	-0.61043700
H	-2.80892900	5.33312600	1.22759400
H	-1.82928300	5.48477500	-0.22212900
H	-4.18467800	6.16633100	-0.69449500
H	-3.78008200	4.71577500	-1.61918200
H	-4.76522900	4.58602600	-0.16025700
C	0.58937800	1.83497300	2.33819700
C	1.28895500	0.48859500	2.45925500
H	0.02451400	2.05509100	3.24451200
H	1.31178800	2.64102700	2.20218000
C	2.47617600	0.58087300	3.41945600
H	0.58871700	-0.27868300	2.80323200
H	1.65245300	0.14885800	1.48568800
C	3.13725100	-0.77898400	3.62286500
H	3.21374000	1.28200200	3.01480700
H	2.13728900	0.98208200	4.38185300
H	3.95618000	-0.71088000	4.34025400
H	2.41632700	-1.51422600	3.98957200
H	3.56027700	-1.13846600	2.68229400
C	0.35298600	1.79719800	-0.14132700
C	1.64741800	2.58951000	-0.27135600
H	-0.36010800	2.07821900	-0.91446200

H	0.54095700	0.73108100	-0.27432200
C	2.12238200	2.56110200	-1.72921600
H	1.51871200	3.63459700	0.02964200
H	2.43430000	2.17521000	0.37052800
C	3.55113200	3.07920500	-1.86678200
H	2.06768400	1.54204200	-2.12483400
H	1.43523900	3.15537600	-2.33979200
H	3.86716600	3.07599400	-2.91109200
H	3.63477900	4.10346800	-1.49278700
H	4.24406500	2.45331600	-1.29730300
C	-1.39883100	0.81123800	1.24643900
C	-2.27249800	0.79274400	2.49047700
H	-0.83759900	-0.12190400	1.17727900
H	-1.99066700	0.89219100	0.33371000
C	-3.16266000	-0.45225200	2.44649900
H	-1.66382600	0.75056600	3.39979100
H	-2.89757900	1.69004300	2.55836200
C	-4.13071400	-0.51802500	3.62217200
H	-3.71633800	-0.47792200	1.50123800
H	-2.51616900	-1.33376800	2.43932300
H	-4.73929800	-1.42267300	3.57260000
H	-3.59455600	-0.52548100	4.57496900
H	-4.80725400	0.34079600	3.62498000
C	1.25480500	-0.96098200	-2.25425600
O	1.33252400	-1.24209500	-0.99714000
O	0.24319800	-0.77846900	-2.90685700
H	0.71102300	-4.57360600	0.05241200
H	-0.22205400	-4.48225600	2.38958800
H	-1.74064400	-5.12555600	1.74333600

H	-0.85058400	-5.04002400	-0.66504600
H	-0.02333600	-3.57797600	-1.22550800
H	-1.74552600	-3.64202000	2.72075600
H	-4.00193000	1.98313200	-2.62278500
H	-5.21497800	0.73677400	-2.28955800
H	-4.24134100	1.39541200	-0.96251300
H	-3.08790900	0.41601500	-4.39142600
H	-4.09644400	-0.97422800	-3.91920800
H	-2.32758000	-1.10867200	-3.88912100