

Electronic Supplementary Information for

A Propargylbenzene Dimer: C–H \cdots π Assisted π – π Stacking

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Table S1. Stabilization energies (kJ mol⁻¹) of PrBz dimers at HF and electron correlation levels without ZPE and BSSE correction.

Structure	ΔE_{HF}	ΔE_{Corr}
P1	-15.3	-29.6
P2 (1)	-11.2	-30.4
P3	-13.0	-28.4
P4	-11.1	-30.1
P5	-10.1	-30.2
P6	-9.4	-30.4
P7	-7.3	-30.4
P8	-7.6	-30.7
P9 (1)	-6.8	-29.8
P10	-7.5	-29.2
P11	-9.3	-22.2
P12 (1)	-12.6	-18.7
P13	-1.3	-28.0
P14	-4.5	-19.5
P15	-6.6	-15.4

Optimized coordinates of various structures of PrBZ dimer calculated at M06-2X/aug-cc-pVDZ level of theory.

P1

C -0.33068700 -2.70381000 -1.19504100
 C 0.10127400 -1.42019800 -0.87438300
 C -0.80258900 -0.45322100 -0.41865400
 C -2.14683100 -0.79771600 -0.27826600
 C -2.58204000 -2.08759900 -0.59551900
 C -1.67859800 -3.04276700 -1.05730600
 H 0.38803100 -3.44744800 -1.53417500

H	1.15765600	-1.16483600	-0.96571600
H	-2.85593700	-0.05329300	0.07983900
H	-3.63456700	-2.34321900	-0.48207800
H	-2.01841500	-4.04754200	-1.30215200
C	-0.26803600	0.93072000	-0.09368300
H	0.20512100	1.34774200	-0.99305600
C	-1.27069400	1.88158700	0.38637700
C	-2.11135400	2.66082700	0.77155300
H	-2.84304600	3.36316000	1.11054200
H	0.52248900	0.83821100	0.66414100
C	-0.03438900	0.95658300	3.39440400
C	-0.46486200	-0.32736500	3.07315900
C	0.44056800	-1.29386400	2.61946500
C	1.78487200	-0.94860300	2.48184600
C	2.21861500	0.34162600	2.79976100
C	1.31361600	1.29633800	3.25941900
H	-0.75429000	1.69989300	3.73175100
H	-1.52128500	-0.58335800	3.16225700
H	2.49516200	-1.69265900	2.12532700
H	3.27122900	0.59786600	2.68853600
H	1.65229700	2.30138700	3.50471700
C	-0.09257100	-2.67819700	2.29385200
H	-0.88277700	-2.58620300	1.53565000
C	0.91105000	-3.62795900	1.81365300
C	1.75305900	-4.40331400	1.42359400
H	2.48590600	-5.10320500	1.08206400
H	-0.56591100	-3.09575000	3.19289200

P2

C	-7.94169800	1.99612800	2.66598700
C	-7.61055800	0.72386200	2.21240200
C	-6.57052400	0.54070600	1.29289000
C	-5.88471400	1.65565100	0.81736500
C	-6.21227500	2.93522100	1.27458900
C	-7.23507100	3.10991600	2.20185900
H	-8.74874700	2.12268600	3.38673900
H	-8.14780700	-0.14653300	2.59170400
H	-5.08106500	1.52752300	0.09357800
H	-5.65236300	3.79451600	0.90871800
H	-7.48662000	4.10665900	2.56157200
C	-6.21305400	-0.88203700	0.90086600
H	-7.09768800	-1.37330600	0.47286300
C	-5.10569900	-1.00704400	-0.04834500
C	-4.19252600	-1.11609800	-0.83472200
H	-3.38395000	-1.21661100	-1.52833400
H	-5.95180000	-1.43593500	1.81571500
C	-4.10047200	-2.41921200	3.66201300
C	-3.33356900	-1.52390600	2.92080500
C	-3.57661300	-0.14654700	2.98931100
C	-4.60073200	0.32123300	3.81193900

C	-5.37482500	-0.57516900	4.55187200
C	-5.12825800	-1.94496700	4.48180300
H	-3.89929600	-3.48756200	3.59987200
H	-2.54162400	-1.89722300	2.26979600
H	-4.80984700	1.39006500	3.85666100
H	-6.17843900	-0.19552900	5.18304600
H	-5.72942900	-2.64218000	5.06368500
C	-2.74102800	0.77911100	2.12297000
H	-3.05581900	0.65124800	1.07761000
C	-2.82458400	2.19668100	2.47504300
C	-2.89956900	3.36540200	2.77776000
H	-2.96287500	4.39901800	3.04044100
H	-1.69090400	0.46441800	2.17215900

P3

C	-2.69236300	-1.29837400	-0.42025300
C	-1.32651500	-1.15217900	-0.63936600
C	-0.62653300	-0.06711800	-0.09930000
C	-1.32494800	0.88158400	0.64584400
C	-2.69696500	0.73693300	0.86959400
C	-3.38364300	-0.35383700	0.34322600
H	-3.22153400	-2.15191800	-0.84199900
H	-0.78533900	-1.90081000	-1.21933300
H	-0.79190000	1.73837100	1.05585000
H	-3.22922600	1.48399200	1.45683400
H	-4.45203200	-0.46796600	0.51982300
C	0.87080200	0.01532600	-0.34172400
H	1.05651400	0.17307300	-1.41298400
C	1.55392900	1.06096900	0.42059900
C	2.10023000	1.91836600	1.07530400
H	2.59749000	2.65696600	1.66788600
H	1.31995800	-0.95395300	-0.07990000
C	0.40748700	-3.16948400	1.56403300
C	0.10209600	-2.05929600	2.34804500
C	1.11685000	-1.22884400	2.83402700
C	2.44466000	-1.52648700	2.52299600
C	2.75271400	-2.63591300	1.73469500
C	1.73644900	-3.46139500	1.25282900
H	-0.39599400	-3.80137600	1.18789000
H	-0.94029000	-1.81988300	2.56448000
H	3.23797100	-0.87787000	2.89006700
H	3.79226700	-2.85521000	1.49586000
H	1.97858700	-4.32802700	0.63959600
C	0.71963700	-0.01402100	3.65396700
H	0.03684600	-0.32888300	4.45405500
C	1.83360600	0.72202300	4.25216400
C	2.75760500	1.32028600	4.75263000
H	3.56682800	1.85258100	5.20595500
H	0.15410100	0.67047900	3.00643200

P4

C	-1.61889000	-3.36955600	-0.24951700
C	-1.04733100	-2.11994600	-0.47627100
C	-1.64283200	-0.96036500	0.03002700
C	-2.82099500	-1.07053600	0.76854700
C	-3.39271300	-2.32176000	1.00296100
C	-2.79460200	-3.47444100	0.49591000
C	-0.98164800	0.37661000	-0.25897900
C	-1.50857100	1.50389400	0.51153400
C	-1.95605800	2.43186500	1.14473700
H	-1.13455900	-4.26134500	-0.64587200
H	-0.11385600	-2.04926500	-1.03602100
H	-3.28400700	-0.17299100	1.17540900
H	-4.31100200	-2.39472000	1.58428700
H	-3.24376700	-4.45014000	0.67708100
H	-1.08625200	0.60645200	-1.32858800
H	0.09338200	0.28576900	-0.05737300
H	-2.34361700	3.26137300	1.69733000
C	-0.48045900	-0.86914200	3.32610900
C	-0.34077400	-2.21518000	2.99153900
C	0.74964700	-2.64835200	2.23613800
C	1.70793400	-1.71763700	1.82756300
C	1.57833400	-0.37346500	2.17628800
C	0.48058900	0.05682600	2.92228500
C	0.87836300	-4.12161100	1.89087100
C	1.53285200	-4.37643600	0.60440300
C	2.07772300	-4.57608100	-0.45671100
H	-1.35204200	-0.53961000	3.88962800
H	-1.10701900	-2.93048300	3.29113100
H	2.55217400	-2.04745100	1.22306400
H	2.33294200	0.34339900	1.85440600
H	0.36450400	1.11000900	3.17049900
H	-0.12250800	-4.57054600	1.87131300
H	1.44533000	-4.63751900	2.67893800
H	2.56106300	-4.76568100	-1.39176400

P5

C	0.11190600	-4.73907800	0.81589600
C	-0.83781200	-3.82059100	1.25411300
C	-0.60418500	-2.44549600	1.14620600
C	0.60247700	-2.00618200	0.60061000
C	1.55579700	-2.92535700	0.15973900
C	1.31256000	-4.29252600	0.26150700
H	-0.08476300	-5.80653400	0.90658800
H	-1.77330500	-4.17064500	1.69178700
H	0.79697900	-0.93760600	0.51928100
H	2.49408400	-2.56809100	-0.26197600
H	2.05720900	-5.00931600	-0.08181800
C	-1.70190100	-1.48464200	1.57462500
H	-2.16698400	-1.84883600	2.50053600

C	-1.25432100	-0.10589400	1.78038500
C	-0.86933200	1.03068200	1.93273400
H	-0.54662100	2.04142500	2.06691300
H	-2.48851800	-1.47978500	0.80691800
C	-2.61260000	-1.19583700	5.29871000
C	-1.27557700	-0.95433900	4.99687300
C	-0.42768000	-2.00118200	4.61746300
C	-0.93518500	-3.29926700	4.56790000
C	-2.27605500	-3.54494600	4.87218000
C	-3.11999700	-2.49583700	5.23157100
H	-3.26282700	-0.36907200	5.58036500
H	-0.88758000	0.06371600	5.02768700
H	-0.28111500	-4.11680200	4.26948800
H	-2.66201800	-4.56245400	4.82409700
H	-4.16666400	-2.68755600	5.46258800
C	1.00425400	-1.66527000	4.23933000
H	1.48888100	-1.15399800	5.08192700
C	1.81850700	-2.81522900	3.84790500
C	2.48172600	-3.77573800	3.53427100
H	3.07296200	-4.61568000	3.23768800
H	0.98152500	-0.94800100	3.40555800

P6

C	-2.34336000	-0.06652100	-0.54661200
C	-3.31057200	0.91636200	-0.36234200
C	-4.20744400	0.84206900	0.70968300
C	-4.11002100	-0.22559300	1.60022900
C	-3.13439200	-1.20899900	1.42148700
C	-2.25336300	-1.13579200	0.34712300
C	-5.26210200	1.92917500	0.84363300
C	-6.00444300	1.91207700	2.10565200
C	-6.60264700	1.89024100	3.15650200
H	-1.65091900	0.00578100	-1.38418000
H	-3.36862000	1.75930200	-1.05143500
H	-4.79331900	-0.28435200	2.44615700
H	-3.05874800	-2.02860000	2.13423100
H	-1.48699700	-1.89768400	0.21432100
H	-5.97936000	1.84023500	0.01617300
H	-4.77560000	2.90837500	0.73367500
H	-7.14771600	1.88054600	4.07674900
C	-1.01054800	-0.41331600	4.28569300
C	-1.82891900	0.69999400	4.12712400
C	-1.63032100	1.58811600	3.06308900
C	-0.60037100	1.34095700	2.15900700
C	0.22425200	0.22446800	2.31773400
C	0.02397900	-0.65445600	3.37805800
C	-2.55061000	2.79181900	2.95704400
C	-2.35972700	3.61741700	1.76414700
C	-2.19462000	4.30422600	0.78235800
H	-1.17774100	-1.09582000	5.11792800

H	-2.64072300	0.88274000	4.83255400
H	-0.44857000	2.01816000	1.32025500
H	1.02410600	0.04107400	1.60141300
H	0.66742800	-1.52458700	3.49973800
H	-2.40984400	3.42804100	3.84188200
H	-3.59421600	2.44920300	2.99031500
H	-2.05094600	4.92231900	-0.07850300

P7

C	-2.37671400	3.32317200	4.80342500
C	-3.58540500	3.17287300	4.12914900
C	-3.61428700	2.70008000	2.81162800
C	-2.41495400	2.38334200	2.17883900
C	-1.20271900	2.52552400	2.85762300
C	-1.17679800	2.99337600	4.16863100
H	-2.36870600	3.69442400	5.82766600
H	-4.52139800	3.42459700	4.63013500
H	-2.42984100	2.00206300	1.15941100
H	-0.27340700	2.25437900	2.35871900
H	-0.23182200	3.09020500	4.69939100
C	-4.96779500	2.52858900	2.14336500
H	-5.50333800	3.48745100	2.16218600
C	-4.92586600	2.04554300	0.76258600
C	-4.88655900	1.65066500	-0.37937800
H	-4.86213600	1.30655700	-1.39168700
H	-5.56701100	1.82610300	2.74008700
C	-4.07686300	-0.74873200	2.60654200
C	-3.66574900	-0.44134300	3.90055400
C	-2.31058200	-0.47233100	4.24616300
C	-1.37423500	-0.83435600	3.27871900
C	-1.78381200	-1.14364100	1.98057200
C	-3.13302200	-1.09472700	1.63832700
H	-5.13324600	-0.70828200	2.34310000
H	-4.40312400	-0.15635300	4.65283900
H	-0.31712200	-0.85554100	3.53861500
H	-1.04124500	-1.41748000	1.23219800
H	-3.45252400	-1.31808900	0.62190500
C	-1.92069300	-0.12127300	5.67189000
H	-2.27675300	-0.91017100	6.34920900
C	-0.48552900	0.06512700	5.89024100
C	0.70210700	0.20895800	6.06620300
H	1.75037000	0.33752300	6.23466100
H	-2.43997300	0.80243500	5.95854800

P8

C	1.85823000	-0.42300300	0.76383600
C	1.68457200	-1.75673800	0.40618000
C	0.64428200	-2.51508200	0.95663000
C	-0.21650500	-1.91624500	1.87294400
C	-0.04701200	-0.57678600	2.23096600

C	0.98836900	0.17320700	1.68089200
H	2.67391000	0.15297100	0.32813000
H	2.36163100	-2.21739300	-0.31473000
H	-1.03590900	-2.49466900	2.29564200
H	-0.74028400	-0.11260600	2.93037100
H	1.11058600	1.21981000	1.95762500
C	0.49894400	-3.96239400	0.51727000
H	1.42259900	-4.50624300	0.75828600
C	-0.63141100	-4.68014000	1.10797700
C	-1.56638400	-5.26733800	1.60066900
H	-2.38650400	-5.79882500	2.03503300
H	0.39483900	-3.98936100	-0.57606900
C	-1.32912400	-2.08086700	-1.83222200
C	-1.01750400	-0.74636500	-1.58069200
C	-1.74668600	-0.00915900	-0.64444100
C	-2.79585800	-0.62795600	0.03676600
C	-3.10146100	-1.96690500	-0.20514400
C	-2.36965000	-2.69906800	-1.13916100
C	-1.37923600	1.44837500	-0.42359700
C	-1.87805500	2.02659400	0.82570000
C	-2.29548900	2.50517700	1.85487800
H	-0.75128500	-2.64141800	-2.56662100
H	-0.18877300	-0.27399300	-2.10897700
H	-3.35934000	-0.06346600	0.77837000
H	-3.91023200	-2.44441500	0.34606500
H	-2.60181100	-3.74803500	-1.31544900
H	-1.75978200	2.05015100	-1.26132000
H	-0.28552600	1.54049400	-0.43729600
H	-2.66218200	2.93921600	2.76087800

P9

C	-1.57929700	-1.47269000	-0.89855900
C	-1.58328300	-0.08179000	-0.96027700
C	-2.38945900	0.66789000	-0.09575100
C	-3.19341400	0.00225400	0.82776600
C	-3.18567700	-1.39256400	0.89317700
C	-2.38095500	-2.13408300	0.03290200
H	-0.94038200	-2.04329600	-1.57177400
H	-0.94950800	0.43078800	-1.68491000
H	-3.80882500	0.57539100	1.51963200
H	-3.80061700	-1.89701100	1.63595800
H	-2.36247700	-3.22074500	0.09716500
C	-2.38327700	2.18512400	-0.21444000
H	-2.98380300	2.48726000	-1.08651600
C	-2.89332700	2.87863600	0.97176900
C	-3.32411600	3.41010300	1.96954000
H	-3.70092700	3.88135100	2.85378800
H	-1.35700300	2.52841700	-0.41138500
C	0.61226800	-2.13395900	1.81884800
C	0.13163200	-0.87765000	2.17805200

C	-0.86739900	-0.74825400	3.14607000
C	-1.37718000	-1.89820400	3.75134300
C	-0.89733200	-3.15798800	3.39236100
C	0.09824100	-3.28088100	2.42564900
H	1.38274200	-2.21934700	1.05353800
H	0.52362200	0.01501000	1.68724200
H	-2.16675100	-1.80656000	4.49486700
H	-1.30661700	-4.04790700	3.86943000
H	0.46906800	-4.26481300	2.14258200
C	-1.34873500	0.64447200	3.51432400
H	-1.38128800	1.26807000	2.61116700
C	-2.67225400	0.68625500	4.13967600
C	-3.76637300	0.70610000	4.65598600
H	-4.73265200	0.73528500	5.11448400
H	-0.62459400	1.11269900	4.19590900

P10

C	-2.40144200	-0.20165100	-0.30713100
C	-3.35076700	0.80612000	-0.16144700
C	-4.25095000	0.79115000	0.91148900
C	-4.18316400	-0.25086800	1.83428700
C	-3.23403200	-1.26534700	1.68596600
C	-2.34164200	-1.24543500	0.61881900
C	-5.25064100	1.92960800	1.03307200
C	-6.32430100	1.70685300	2.00238500
C	-7.21498600	1.51259600	2.79685300
H	-1.70759600	-0.17529500	-1.14634600
H	-3.40019800	1.61432800	-0.89291600
H	-4.87537800	-0.26667500	2.67436800
H	-3.18675100	-2.06922000	2.41880100
H	-1.59477800	-2.03028000	0.51334200
H	-5.70308400	2.11472000	0.05005100
H	-4.71705500	2.84752000	1.31828000
H	-8.01269800	1.34683700	3.48955600
C	0.74471100	-0.27163400	2.08517300
C	0.01851300	0.90797600	1.94717300
C	-0.99897400	1.23046600	2.85032100
C	-1.27466100	0.35518500	3.89995200
C	-0.54841800	-0.82826600	4.04097500
C	0.46059100	-1.14712400	3.13460200
C	-1.75092600	2.53643200	2.65606600
C	-2.95649800	2.67859700	3.47350800
C	-3.95819800	2.78144100	4.14290400
H	1.53091100	-0.51142200	1.37049600
H	0.23414400	1.58347000	1.11833200
H	-2.07422100	0.59347200	4.59955800
H	-0.77605200	-1.50558300	4.86306100
H	1.02513100	-2.07191900	3.24436600
H	-2.03382200	2.62237500	1.59796500
H	-1.07656900	3.37687900	2.87202300

H	-4.86144000	2.87178000	4.70850900
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P11

C	-6.54712200	2.14829800	2.83852600
C	-6.16390700	0.84066400	3.12105100
C	-6.04302300	-0.10655200	2.09856000
C	-6.33236200	0.27277400	0.78910000
C	-6.71646900	1.58472400	0.50172100
C	-6.82066000	2.52727000	1.52201600
H	-6.63312300	2.87551100	3.64488900
H	-5.93627800	0.55126700	4.14793700
H	-6.24360900	-0.45938200	-0.01191400
H	-6.93588800	1.86901500	-0.52658700
H	-7.11868400	3.55011800	1.29680700
C	-5.54721000	-1.49451500	2.46284700
H	-6.18568600	-1.91179400	3.25282400
C	-5.49561900	-2.44292800	1.35013000
C	-5.46174100	-3.21883600	0.42338200
H	-5.42984100	-3.91851500	-0.38472200
H	-4.53622100	-1.40051100	2.88715900
C	-2.99672300	0.81904400	1.74668900
C	-2.57185700	0.75321800	3.07067300
C	-1.92955700	-0.39054400	3.55969300
C	-1.71882100	-1.46974800	2.70023400
C	-2.14506600	-1.40472900	1.37164300
C	-2.78412000	-0.26369700	0.89192200
H	-3.52414700	1.70331400	1.38981000
H	-2.75088900	1.59738300	3.73801100
H	-1.22817500	-2.36631500	3.07478200
H	-1.99268900	-2.25950900	0.71491000
H	-3.13755800	-0.22495000	-0.13712000
C	-1.47400600	-0.39548500	5.01035900
H	-2.31352200	-0.09340500	5.65080500
C	-0.95524200	-1.67630000	5.49239800
C	-0.52807600	-2.73879400	5.87912200
H	-0.14846100	-3.67370800	6.23388000
H	-0.69522800	0.36874300	5.14190900

P12

C	2.76386900	2.69369100	4.37151900
C	2.50812400	1.34028100	4.15444300
C	2.18238400	0.87227200	2.87902900
C	2.11415600	1.78103200	1.82002500
C	2.36674700	3.13572400	2.03494800
C	2.69311500	3.59582200	3.31072400
H	3.01278600	3.04403500	5.37237200
H	2.55736100	0.63982400	4.98876900
H	1.85449500	1.42916200	0.82081500
H	2.29658700	3.83089700	1.20000600
H	2.88739100	4.65406400	3.47885000

C	1.95007200	-0.61341800	2.66256600
H	1.62924800	-1.07013700	3.60699100
C	0.95721000	-0.91764700	1.62806900
C	0.13496000	-1.15627600	0.77415800
H	-0.59669900	-1.36942500	0.01996400
H	2.90100500	-1.09367000	2.38941400
C	-3.24162200	-0.49671000	-0.46252300
C	-2.65064100	0.64408300	0.07261900
C	-1.58461300	1.27092800	-0.58242400
C	-1.13065600	0.74663300	-1.79193800
C	-1.72088200	-0.39895100	-2.33088500
C	-2.77319700	-1.02698200	-1.66751400
H	-4.06477200	-0.97833500	0.06292000
H	-3.00654900	1.04443000	1.02236600
H	-0.30152400	1.22756200	-2.30753900
H	-1.35181500	-0.80290700	-3.27233200
H	-3.23003200	-1.92222700	-2.08596500
C	-0.93779400	2.47181400	0.08516000
H	-0.50677400	2.14926200	1.04464700
C	0.11309400	3.11543100	-0.70336000
C	0.97975200	3.62883300	-1.37254100
H	1.74496400	4.09596800	-1.95589600
H	-1.70961400	3.21658400	0.32032100

P13

C	3.52574500	2.35334700	1.09111500
C	3.20050000	1.14150600	0.48905500
C	2.08841900	0.40709400	0.91527700
C	1.29981100	0.91431300	1.94700300
C	1.62383500	2.13118100	2.55115300
C	2.73671700	2.85251400	2.12900300
H	4.39825400	2.91031000	0.75165000
H	3.82276800	0.75280600	-0.31822400
H	0.43161000	0.34741300	2.28141500
H	1.00116500	2.51548800	3.35842300
H	2.98764700	3.80111200	2.60085300
C	1.80642100	-0.92922100	0.24843600
H	2.69087000	-1.57152500	0.35774700
C	0.64169600	-1.64147700	0.77287300
C	-0.32022600	-2.21991200	1.22101500
H	-1.17755100	-2.73673500	1.59641700
H	1.66286400	-0.77152300	-0.82911500
C	-2.95560000	-0.78705000	-0.60335600
C	-2.63081200	0.42455900	-0.00060200
C	-1.51847700	1.15920200	-0.42578800
C	-0.72916600	0.65245400	-1.45720000
C	-1.05270900	-0.56420400	-2.06202900
C	-2.16581600	-1.28577100	-1.64089800
H	-3.82826200	-1.34424400	-0.26467100
H	-3.25360500	0.81289700	0.80644900

H	0.13924200	1.21953600	-1.79077000
H	-0.42949100	-0.94813900	-2.86905500
H	-2.41636600	-2.23419000	-2.11330500
C	-1.23686600	2.49516800	0.24185300
H	-1.09310300	2.33687700	1.31929300
C	-0.07243700	3.20812200	-0.28236300
C	0.88830600	3.78833100	-0.73075000
H	1.74488600	4.30632000	-1.10629100
H	-2.12146500	3.13733300	0.13300400

P14

C	-0.94353900	-1.42415600	-2.09855700
C	-1.09268800	-0.05018100	-1.93342200
C	-1.98851600	0.46073200	-0.98881100
C	-2.73005900	-0.42561100	-0.20830600
C	-2.58284800	-1.80328300	-0.37438000
C	-1.69316300	-2.30631100	-1.31983400
H	-0.23778200	-1.80725100	-2.83395200
H	-0.50230900	0.63578900	-2.54248200
H	-3.41892600	-0.03669000	0.54004000
H	-3.16331000	-2.48455000	0.24562400
H	-1.57427000	-3.38108800	-1.44400700
C	-2.12805000	1.96965400	-0.86222100
H	-2.68840200	2.35525400	-1.72666300
C	-2.79099600	2.42539900	0.36305200
C	-3.34675700	2.78889200	1.37484300
H	-3.84079900	3.12532100	2.26388500
H	-1.13183500	2.43087400	-0.91207800
C	1.28311100	3.78460700	3.46448600
C	0.59488800	2.95717000	2.58135600
C	0.99729600	1.63018000	2.38811700
C	2.09407200	1.14160600	3.09723200
C	2.78590700	1.97128100	3.98297900
C	2.38506500	3.29275200	4.16840700
H	0.95895200	4.81505200	3.60728600
H	-0.27187500	3.33758700	2.03652000
H	2.40487200	0.10695900	2.95661700
H	3.64195100	1.57956700	4.53171500
H	2.92500800	3.93793500	4.86036100
C	0.22512600	0.79346900	1.38541000
H	0.41552000	1.18361100	0.37489900
C	0.53405400	-0.63649900	1.37810300
C	0.79670900	-1.81722600	1.36585700
H	1.00756300	-2.86547000	1.34372200
H	-0.85040200	0.91983900	1.56671000

P15

C	-1.44187500	-1.18503300	-2.59499400
C	-0.65508900	-0.39201000	-1.76385600
C	-1.12026100	0.00584100	-0.50629200

C	-2.39442900	-0.38718400	-0.10009100
C	-3.18654800	-1.18046500	-0.93250100
C	-2.71320300	-1.58640900	-2.17855200
H	-1.06220700	-1.49444400	-3.56785800
H	0.34324500	-0.09345500	-2.08605100
H	-2.75802700	-0.09312400	0.88286000
H	-4.17704100	-1.48790300	-0.60015400
H	-3.32942500	-2.21048300	-2.82407700
C	-0.19145500	0.82105500	0.37622100
H	0.01138700	1.78926900	-0.10173600
C	-0.68247100	1.06131900	1.73362800
C	-1.09451900	1.25637300	2.85357700
H	-1.45330200	1.44088400	3.84403000
H	0.76879900	0.29144200	0.44346700
C	4.08840700	-2.78990000	5.19104700
C	3.01437600	-2.05766700	4.69391200
C	2.29501600	-2.50839600	3.58091800
C	2.66979200	-3.70674400	2.97466700
C	3.74696000	-4.44327700	3.47216500
C	4.45891400	-3.98932300	4.57939800
H	4.63866500	-2.42515200	6.05748600
H	2.72859200	-1.12066800	5.17397600
H	2.11610500	-4.06377800	2.10786200
H	4.02902700	-5.37750300	2.98842100
H	5.29921000	-4.56411100	4.96583100
C	1.12951100	-1.66858200	3.08604300
H	1.47481000	-0.64407700	2.88906000
C	0.46365400	-2.17676000	1.88611400
C	-0.08445700	-2.60270300	0.89579000
H	-0.60125500	-2.94146700	0.02083700
H	0.38027600	-1.58061900	3.88508900

Optimized coordinates of various structures of phenylacetylene dimer calculated at M06-2X/aug-cc-pVDZ level of theory.

PA1

C	-1.29824300	-0.02849400	-1.54243400
C	-0.27883100	-0.18253900	-2.48266200
C	0.77762800	0.72819900	-2.51807400
C	0.82144800	1.78588300	-1.61377000
C	-0.19756200	1.93746400	-0.66267400
C	-1.26248400	1.02572600	-0.63553100
H	-0.30252700	-1.02014700	-3.17758900
H	1.57429600	0.61223300	-3.25135800

H	1.64532900	2.49699200	-1.62910300
C	-0.13448800	3.00179500	0.30061000
H	-2.04261400	1.14100500	0.11430900
H	-2.11432300	-0.74837300	-1.50307300
C	-0.06933200	3.88485300	1.12683000
H	-0.02120300	4.67696700	1.84376100
C	1.29728100	0.02923700	1.54187000
C	1.26162900	-1.02486200	0.63482000
C	0.19674000	-1.93664200	0.66176400
C	-0.82234400	-1.78522700	1.61281100
C	-0.77863100	-0.72766500	2.51726000
C	0.27779200	0.18312200	2.48204000
H	-1.57535500	-0.61183100	3.25050300
H	-1.64620100	-2.49636800	1.62798500
C	0.13377200	-3.00082100	-0.30168800
H	2.04182200	-1.14001400	-0.11497500
H	2.11334000	0.74914700	1.50267100
H	0.30140300	1.02063300	3.17708700
C	0.06857900	-3.88359200	-1.12819700
H	0.02053000	-4.67550000	-1.84535700

PA2

C	0.33446300	2.23392900	-3.84242300
C	1.40899300	1.38255600	-4.13763700
C	2.68404500	1.68247600	-3.66759300
C	2.89682500	2.82500500	-2.89554600
C	1.82874000	3.67107400	-2.59407000
C	0.55271400	3.38160200	-3.06652700
C	-0.98291100	1.93117400	-4.33027100
C	-2.09291400	1.67782800	-4.74265800
H	1.23071800	0.48853300	-4.73196100
H	3.51476900	1.01777500	-3.89973000
H	3.89522200	3.05506300	-2.52644500
H	1.98677000	4.55587900	-1.97979300
H	-0.28781500	4.02847700	-2.82285200
H	-3.07173100	1.45942900	-5.11381200
C	1.29164900	-0.48631500	-1.16167700
C	0.19498000	-1.08856500	-1.78034600
C	-1.04851800	-0.45698300	-1.76141100
C	-1.20003800	0.77064500	-1.12392100
C	-0.10039800	1.37830600	-0.50221400
C	1.14972700	0.74270500	-0.52592300
C	-0.24780800	2.65563100	0.13956900
C	-0.36886900	3.73751700	0.67016100
H	-2.16316600	1.27707800	-1.11776400
H	-1.90296900	-0.91582900	-2.25569600
H	0.31103000	-2.04835900	-2.28148600
H	2.26575600	-0.97252400	-1.18331200
H	2.00189700	1.22677500	-0.05317900
H	-0.48137600	4.68538400	1.15231600

PA3

C	1.13319200	3.65279700	-2.67652400
C	1.31640500	2.59709200	-3.58037600
C	2.56194900	1.98696700	-3.69456400
C	3.63050900	2.42038300	-2.90941000
C	3.45002400	3.46869600	-2.00547900
C	2.20862500	4.08608700	-1.88733400
C	-0.15493500	4.27471700	-2.54317000
C	-1.23874600	4.79929700	-2.41672800
H	0.47348400	2.25648600	-4.17836600
H	2.69649500	1.16341300	-4.39411900
H	4.60366100	1.93971900	-2.99915400
H	4.28132900	3.80710600	-1.38895800
H	2.05307400	4.89528600	-1.17717700
H	-2.19377400	5.26770600	-2.30799400
C	1.42663600	-0.22968900	-1.32111700
C	0.27928500	-0.55457100	-2.04506300
C	-0.87705500	0.21367600	-1.89894200
C	-0.89101700	1.30036800	-1.02993700
C	0.26074300	1.62769800	-0.29958600
C	1.42191200	0.85736700	-0.45219900
C	0.25667800	2.75916200	0.58543900
C	0.25740900	3.72009000	1.32189700
H	-1.78231400	1.91389400	-0.91790300
H	-1.77308300	-0.03528400	-2.46537500
H	0.28600700	-1.40484800	-2.72552000
H	2.33334700	-0.82099100	-1.43951700
H	2.31621900	1.12699400	0.10600200
H	0.25038200	4.56430100	1.97805800

PA4

C	-0.86036400	0.89144800	-2.05820800
C	1.50965100	4.10165500	0.77800400
C	-1.77306900	0.24792800	-1.22172700
H	-0.78715300	0.60704700	-3.10675500
C	-0.03234800	1.89030100	-1.55480400
C	-1.85943600	0.60980000	0.12274200
H	-2.40958100	-0.54274000	-1.61563600
H	0.68574200	2.39485400	-2.19853300
C	-0.10982400	2.24929000	-0.20112800
H	-2.55709400	0.09839800	0.78416300
C	-1.03258600	1.60466000	0.63550300
H	-1.08102900	1.87683400	1.68802000
C	0.76428100	3.25959500	0.32918200
H	2.16263100	4.85010600	1.17460700
C	0.13963600	-3.05995000	-1.09941100
C	-0.57527200	-1.21626000	3.37990800
C	1.11588800	-2.25434700	-1.68644000
H	-0.29583100	-3.88631500	-1.65921500

C	-0.28085000	-2.81202500	0.20433400
C	1.67333900	-1.19796200	-0.96481400
H	1.44113600	-2.44923500	-2.70729800
H	-1.04408900	-3.43276300	0.66993100
C	0.27631900	-1.74995800	0.93031800
H	2.42883200	-0.56139200	-1.42252800
C	1.25929900	-0.94367600	0.33862000
H	1.67804600	-0.11199500	0.90219500
C	-0.17783900	-1.46883300	2.26425000
H	-0.91181600	-1.00416500	4.37268700

PA5

C	-2.08357300	0.45361800	-0.71068500
C	-2.02791700	1.61324400	0.07556400
C	-1.08152500	2.59620300	-0.19955600
C	-0.18797300	2.43288800	-1.25900000
C	-0.24357400	1.28111100	-2.04465500
C	-1.18535300	0.29329300	-1.77516200
C	-3.03013600	-0.58451900	-0.41127400
C	-3.79739800	-1.48407200	-0.15123900
H	-2.72713900	1.73039300	0.90134300
H	-1.04223400	3.49482000	0.41432600
H	0.55170700	3.20337500	-1.47136800
H	0.45765200	1.14641100	-2.86670800
H	-1.22607000	-0.61619200	-2.37152300
H	-4.47545700	-2.28121900	0.06851300
C	0.02205600	-2.59159800	-0.13179400
C	1.11413600	-2.33750500	-0.97621800
C	1.93097300	-1.23507600	-0.74628400
C	1.66576300	-0.37552300	0.32132300
C	0.58519200	-0.62811600	1.16582400
C	-0.23315300	-1.73295700	0.94620100
C	-0.83046200	-3.72226000	-0.37629700
C	-1.54617700	-4.67397400	-0.59494200
H	1.31016700	-3.01125900	-1.80830700
H	2.77535700	-1.04212700	-1.40636700
H	2.29753400	0.49497300	0.49069600
H	0.37203700	0.04454500	1.99477800
H	-1.08887400	-1.92845500	1.58900400
H	-2.17496000	-5.51800900	-0.78377100

PA6

C	-1.49849000	0.12694200	-1.75338900
C	-0.55882100	0.02318900	-2.77962700
C	0.49861300	0.93085200	-2.84922300
C	0.61475400	1.94405300	-1.90271800
C	-0.33246300	2.05709900	-0.87507100
C	-1.38851400	1.13748500	-0.80324700
H	-0.64945200	-0.76675400	-3.52401000
H	1.23663100	0.84921700	-3.64575500

H	1.43581100	2.65700600	-1.94860700
C	-0.22265600	3.10993600	0.09594700
H	-2.11633800	1.22690400	0.00102100
H	-2.32191500	-0.58307500	-1.69305800
C	-0.13222400	3.99992600	0.91119600
H	-0.04590700	4.77876900	1.63835900
C	2.76700900	2.53437400	2.45173900
C	2.65598300	1.52381100	1.50177500
C	1.60045800	0.60375000	1.57529600
C	0.65475600	0.71649000	2.60437000
C	0.77194400	1.72969200	3.55067900
C	1.82891000	2.63774800	3.47942600
H	0.03516100	1.81098200	4.34837100
H	-0.16591300	0.00318700	2.65154500
C	1.48949700	-0.44954000	0.60485000
H	3.38262500	1.43469300	0.69642400
H	3.59005400	3.24470600	2.39014900
H	1.92041700	3.42770100	4.22366500
C	1.39839500	-1.33984600	-0.21011400
H	1.31087000	-2.11920300	-0.93658900

Optimized coordinates of various structures of PrBZ dimer calculated at M06-2X/aug-cc-pVDZ level of theory.

TU1

C	-2.28071100	-0.76829700	-0.51086300
C	-0.90605500	-0.78733200	-0.27339200
C	-0.16430600	0.39547100	-0.26011600
C	-0.83348000	1.60396200	-0.48836600
C	-2.20651200	1.62977100	-0.72187400
C	-2.93705400	0.43996700	-0.73484000
H	-2.84140000	-1.70262200	-0.50934200
H	-0.40493800	-1.73513600	-0.07714800
H	-0.26999700	2.53790900	-0.47436500
H	-2.70922500	2.58073000	-0.89469800
H	-4.01115400	0.45757800	-0.91446700
C	1.32115500	0.37971200	-0.00795600
H	1.87654600	0.55950000	-0.93785900
H	1.60447700	1.16289800	0.70600300
H	1.63817000	-0.58666100	0.39912000
C	-0.46705200	-1.67136200	3.27195400
C	-1.83996300	-1.64691000	3.03794300
C	-2.51006000	-0.43912000	2.80823400
C	-1.76931100	0.74425400	2.82057400
C	-0.39464400	0.72658400	3.05844100
C	0.26253900	-0.48088500	3.28394100
H	0.03635100	-2.62170200	3.44606200
H	-2.40274400	-2.58131100	3.02481800

H	-2.27113600	1.69147300	2.62314300
H	0.16528800	1.66137600	3.05610000
H	1.33654500	-0.49742200	3.46411200
C	-3.99525500	-0.42545400	2.55437700
H	-4.55142600	-0.62040500	3.48065800
H	-4.31541700	0.54510700	2.16003400
H	-4.27426800	-1.19961400	1.82899100