

# The non-aromatic endocyclic angle at the fusion with the aromatic ring in benzocyclopentene and -hexene revisited.

Dirk J.A. De Ridder & Hans-Beat Bürgi

**Table 1** CSD reference codes for both data sets, indicating to which subset(s) the compound is belonging.

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Benzocyclopentenes					
ACINDN	522C	FULZIV	533C	PHTGLY	522N
BAHMIG	523C	FUPCAU	523N	PHTGLY01	522N
BASKEL	533C	GAKSIU	523O	PHTHAO	522O
BDTPIM	522N	GATTOK	533C	PHTHIB	522N
BEBCUG	533N	GAVMOF	533O	PINDON	522C
BEDNON	533C	GAXTII	523C	PIVIND01	522C
BEJBUN	533O	GEFPFM	533O	PIVIND10	522C
BEJMIM	522C	GEXWOV	533C	PLBULC	522N
BERKOY	523C	GEZFIA	533C	PLBULC01	522N
BEXLOF	523O	HACMIH	522N	PNPSXI	522N
BIBWAK	523C	HACTOU	523N	PTHPAL	522N
BICDIA	533C	HADMEE	533C	PYINDO	522C
BICHOK	522N	HDMNAC	533C	SACSUK	523N
BIINDO	522C	HNOBCH	533C	SARSOT	522N
BIJVEV	523C	HPIPZO10	523C	SARSUZ	523O
BIPHIM	522N	HPNFLO	523C	SAXFAY	522C
BITTED	522C	HPRIND	523N	SAXHUU	522N
BITTED10	522C	HXPBIM	523N	SAZCUR	523O
BIYMAX	533O	IMEPIM	522N	SAZTUI	522N
BOSSAD	533C	INDDON	522C	SEDBEI	533C
BOXFEZ	533C	INDSAZ	522C	SEDRIC	533C
BPHIPH	522C	INTRBP	522C	SEFLIY	523O
BTCODD	533C	JABXUF	522N	SEGYEI	533N
BUI NPR	522C	JECBOI	533C	SEKKOI	523N
BURKAA	522N	JECCEZ	533C	SEMCUI	533C
BZCYDT	533C	JECCID	533C	SEMDAP	533C
BZMADN	522N	JECCOJ	533C	SEMJID	522O
BZYIND	523C	JEGMEN	533C	SERNOS	523N
CAHBAO	533C	JEJEN	533C	SIDJUK	533O
CANLOS	522C	JEJEN10	533C	SIKFEX	522N
CAPYUN	522C	JIFZIH	522N	SISZOJ	522N
CEDJIE	523N	JIGGEL	523O	SIVYOL	533C
CELLIO	523C	JIRDET	522N	SIWFEJ	533C

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CEMBOL	533C	JIRDIX	522N	SIWXUR	522N
CESBUX	533C	JISWAJ	533N	SIZCOT	523O
CESYEE	533C	JIWMEH	523N	SIZCUZ	523O
CIGHEF	533O	JOPLAB	523C-522C	SOCKAW	523C
CIGHIJ	533O	JORYUK	522N	SOJCEZ	523C
CIGHOP	533O	JOTGII	522C	SOJJAC	522O
CIKMUE	522N	JUBLOH	522N	SOJPUC	523O
CILHAG	522C	JUCYAH	523N	SOWCOW	522N
CIMMAM	533C	JULVER10	522C	SOWWUW	523C
CIYYOY	533C	JURKOW	523N	SUBXIW	522N
CLMIND	533N	JUYGAL	523C	SUBXOC	522N
CLPXCN	533O	KAJSET	533O	SUFLAG	522C
CNINDO	522C	KAJSOD	533O	SUHRAO	522C
COMGOA	522N	KAJSUJ	533O	TAPTEJ	533C
COMGUG	522N	KALGOT	533C	TCDMSP10	533C
CONJUK	523O	KALGUZ	533C	THALID10	522N
COXMIL	533C	KERXIO	523N	VAFCIO	533C
COXMIL01	533C	KETLEA	523C	VAFCOU	533C
COYNAF	522N	KETLIE	523C	VAGXIK	522O
COZFOM	522N	KEWGOI	523C	VAJHAP	533C
CPIBFC	533O	KICRAP	523C	VALFOD	533C
CPISIN	533N	KIHVOM	533C	VALGEU	533C
CTSGLM	522N	KIVLIK	533C	VALGIY	533C
CUDMIX	523N	KOBFOW	533O	VALGOE	533C
CUFFAK	523O	KOCHIT	522N	VALGUK	533C
CUMFEV	533C	KOKMOM	522N	VALHAR	533C
CUMFIZ	533C	KONHOK	533C	VANBIV	523N
CUMFOF	533C	KOTWUL	533N	VANGEW	533C
CYMINO01	522C	KOTXAS	533N	VASWOB	523C
DADDER	522O	KOWTIZ	522C	VASXAO	523C
DANREP10	533N	KUFWUD	533C	VAWVIY	523C
DASPIW	522C	KUKDID	533C	VAYVOG	522N
DEPVUP	533C	KUTGEL	533C	VEFYUA	533O
DETGOY	522N	LABWAM	523C	VEGZUC	533N
DEZKIC	533C	LAGYOH	523N	VEKZUG	522N
DIJZOL	533C	LAGZAU	523N	VEMCOF	522C
DIVDER	522C	LAGZEY	523N	VICBEO	522N
DOLJET	522C	LALWEA	533C	VICBIS	522N
DOLJET01	522C	LALYEC	522C	VICPAY	533C

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DOMSUT	522N	LATXAF	533C	VIFWUC	522N
DOTRAF	533C	LAVCUG	523C	VIHTAH	522N
DOYFEC	523C	LAVKAU	533C	VIKLIK	523C
DOZSIU	522C	MAPIND	522C	VIMPEN	523O
DPBFSO	533O	MAYPIB	533O	VOFVOB	522N
DUCWUT	522C	MAZKBN	533C	VOGFEC	522C
DUDLUJ	523N	MBPHIN	533C	VOJSIW	522N
DUNPOR	522N	MBYINO	522C	VOPDIN	522N
DUVMEM	522C	MBYINO02	522C	VOPFUB	522N
DUZZAZ	533C	MPHTPA	522N	VOPYII	522C
DUZZED	533C	MSULIN	522C	VOYZEO	522N
EOPTHL	522N	NAPINO	522C	VUCHIK	523C
EPINDO	522C	NINDOD	522C	VUFNAL	533O
EPNPHD10	533O	NINDOD01	522C	VUGWAV	523O
EPHPZ	522N	NINDOD10	522C	VUJCUY	533C
EXMTCV	533C	NINHYD	522C	VUJSUO	523C
FADMAY	533C	NISTHD10	533C	VUJTUP	533C
FAFJOL	533C	NMYPHD	522O	VUJVAX	533C
FARLEP	533C	NPHTNS	522N	VUKHUE	522N
FAYWUX	522N	NPINDO	522C	VUKJAM	522N
FEKFIK	522C	OTLPTH	523O	VUKJIU	522N
FEMLUE	533C	OXINET	533O	VUKVEC	523C
FETXOR	522N	PACZOI	533C	VUXYUI	523C
FIJJUD	522N	PAJPAR	533C	WACHUD	522N
FIKFAG	523C	PAPPHI	522N	WAMZEP	523C
FIKFEK	523C	PAPPOL	523O	WAMZEP	533C
FIMPOG	522C	PATMUS	523N	XPINO	522C
FIZFAV	522N	PBBSHD	522C	XSBFIC	533O
FIZJON	533C	PEBHAF	522N	YAMHAV	533C-523C
FLSCAC	523O	PEJHOB	522N	YAPHEC	533C
FOWDUQ	533C	PHALIM01	522N	ZZZAWJ10	522N
FOWFAY	533C	PHISOR	522N	ZZZAWP10	522N
FUDLUL	523N	PHRCGE	522N	ZZZAWV10	522N
Benzocyclohexenes					
AHMHPC	633C	DOSMUT	623C	KOMVIR	633C
ALENPR	633C	DPBFSO	633C	KOMVOX	633C
BAPGEE	633C	DUBPUL	622N	KUFBAO	633C
BAPGII	633C	DUFKIY	633O-623O	KUGXOZ	633N
BCOCAN	633C	DUTTAN10	622C	KUKDID	633C

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BEBCUG	633C	DUZZAZ	633C	LACTUE	622C
BEDNON	633C	DUZZED	633C	LAJNIT	633C
BEOBCN10	633O	EABPAY	633O	LATXAF	633C
BHPHOL	623C	EHMBCX	633C	MAYPIB	633C
BICDEW	633C	EMZHAN	622N	MBZHOA	633C
BIVLAT	622C	EPIPNL	633C	MBZHOB	633C
BIYMAX	633C	EPNPHD10	633C	MDZANO	622N
BMPYNP	633C	ETZAND	622N	MHCSTY	623N
BOMNAS	633C	EXMENC	633C	MNAPOD10	633C
BOMPUE	633C	FAFXIT	633C	MPANPL	633C
BOPRIH10	633C	FASDEI	633N	MTHANQ	622C
BOSSAD	633C	FATJAL	633C	MTNCBX	633C
BOYKEF	633C	FEHCAW	623C	MXCHCH	633C
BTCDOD	633C	FIBKEG	633C	MXCVPN	633C
BUKYIP	633C	FIKFAG	623C	OHBZBP	633C
BUKYOV	633C	FIKFEK	633C	OHLACT10	633C
BUKZIQ	633C	FITYOW	633C	PEKZEK	633C
BUKZOW	633C	FITYUC	633C	PHENON	633C
BUMRIK	633O	FODVOJ10	633C	PHTRPH	633C
BUYRUI01	633C	FOHPUN	633C	SABNAK	633C
BUYRUI02	633C	FOMTAC	633C	SABNEO	633C
BUYRUI03	633C	FOYTIW	633C	SABNIS	633C
BZCYDT	633C	FUWHOU	633C	SAMRON	633N
BZEHPN	633C	FUWHUA	633C	SATCIZ	623C
BZOCND	633O	FUWJEM	633C	SAXFUS	633C
BZTETO	623C	FUWTIA	633C	SAXJIK	633C
CABZIO	633C	FUWTOG	633C	SEBPOE	633C
CANCID	633C	FUXYIG	633C	SEBRAS	633C
CANCID10	633C	GACFAR	623C	SEBREW	633C
CANCOJ	633C	GAFHIE	633C	SEBRIA	633C
CANCOJ10	633C	GASHUD	623C	SEDRIC	633C
CAWYII	633O	GATTOK	633C	SEWGEG	633C
CEGSAI	633N	GEFPEM	633C	SIDJUK	633C
CEJXAQ	623C	GEJCIH	633O	SIWFAF	633C
CEKWOE	633C	GEJCON	633C	SIWFEJ	623C
CELNUC	622C	GICKAE	633N	SIZBOS	623C
CELPEO	622C	GIGJAH	633N	SONVIA	622C
CETTOK	622C	GIGKOW	633O	SUCHAZ	633C
CEWDEN10	633C	GIGYOK	633N	SUKSAS	633N

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CIBWAL	633N	GOJDEO	633C	SUKSEW	633N
CIBWEP	633N	HACCOD	633O	SUKTAT	633O
CICWEQ	633O	HDMBZD	633C	TAHBIN	623O
CIGHIJ	633C	HDMNAC	633C	TAKMIB	633C
CIGHOP	633C	HEPANT	633C	TBTRCP10	633C
CIRXUW	633C	HMZHAN	622N	TETSUA	633C
CIRYAD	633C	HNFMNO	623C	VAKBAK	633C
CISSAY	633C	HNOBCH	623C	VAMPOO	633O
CIYYOY	633N	HPMTIQ	633N	VANGEW	633C
CIYYUE	633C	HYBOTZ	633N	VAWVOE	623C
CIYYUE	633N	JABCUK	623O	VEDNUN	633C
CLPXCN	633C	JAWZAI	633C	VEDNUN10	633C
CNMTOC	633C	JEDVIX	623C	VEDSOM	633N
COMFOZ	633N	JEZRIP	633C-623C	VEDZEJ	622C
COMXOR	633C	JIGGOV	633C	VEFPEB	633C
CORYUD	633N	JIGGUB	633C	VEFYUA	633C
COVFUO	633C	JIMHES	633O	VELDAR	633N
COVFUO10	633C	JOBZEF	633C	VEPHED	633C-633N
CUXHOS	633N	JUKWAN	633N	VEVLAJ	633C
CUYPIV	622C	JUPVAR	633C	VEVLIR	633C
DAFVIP	633C	KAFDEA	623C	VEVLUD	633C
DAFVOV	633C	KAMLAL	633C	VEVMEO	633C
DARVOH	623O	KAMTEX	623C	VEXPUJ	633C
DARVUN	623O	KEFZAW	633C	VICXOU	633C
DAWHEO	633C	KEPFAM	623C	VICXOU10	633C
DEFXER	633C	KEPFOA	623C	VIKLAC	623C
DEPJOX	622N	KEPFUG	633C	VIKLEG	623C
DEPVUP	633C	KEPTUU	623C	VINJAD	633C
DEXCOY	633C	KETVOU	633O	VOBVOX	633N
DHTRYP10	633C	KEXCUL	633O	VOLMOY	633C
DITWOS	633C	KEXLUU10	633N	VONCIK	633C
DITWUY	633C	KIHVOM	633C	VUJVEB	633C
DIZCOE	633O-623O	KINFIW	633C	VUSRIK	623C
DMBMOR	633C	KITLII	633C	VUYXES	633C
DOBSES	633C	KOBFOW	633C	XSBFIC	623O
DOFCUW	623C	KOCKES	633C	YAFYUZ	633O-623O
DOJROJ10	633C-622C	KOCKIW	633C	YAKGAS	633C
DOMNOI	633C	KOHHOE	623C	ZBUNDO	633C
DOPREF	623C	KOHZAI	633C		

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**The non-aromatic endocyclic angle at the fusion with the aromatic ring in benzocyclopentene and -hexene revisited.**

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*Supplementary material: CSD Reference codes with full reference of the benzocyclopentenes*

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**The non-aromatic endocyclic angle at the fusion with the aromatic ring in benzocyclopentene and -hexene revisited.**

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