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Supporting information for article:

**An enhanced set of displacement parameter restraints in
*CRYSTALS***

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1 supplementary material

1.1 Ar''₂PBr structure

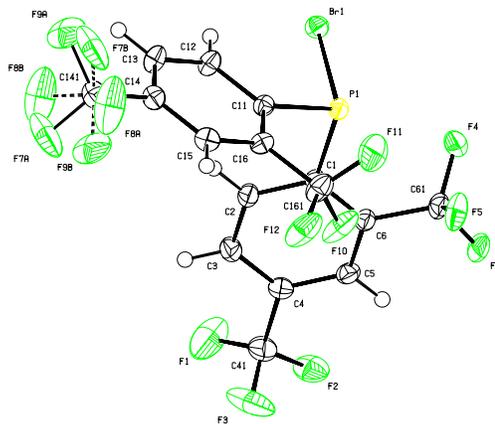


Figure S1: ORTEP plot of Ar''₂PBr

1.1.1 List of restraints

List of restraints used for the refinement of Ar''₂PBr noted **4** in Batsanov, A. S., *et. al.* **2002**. *J. Chem. Soc., Dalton Trans.* pp. 4622–4628.

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#LIST      16
DISTANCE 0.0, 0.001 = MEAN C(141) TO F(71),
CONT C(141) TO F(81),
CONT C(141) TO F(91),
CONT C(141) TO F(72),
CONT C(141) TO F(82),
CONT C(141) TO F(92)
DISTANCE 0.0, 0.001 = MEAN F(71) TO F(72),
CONT F(72) TO F(81),
CONT F(81) TO F(82),
CONT F(82) TO F(91),
CONT F(91) TO F(92),
CONT F(92) TO F(71)
UTLS 0.0001 3 F(72) F(82) F(92) C(14) C(141) F(71) F(81) F(91)
PLANAR 0.001000 F(71) F(81) F(91) F(72) F(82) F(92)
END
# Remove space after hash to activate next line
# USE LAST
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1.1.2 CF₃ search in the CCDC database

List of the hits from the search of the CCDC database with the corresponding R1-Factor (%) of the fit of a TLS model on a CF₃ group.

Ref code	R1-Factor						
ACEXUB	6.20	EVAJAN	1.32	HOYZOL	2.99	LAQKEV	5.07
ADECES	2.14	EVAMUK	1.40	HOZCAB	5.46	LEDZUR	1.86
ADIHOL	1.99	EVATOL	3.77	HUDDEQ	3.19	LEGJIS	2.34
AFAWUB	1.63	EVEBAJ	1.59	HUGCOC	1.94	LEHMUI	2.54
AFEKUS	3.71	EVEDEP	2.03	HULCUM	3.00	LEHTOI	1.86
AFIHUT	2.16	EVEQEC	1.77	HULDAT	1.54	LEQQAB	16.08
AFITAM	1.04	FACQIK	5.07	HUPPOZ	2.21	LEQQEF	16.08
AFOGAF	2.02	FAXKAR	2.50	HUYXUU	3.60	LESCOD	1.17
AGAPOP	2.99	FAXVAC	2.91	ICACIY	3.43	LESGAT	2.90
AYUMOX	1.99	FAXZUA	6.09	IDATAK	2.49	LESRAE	3.32
AZAHAL	4.37	FICTUI	3.17	IDODUB	1.69	LESREI	1.24
AZOZEV	1.39	FICZIC	3.61	IDODUC	4.68	LJLJUM	1.29
AZURUJ	2.41	FIWHEZ	6.29	IDOGOZ	2.83	LJPIE	2.81
BEMWIB	6.21	FOBYEB	4.08	IDUNUS	1.29	LIWCIE	2.15
BIKHIN01	1.13	FOCCUW	3.06	IFOTAA	2.50	LOHZUE	3.47
BIZROS	2.98	FOGVII	5.27	IJOHUL	3.39	LOJJAW	2.09
BOVCEV01	6.01	FOHROK	7.32	IJUDAT06	2.06	LOJKEB	2.24
BUFCIP	2.44	FOLJIB	2.66	IJUMUW	2.15	LOSDAZ	2.86
BUFMEV	1.32	FOVLOS	2.27	IKEBUW	2.46	MAVKUQ	7.33
CEGTEP	2.31	FUHQUV	1.62	IKEYUS	4.72	MEBJOT	3.05
CIPSOK	2.81	GAQDAF	1.83	ILIQID	1.14	MEHCOS	1.46
CORZEQ	1.17	GAQYII	1.48	IROYET	2.49	MEMWOR	4.82
CUCYEF	2.78	GARCIN	1.43	IWOMUC	1.63	MENRED	3.06
DIXZUH	2.29	GARJAM	1.83	IXAVOS	4.25	MEWZIZ	1.12
DIYBAQ	5.96	GAVTED	6.57	IYEBAP	4.13	MEWZOF	1.31
DOKSUS	4.21	GISMIF	1.99	IYUWEE	3.25	MIGGIT	2.56
DOKVEF	4.05	GISWOV	2.41	JAYCES	1.98	MIGNIA	3.24
DUHPIG	4.47	GIWBOF02	2.05	JEVVIQ	2.81	NAMQIC	1.52
DUKJUP	3.03	GUVXAY	2.58	JEYVIT	2.43	NAYWIU	9.45
DUNLOO	4.40	HANCUV	3.35	KAGXIC	1.34	NEFRIA	2.68
EBOXIF	3.13	HAYJOI	1.80	KAMQOF	1.77	NENKIB	1.26
EBOXOL	3.13	HESKOG	2.42	KERSOQ	2.50	NENMUP	3.48
EDAVEK	2.39	HIFCUV	2.81	KIKGAN	2.28	NEQSOS	3.13
EDUYAF	1.82	HIQWEK	2.04	KIKJUK	1.98	NIFGEP	4.00
EFAJOM	1.62	HIRHIA	1.94	KOFFER	1.52	NIPDOH	1.78
EFAXIU	1.53	HIRYOX	2.14	KUSVAW01	1.88	NIQSOW	1.78
EFAXOA	1.04	HODQEX	2.73	KUYVOQ	1.61	NUNMAL	1.60
ENIPUO	2.86	HOFCAH	1.52	LANHOZ	2.43	NUPYIH	1.90
EROPUX	2.28	HOFJAP	2.75	LANJAN	2.17	NUQGIQ	1.55
ETUDED	1.69	HOFKAP	25.55	LANLET	2.42	NUQMOC	1.01
EVABAF	2.56	HOLHOG	1.18	LAPTUT	4.57	NURFIQ	2.25

Ref code	R1-Factor						
OBOBUE	5.44	QIRQAL	2.88	SOLWIA	3.32	VICXOV	2.19
OBOYOV	2.38	QOFJEB	2.93	SOYPUS	1.31	VIZZUB	1.99
OBUYUH	2.67	QQQAUD01	4.21	SUYDAS	1.36	VOJHEI	1.62
OCADIH	2.40	QUXPEF	7.11	SUZMUW	1.77	VUYMAE	8.76
OCAPEP	1.15	QUYGAT	2.30	TAKWIO	4.57	VUZTAM	6.67
OCEHUB	3.46	QUYSEJ	1.48	TAQQIM	2.75	WABFOV	1.22
OFEKAM	2.23	QUZBAP	3.48	TECHAL	5.26	WABJAL	2.22
OFEKOA	2.89	QUZBOD	2.63	TERPAI	3.04	WACNUL	3.73
OGELUI	3.20	QUZKIG	1.30	TEVMOX	3.33	WAWSET	7.55
OLOKAB	1.67	QUZSUA	1.48	TIBXUY	1.55	WENRUD	7.16
PAGFOV	5.57	QUZTAH	1.91	TICGIW	1.51	WIGZES	1.54
PAWDOI	1.38	QUZTIP	2.65	TIGNIH	1.69	WIHHIF	3.28
PAWZAQ	1.69	RAZZUO	5.78	TOBKOL	2.27	WIHJUT	2.30
PAXZUL	1.80	REBJOY	1.18	TOBMED	2.01	WINKEK	3.39
PAZCEZ	1.82	RIGTUX	2.57	TOTBIP	1.81	WINKIO	4.82
PELNUQ	4.02	RIGVAF	1.93	TUPNOI	3.54	WIZZOV	1.58
PELQIH	2.92	RIHGAR	1.74	TUPZIO	3.04	WOGXOG	11.38
PELQON	2.08	RIRWIZ	5.79	TUQHUI	8.04	WOJMAL	1.58
PEMFOD	2.54	RISMUC	3.06	UBABUX	2.05	WUZWOE	6.08
PILRUY	3.03	RITLIR	2.28	UGUMUE	2.36	XAKFOG	4.15
PODZEO	2.11	ROFYUH	1.90	ULEFAT	4.19	XALYAL	1.88
POMLEJ	2.76	ROLVEV	1.04	ULEPUX	1.12	XALYEP	3.81
PONYOH	3.21	ROMMUC	1.55	ULIKUW	1.83	XAZCUY	1.13
PUGJOR	2.61	RUJPAO	3.75	UNIZOH	2.97	XAZXOM	2.79
PUGWOE	1.50	SABBUU	4.42	UNOXIF	3.97	XECBIS	1.21
PUHNUC	2.50	SAFXAA	3.75	UNOZON	1.93	XECDAM	2.73
PUHVAQ	5.54	SAGRAV	4.85	UNUZIN	1.90	XENFIG	10.88
PUJFEG	1.88	SAPBAN	2.94	UREMOU	1.08	XEYVAZ	2.34
PUKKUC	1.66	SAPHOH	2.93	UREXIZ	1.61	XEYZAD	1.61
QABCEE	2.28	SECWOO	1.34	UXOHUM02	1.52	XIFPOS	1.57
QABCII	2.28	SEDGEP	4.62	UXOHUM	1.52	XISQUM	1.32
QAHVOM	3.15	SESQOX	3.29	UZUZUM	2.05	XOFKUA	1.97
QAJSOL	1.98	SILDAT	3.29	VABHEN	3.00	XOYYIU	3.15
QAJSUR	2.69	SIMKAB	2.46	VABWUS	3.18	YAFMID	4.27
QANYIO	1.34	SIMQIP	9.54	VACBAE	1.48	YAFRII	1.53
QAYTEQ	1.62	SIMTEO	1.16	VELXOA	3.40	YAFSUV	1.50
QEDHOY	2.66	SIMZEU	4.13	VENGEB	1.98	YAHFIY	3.86
QILFIC	1.34	SISWAT	4.42	VENKEF	2.66	YAHLEA	11.28

Ref code	R1-Factor
YAHYIR	1.92
YAHZUE	1.83
YAMSAH	2.11
YAVTUM	2.30
YAWQEU	1.65
YAXHAI	4.20
YAXNES	2.59
YEDXEL	1.86
YEDXIP	3.92
YEJYOB	1.62
YIFLEF	1.96
YIRSOI	1.86
YOTSIK	3.39
YUQKAX	13.34
ZANZUL	2.72
ZAPBEZ	3.48
ZAQDOM	4.24
ZAQLIO	1.83
ZAQRAM	1.40
ZAQSAN	3.88
ZIJXIB	1.99
ZIYSUX	1.69
ZIZWAI	24.98
ZIZWIQ	47.08
ZIZXAJ	27.72
ZIZXEN	7.35
ZUKQAZ	6.65

1.2 wm5234 structure

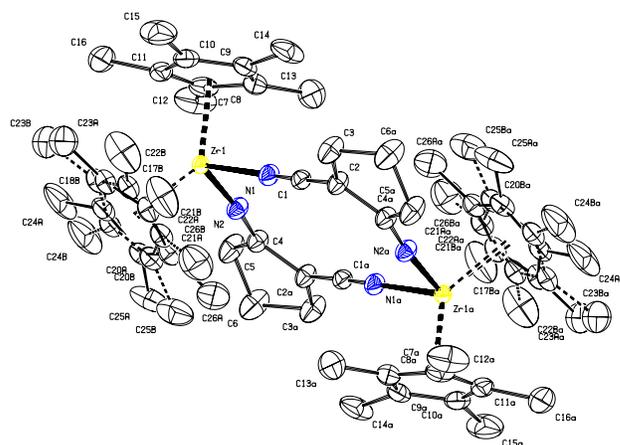


Figure S2: ORTEP plot of **wm5234** (hydrogen atoms omitted for clarity)

1.2.1 pentamethylcyclopentadienyl restraints using UPERP, UPLANE and ULIJ

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#LIST 16
REM === MINOR COMPONENT INNER RING ===
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UPERP 0.001 C(172) TO C(212) TO C(182)
UPERP 0.001 C(182) TO C(172) TO C(192)
UPERP 0.001 C(192) TO C(182) TO C(202)
UPERP 0.001 C(202) TO C(192) TO C(212)
UPERP 0.001 C(212) TO C(202) TO C(172)
UPLANE 0.001 C(172) TO C(212) TO C(182)
UPLANE 0.001 C(182) TO C(172) TO C(192)
UPLANE 0.001 C(192) TO C(182) TO C(202)
UPLANE 0.001 C(202) TO C(192) TO C(212)
UPLANE 0.001 C(212) TO C(202) TO C(172)
ULIJ 0.001 C(172) TO C(182) TO C(192),
CONT C(182) TO C(192) TO C(202),
CONT C(192) TO C(202) TO C(212),
CONT C(202) TO C(212) TO C(172),
CONT C(212) TO C(172) TO C(182)
REM === MINOR COMPONENT OUTER RING
UPERP 0.001 C(222) TO C(172)
UPERP 0.001 C(232) TO C(182)
UPERP 0.001 C(242) TO C(192)
UPERP 0.001 C(252) TO C(202)
UPERP 0.001 C(262) TO C(212)
UPLANE 0.001 C(222) TO C(172) TO C(182)
UPLANE 0.001 C(232) TO C(182) TO C(192)
UPLANE 0.001 C(242) TO C(192) TO C(202)
UPLANE 0.001 C(252) TO C(202) TO C(212)
UPLANE 0.001 C(262) TO C(212) TO C(172)
ULIJ 0.001 C(222) TO C(232) TO C(242),
CONT C(232) TO C(242) TO C(252) ,
CONT C(242) TO C(252) TO C(262),
CONT C(252) TO C(262) TO C(222),
CONT C(262) TO C(222) TO C(232)
REM #####
REM === MINOR COMPONENT INNER RING ===
UPERP 0.001 C(171) TO C(211) TO C(181)
UPERP 0.001 C(181) TO C(171) TO C(191)
UPERP 0.001 C(191) TO C(181) TO C(201)
UPERP 0.001 C(201) TO C(191) TO C(211)
UPERP 0.001 C(211) TO C(201) TO C(171)
UPLANE 0.001 C(171) TO C(211) TO C(181)
UPLANE 0.001 C(181) TO C(171) TO C(191)
UPLANE 0.001 C(191) TO C(181) TO C(201)
UPLANE 0.001 C(201) TO C(191) TO C(211)
UPLANE 0.001 C(211) TO C(201) TO C(171)
ULIJ 0.001 C(171) TO C(181) TO C(191),
CONT C(181) TO C(191) TO C(201),
CONT C(191) TO C(201) TO C(211),
CONT C(201) TO C(211) TO C(171),
CONT C(211) TO C(171) TO C(181)
REM === MINOR COMPONENT OUTER RING ===
UPERP 0.001 C(221) TO C(171)
UPERP 0.001 C(231) TO C(181)
UPERP 0.001 C(241) TO C(191)
UPERP 0.001 C(251) TO C(201)
UPERP 0.001 C(261) TO C(211)
UPLANE 0.001 C(221) TO C(171) TO C(181)
UPLANE 0.001 C(231) TO C(181) TO C(191)
UPLANE 0.001 C(241) TO C(191) TO C(201)
UPLANE 0.001 C(251) TO C(201) TO C(211)

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UPLANE 0.001 C(261) TO C(211) TO C(171)
ULIJ 0.001 C(221) TO C(231) TO C(241)
CONT C(231) TO C(241) TO C(251),
CONT C(241) TO C(251) TO C(261),
CONT C(251) TO C(261) TO C(221),
CONT C(261) TO C(221) TO C(231)
REM #####
REM === DISTANCES AND ANGLES RESTRAINTS ===
DISTANCE 0.0,.00200 = MEAN C(222) TO C(182),
CONT C(222) TO C(212) ,
CONT C(232) TO C(192) ,
CONT C(232) TO C(172) ,
CONT C(242) TO C(202) ,
CONT C(242) TO C(182) ,
CONT C(252) TO C(212) ,
CONT C(252) TO C(192) ,
CONT C(262) TO C(172) ,
CONT C(262) TO C(202)
SAME 0.01, 0.1
CONT C(171) C(181) C(191) C(201) C(211) C(221) C(231) C(241) C(251) C(261) AND
CONT C(172) C(182) C(192) C(202) C(212) C(222) C(232) C(242) C(252) C(262)
PLANAR 0.0010000 C(171) C(181) C(191) C(201) C(211)
CONT C(221) C(231) C(241) C(251) C(261)
CONT C(172) C(182) C(192) C(202) C(212)
CONT C(222) C(232) C(242) C(252) C(262)
DISTANCE 0.0, 0.002 = MEAN C(221) TO C(231), C(231) TO C(241),
CONT C(241) TO C(251),
CONT C(251) TO C(261), C(261) TO C(221),
CONT C(222) TO C(232), C(232) TO C(242), C(242) TO C(252),
CONT C(252) TO C(262), C(262) TO C(222)
END
# Remove space after hash to activate next line
# USE LAST

```

1.3 pentamethylcyclopentadienyl restraints using UTLS

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#LIST      16
UTLS 0.0005 C(222) C(232) C(242) C(252) C(262)
CONT C(172) C(182) C(192) C(202) C(212)
DISTANCE 0.0,.00200 = MEAN C(222) TO C(182),
CONT C(222) TO C(212) ,
CONT C(232) TO C(192) ,
CONT C(232) TO C(172) ,
CONT C(242) TO C(202) ,
CONT C(242) TO C(182) ,
CONT C(252) TO C(212) ,
CONT C(252) TO C(192) ,
CONT C(262) TO C(172) ,
CONT C(262) TO C(202)
SAME 0.01, 0.1
CONT C(171) C(181) C(191) C(201) C(211) C(221) C(231) C(241) C(251) C(261) AND
CONT C(172) C(182) C(192) C(202) C(212) C(222) C(232) C(242) C(252) C(262)
PLANAR 0.0010000 C(171) C(181) C(191) C(201) C(211)
CONT C(221) C(231) C(241) C(251) C(261)
CONT C(172) C(182) C(192) C(202) C(212)
CONT C(222) C(232) C(242) C(252) C(262)
DISTANCE 0.0, 0.002 = MEAN C(221) TO C(231), C(231) TO C(241),

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CONT C(241) TO C(251),
CONT C(251) TO C(261), C(261) TO C(221)
CONT C(222) TO C(232), C(232) TO C(242), C(242) TO C(252),
CONT C(252) TO C(262), C(262) TO C(222)
END
# Remove space after hash to activate next line
# USE LAST

```

1.3.1 pentamethylcyclopentadienyl CCDC search

List of the hits from the search of the CCDC database with the corresponding R1-Factor (%) of the fit of a TLS model on the pentamethylcyclopentadienyl ligand.

Ref code	R1-Factor	Ref code	R1-Factor	Ref code	R1-Factor
ACEWEK	8.41	JEWBOD	8.96	SILLEF	14.68
ACUGIQ	16.49	KERMUQ	7.94	SILLEF	6.66
AFECAQ	5.12	KERMUQ	9.56	SUFCUT	4.71
AFUXEG	4.87	KIWHUU	11.61	SUFCUT	5.19
AFUXEG	5.15	KIWHUU	12.29	SUFCUT	5.35
ASUFUP	9.61	KIWNEK	11.91	TIBCAJ	19.81
ASUKOO	11.72	LOYGAJ	6.57	TIBPOK	10.87
ASUKOO	13.26	LOYGAJ	6.57	TIBPOK	4.17
ATUQOV	6.19	LOYGAJ	8.42	TIBVIK	4.67
AWOREK	4.74	LOYGAJ	8.78	TIBVIK	6.17
AWOREK	5.79	METTAH	8.18	WIHLEG	10.61
AWOVOY	2.62	METTAH	9.23	WIHLEG	6.39
AWOXEQ	5.82	MEWDUP	3.67	WIHLEG	8.59
CASPAO	7.20	MOCRAX	4.64	WIHLEG	9.13
CERLUH	8.16	MUVWEF	3.92	WIHLIJ	5.19
CICFEA	6.88	MUVWEF	3.92	WIHLIJ	5.36
DEGNAF	7.39	NAKWIH	3.76	WIHLIJ	5.83
DELTOE	3.40	NAKWIH	6.45	WIHLIJ	6.05
DELTOE	4.32	NIKTEI	3.72	WIHNIL	10.02
DUHQIH	4.69	NIMJAW	5.61	WIHNIL	10.54
DUHQIH	5.62	NOQLEL	1.68	WOZZAM	4.25
EDULOF	6.69	OPEFAS	3.18	WOZZEQ	5.18
ERESUQ	8.52	PEGJAN	4.25	XAKNII	13.98
ETUGIK	6.46	PEGJER	13.60	XAPSOX	6.94
FOBWID	5.66	POFDIY	7.81	XECSIJ	3.74
FOWJUX	3.59	POFDIY	8.94	XIYLEY	5.22
GEPKIW	10.68	POSTAU	12.22	XIYLEY	8.94
HIVDIA	4.45	QUBTUE	6.49	YIDVAJ	12.47
HUYVII	4.76	QUCHEC	15.62	YIDVAJ	16.84
ICAGUO	3.72	REZKIR	4.88	YIDZOB	2.58
IDIMAL	6.46	REZKIR	5.36	YOZKEF	7.62
ISUQUK	4.04	SILLEF	11.45		
JERTIJ02	6.91	SILLEF	12.67		