# Solid Solution of Two Diastereomers of [3a(*R*,*S*),7a(*R*,*S*)]-3-[(1'*R*)-1-phenylethyl]hexahydro-1,3-benzothiazol-2(3H)-iminium chloride

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**Table 1S.** List of crystal structures forming solid solution of two diastereomers.

| **REFCODE** | **Space group** | **Formula** | **References** |
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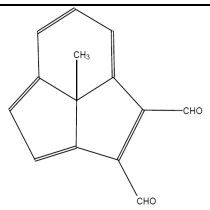
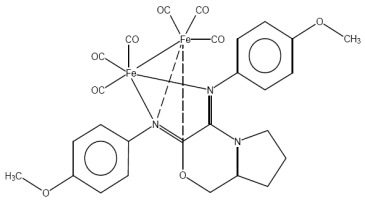
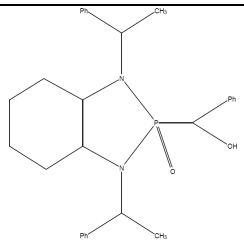
| CIKRET | $P2_1/n$ |  $C_{14}H_{10}O_2$ | R. McCague, C.J. Moody, C.W. Rees, D.J. Williams (1984) *J. Chem. Soc. Perkin Trans.1*, 909–914. |
| CUQLEF | $P$–1 |  $C_{27}H_{23}Fe_2N_3O_9$ | W. Imhof, A. Gobel, R. Beckert, T. Billert, H. Gorls (1999) *J. Organomet. Chem.*, 590, 104–114. |
| EVORUC | $P2_1$ |  $C_{29}H_{35}N_2O_2P_1$ | G.E. Moreno, L. Quintero, S. Bernes, C. Anaya de Parrodi (2004) *Acta Cryst. C*, 60, o411–o414. |

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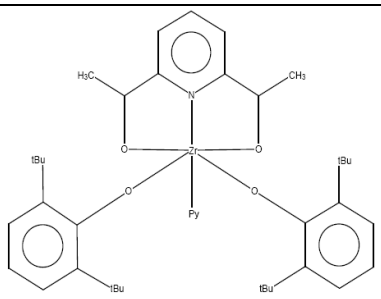
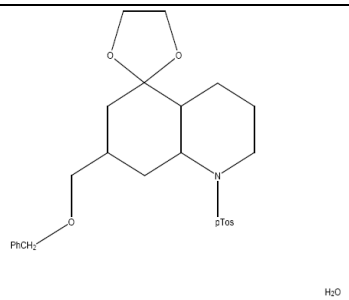
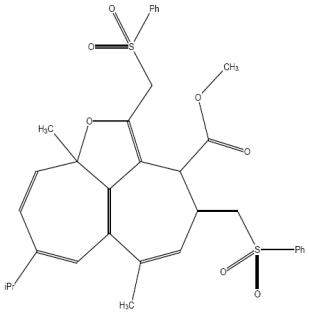
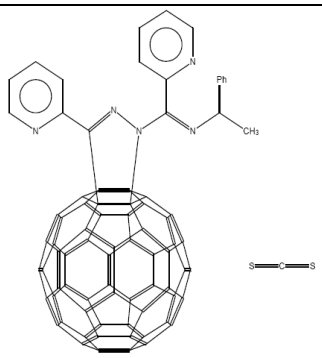
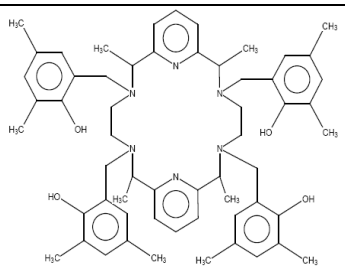
|---|---|---|---|
| FARLIT | $P2_1$ |  $C_{42}H_{58}N_2O_4Zr_1$ | 1. P.E. Fanwick, L.M. Kobriger, A.K. McMullen, I.P. Rothwell (1986) *J. Am. Chem. Soc.*, 108, 8095–8097. |
| IYIVER | *C*2/c |  $C_{26}H_{33}N_1O_5S_1$, $H_2O_1$ | D.F. Taber, P.V. Joshi, K. Kanai (2004) *J. Org. Chem.*, 69, 2268–2271. |
| NEBYAU | *P*–1 |  $C_{34}H_{38}O_7S_2$ | K. Abou-Hadeed, H.-J. Hansen (1997) *Helv. Chim. Acta*, 80, 2535–2564. |
| NEPHAR | $P2_12_12_1$ |  $C_{80}H_{19}N_5$, $2(C_1S_2)$ | G.P. Miller, M.C. Tetreau, M.M. Olmstead, P.A. Lord, A.L. Balch (2001) *Chem. Commun.*, 1758–1759. |
| PIDZUX | *P*–1 |  $C_{58}H_{74}N_6O_4$ | S.W.A. Bligh, N. Choi, W.J. Cummins, E.G. Evagorou, J.D. Kelly, M. McPartlin (1993) *J. Chem. Soc. Dalton Trans.*, 3829–3831. |

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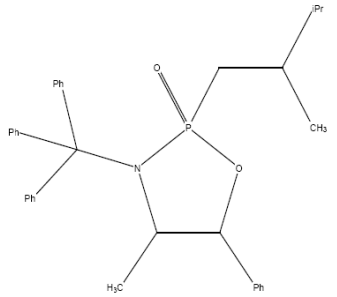
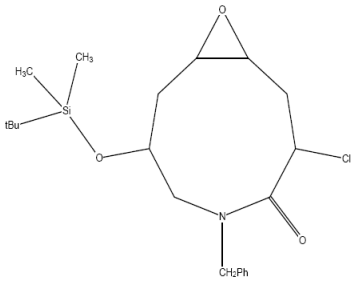
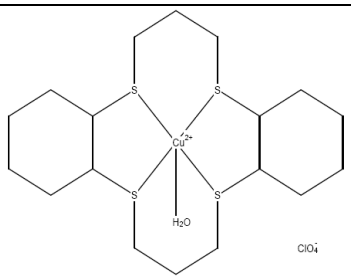
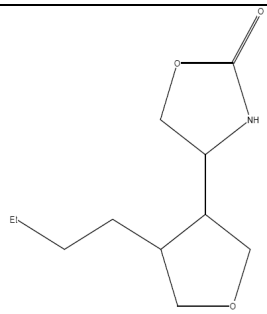
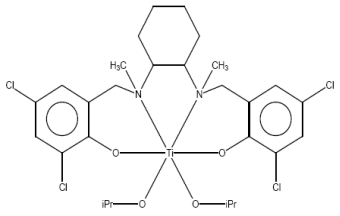
| QAZPAI | $P6_1$ |  <br>$C_{34}H_{38}N_1O_2P_1$ | I. Forristal, J. Lowman, K. Afarinkia, J.W. Steed (2001) CrystEngComm, 3, 53–56. |
| QENVAG | $P2_12_12_1$ |  <br>$C_{21}H_{32}Cl_1N_1O_3Si_1$ | A. Sudau, W. Munch, J.W. Bats, U. Nubbemeyer (2001) *Chem.-Eur.J.*, 7, 611–621. |
| QOXJUI | $P2_1/n$ |  <br>$C_{18}H_{34}Cu_1O_1S_4^{2+}$, $2(Cl_1O_4^{1-})$ | Q. Yu, C.A. Salhi, E.A. Ambundo, M.J. Heeg, L.A. Ochrymowycz, D.B. Rorabacher (2001) *J.Am.Chem.Soc.*, 123, 5720–5729. |
| QUFJEG | $P-1$ |  <br>$C_{11}H_{19}N_1O_3$ | T. Bach, B. Schlummer, K. Harms (2001) *Chem.-Eur. J.*, 7, 2581–2594. |
| RAQLEB | $P4_32_12$ |  <br>$C_{28}H_{38}Cl_4N_2O_4Ti_1$ | A. Yeori, S. Groysman, I. Goldberg, M. Kol (2005) *Inorg. Chem.*, 4, 466–4468. |

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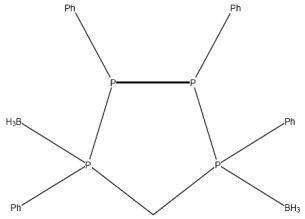
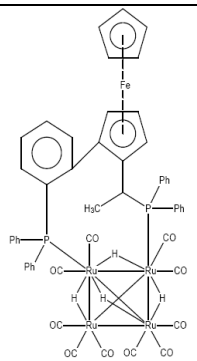
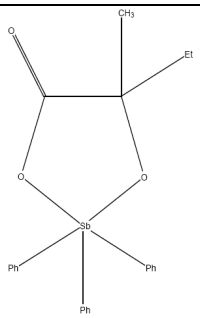
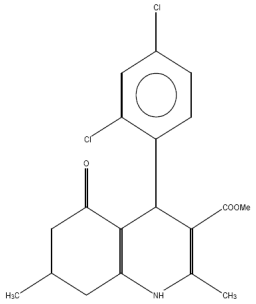
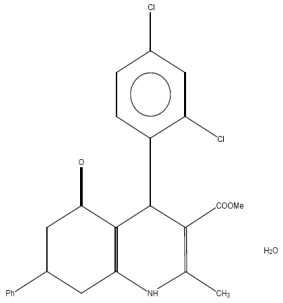
| SEDPAT | *P*–1 |  <br>$C_{25}H_{28}B_2P_4$ | R. Wolf, M. Finger, C. Limburg, A.C. Willis, S.B. Wild, E. Hey-Hawkins (2006) *J. Chem. Soc. Dalton Trans.*, 831–837. |
| SIKLAA | $P2_12_12_1$ |  <br>$C_{52}H_{40}Fe_1O_{10}P_2Ru_4$ | V. Moberg, M. Haukka, I.O. Koshevoy, R. Ortiz, E. Nordlander (2007) *Organometallics*, 26, 4090–4093. |
| UBIYUZ | $P2_1/c$ |  <br>$C_{23}H_{23}O_3Sb_1$ | H. Barucki, S.J. Coles, J.F. Costello, M.B. Hursthouse (2001) *J. Organomet. Chem.*, 622, 265–273. |
| UCOLOO | $P2_1/n$ |  <br>$C_{19}H_{19}Cl_2N_1O_3$ | A. Linden, M.G. Gunduz, R. Simsek, C. Safak (2006) *Acta Cryst.* C62, o227–o230. |
| UCOLUU | *P*–1 |  <br>$C_{24}H_{21}Cl_2N_1O_3, H_2O_1$ | A. Linden, M.G. Gunduz, R. Simsek, C. Safak (2006) *Acta Cryst.* C62, o227–o230. |

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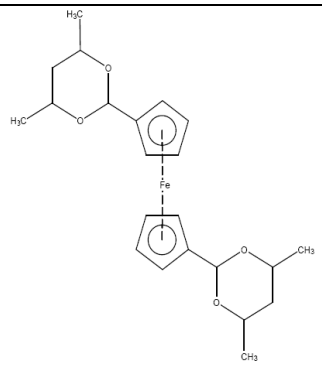
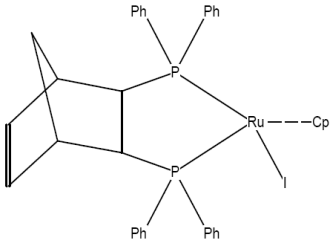
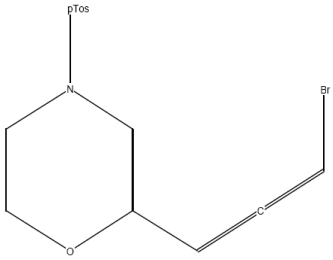
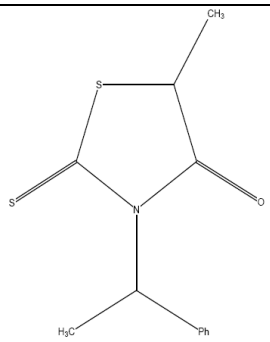
| UJOYOH | $P2_12_12_1$ |   $C_{22}H_{30}Fe_1O_4$ | C.G. Hartinger, A.A. Nazarov, V. Chevchenko, V.B. Arion, M. Galanski, B.K. Keppler (2003) *Dalton Trans.*, 3098–3102. |
| VIMBEY | $P2_12_12_1$ |   $C_{36}H_{33}I_1P_2Ru_1$ | H. Nishiyama, H. Brunner, P.G. Jones (1991) *J. Organomet. Chem.*, 405, 247–255. |
| VIXLIY | $P2_1/c$ |   $C_{14}H_{16}Br_1N_1O_3S_1$ | D.C. Braddock, R. Bhuva, Y. Perez-Fuertes, R. Pouwer, C.A. Roberts, A. Ruggiero, E.S.E. Stokes, A.J.P. White (2008) *Chem. Commun.*, 1419–1429. |
| WOMBUV | $P2_1$ |   $C_{12}H_{13}N_1O_1S_2$ | K. Rang, Fen-Ling Liao, J. Sandstrom, Sue-Lein Wang (1997) *Chirality*, 9, 568–577. |

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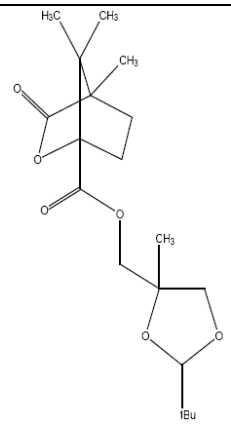
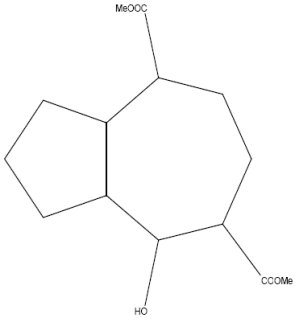
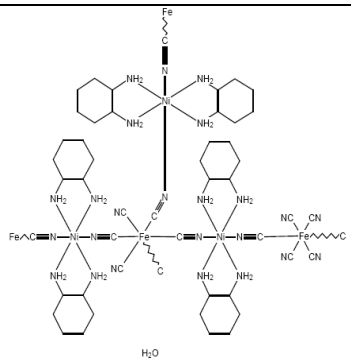
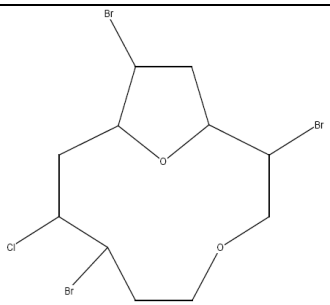
| XATLUZ | $P2_1$ |  <br>$C_{19}H_{30}O_6$ | C. Wattenbach, S. Rabe, U. Muller, H. Frauenrath (2000) *Z. Kristallogr.-New Cryst.Struct.*, 215, 511–512. |
| XOLPUK | *R*–3 |  <br>$C_{14}H_{22}O_5$ | I. Reboul, T. Boddaert, Y. Coquerel, J. Rodriguez (2008) *Eur. J .Org. Chem.*, 5379–5382. |
| XOPGOY | *P*–1 |  <br>$(C_{48}H_{84}Fe_2N_{24}Ni_3)n, 2n(H_2O_1)$ | F. Bellouard, M. Clemente-Leon, E. Coronado, J.R. Galan-Mascaros, C.J. Gomez-Garcia, F. Romero, K.R. Dunbar (2002) *Eur. J. Inorg. Chem*., 1603–1606. |
| XOTPAY | $P2_12_12_1$ |  <br>$C_{11}H_{16}Br_3Cl_1O_2$ | D.C. Braddock, D.S. Millan, Y. Perez-Fuertes, R.H. Pouwer, R.N. Sheppard, S. Solanki, A.J.P. White (2009) *J. Org. Chem.*, 74, 1835–1841. |

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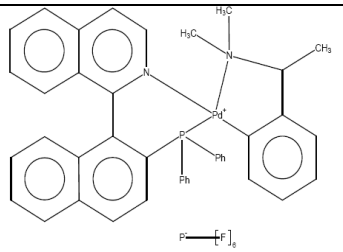
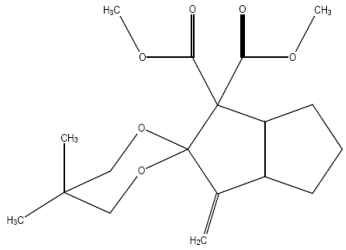
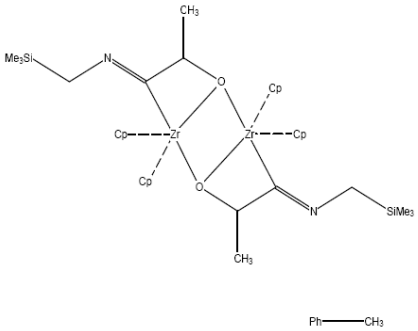
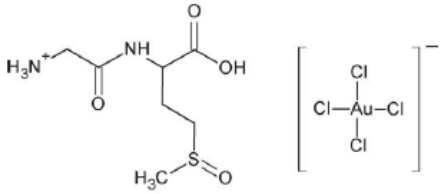
| YIMXOH | *P*–1 |  $C_{41}H_{36}N_2P_1Pd_1^{1+}$, $F_6P_1^{1-}$ | N.W. Alcock, D.I. Hulmes, J.M. Brown (1995) *Chem. Commun.*, 395–397. |
| YUHVAY | *P*–1 |  $C_{18}H_{26}O_6$ | T. Yamada, H. Uekusa, Y. Ohashi, S. Yamago, X.Q. Wang, E. Nakamura (1995) *Acta Cryst.* C, 51, 1137–1139. |
| ZEWTOK | *P*–1 |  $C_{34}H_{50}N_2O_2Si_2Zr_2$, $C_7H_8$ | S. Schmuck, G. Erker, S. Kotila (1995) *J. Organomet. Chem.*, 502, 75–86. |
| | *P*–1 |  $C_7H_{15}N_2O_4S_1^{1+}$, $Au_1Cl_4^{1-}$ | U. Rychlewska, B. Warzajtis, B.D. Glisic, S. Rajkovic, M. Djuran (2010) *Acta Cryst.* C66, m51–m54. |