

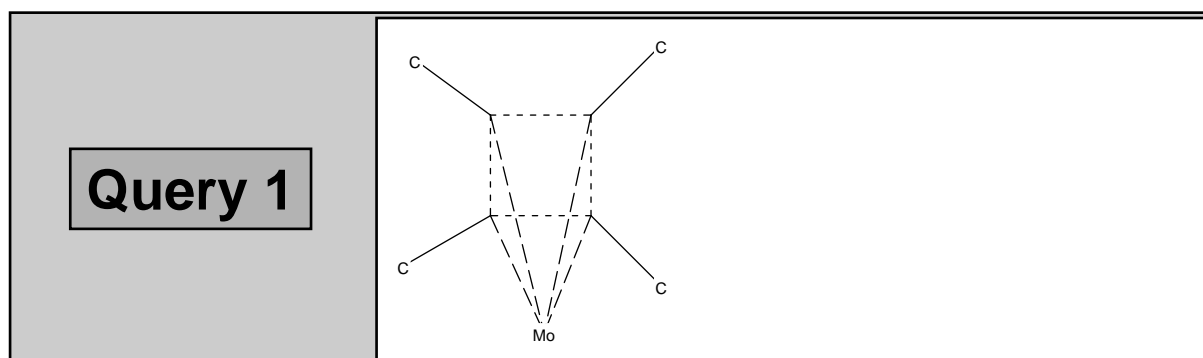
# Search Overview

**Search:** search1  
**Date/Time done:** Tue Feb 1 11:03:45 2005  
**Database(s):** CSD version 5.25 (November 2003)  
**Restriction Info:** No refcode restrictions applied  
**Filters:** Only Organometallic  
**Percentage Completed:** 100%  
**Number of Hits:** 10

*Single query used. Search found structures that:*

match

**Query 1**



# Search: search1 (Tue Feb 1 11:03:45 2005): Hits 1-4

## COXVIU

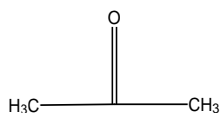
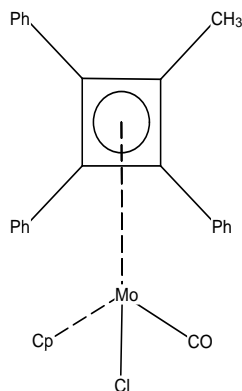
**Reference:** R.P.Hughes, J.W.Reisch, A.L.Rheingold (1984) *Organometallics*, **3**,1761

**Formula:** C<sub>29</sub> H<sub>23</sub> Cl<sub>1</sub> Mo<sub>1</sub> O<sub>1</sub> C<sub>3</sub> H<sub>6</sub> O<sub>1</sub>

**Compound Name:** Carbonyl-chloro-(η<sup>5</sup>-cyclopentadienyl)-(η<sup>4</sup>-1-methyl-2,3,4-trimethylcyclobutadiene)-molybdenum acetone solvate

**Space Group:** P-1 **Cell:** a 11.041(3) b 14.556(4) c 16.969(5)  
**Space Group No.:** 2 **(Å, °)** α 103.29(2) β 92.73(2) γ 107.64(2)

**R-Factor (%):** 5.23 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.527



## GICGUU

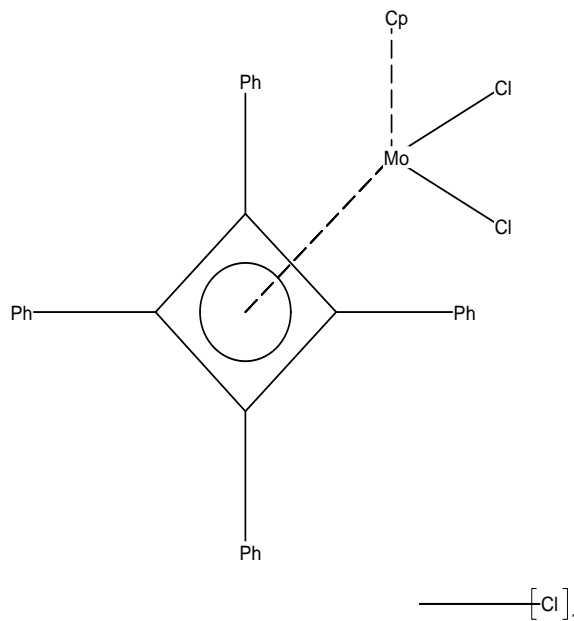
**Reference:** W.Hirpo, M.D.Curtis (1988) *J.Am.Chem.Soc.*, **110**,5218

**Formula:** C<sub>33</sub> H<sub>25</sub> Cl<sub>2</sub> Mo<sub>1</sub> C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>

**Compound Name:** (η<sup>4</sup>-Tetraphenylcyclobutadiene)-(η<sup>5</sup>-cyclopentadienyl)-dichloro-molybdenum dichloromethane solvate

**Space Group:** Pbc<sub>a</sub> **Cell:** a 27.118(39) b 11.420(12) c 19.322(15)  
**Space Group No.:** 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 5.70 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.495



## GICGUU10

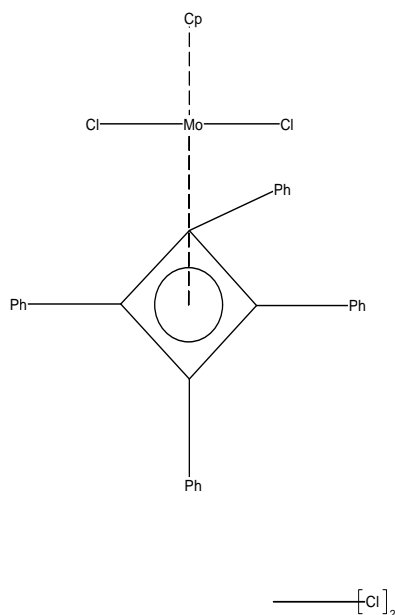
**Reference:** O.J.Curnow, W.Hirpo, W.M.Butler, M.D.Curtis (1993) *Organometallics*, **12**,4479

**Formula:** C<sub>33</sub> H<sub>25</sub> Cl<sub>2</sub> Mo<sub>1</sub> C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>

**Compound Name:** (η<sup>5</sup>-Cyclopentadienyl)-(η<sup>4</sup>-tetraphenylcyclobutadiene)-dichloro-molybdenum dichloromethane solvate

**Space Group:** Pbc<sub>a</sub> **Cell:** a 27.118(39) b 11.420(12) c 19.322(15)  
**Space Group No.:** 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 5.70 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.495



## GIQTIJ

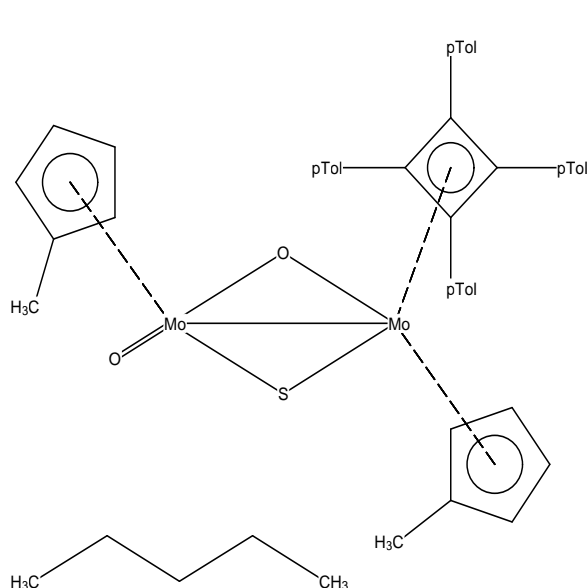
**Reference:** H.Adams, L.J.Gill, M.J.Morris (1998) *J.Chem.Soc.,Dalton Trans.*, 2451

**Formula:** C<sub>44</sub> H<sub>42</sub> Mo<sub>2</sub> O<sub>2</sub> S<sub>1</sub> 0.5(C<sub>5</sub> H<sub>12</sub>)

**Compound Name:** (μ<sub>2</sub>-Oxo)-(μ<sub>2</sub>-sulfido)-(η<sup>4</sup>-tetra-p-tolylcyclobutadiene)-bis(η<sup>5</sup>-methylcyclopentadienyl)-oxo-di-molybdenum n-pentane solvate

**Space Group:** P-1 **Cell:** a 10.955(3) b 11.906(2) c 16.280(2)  
**Space Group No.:** 2 **(Å, °)** α 85.66(1) β 80.06(2) γ 77.42(2)

**R-Factor (%):** 6.34 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.405



# Search: search1 (Tue Feb 1 11:03:45 2005): Hits 5-8

## LUJZOF

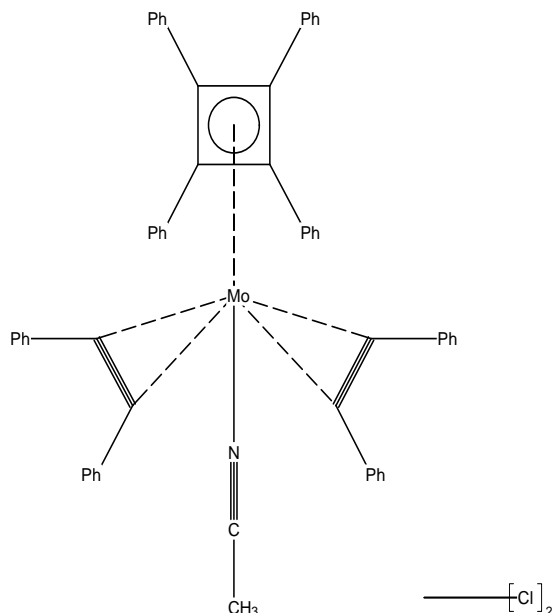
**Reference:** Su-Chin Chang, Wen-Yann Yeh, Gene-Hsiang Lee, Shie-Ming Peng (2002) *J.Chin.Chem.Soc.(Taipei)* **49**,325

**Formula:** C<sub>58</sub> H<sub>43</sub> Mo<sub>1</sub> N<sub>1</sub> C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>

**Compound Name:** (η<sup>4</sup>-1,2,3,4-Tetraphenylcyclobutadiene)-bis(η<sup>2</sup>-1,2-diphenylacetylene)-(acetonitrile)-molybdenum dichloromethane solvate

**Space Group:** P-1 **Cell:** a 12.345(0) b 12.880(0) c 16.472(0)  
**Space Group No.:** 2 **(Å,°)** α 76.67(0) β 84.32(0) γ 75.17(0)

**R-Factor (%):** 6.53 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.261



## LUJZUL

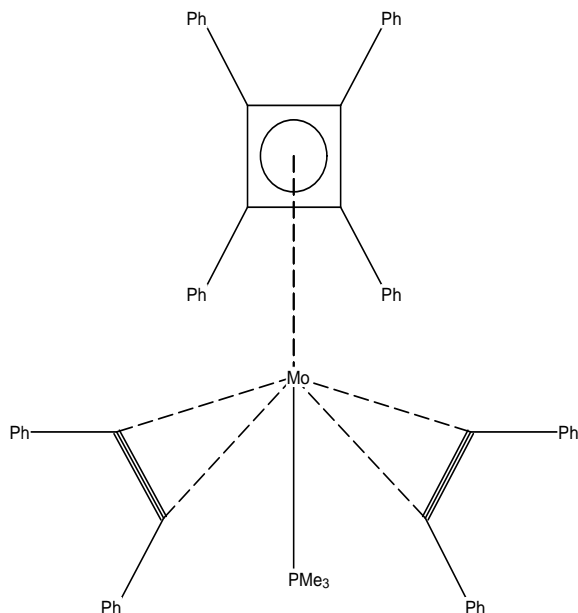
**Reference:** Su-Chin Chang, Wen-Yann Yeh, Gene-Hsiang Lee, Shie-Ming Peng (2002) *J.Chin.Chem.Soc.(Taipei)* **49**,325

**Formula:** C<sub>59</sub> H<sub>49</sub> Mo<sub>1</sub> P<sub>1</sub>

**Compound Name:** (η<sup>4</sup>-1,2,3,4-Tetraphenylcyclobutadiene)-bis(η<sup>2</sup>-1,2-diphenylacetylene)-(trimethylphosphine)-molybdenum

**Space Group:** Pbcu **Cell:** a 18.361(0) b 18.696(0) c 26.265(0)  
**Space Group No.:** 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 3.12 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.304



## LUKBAU

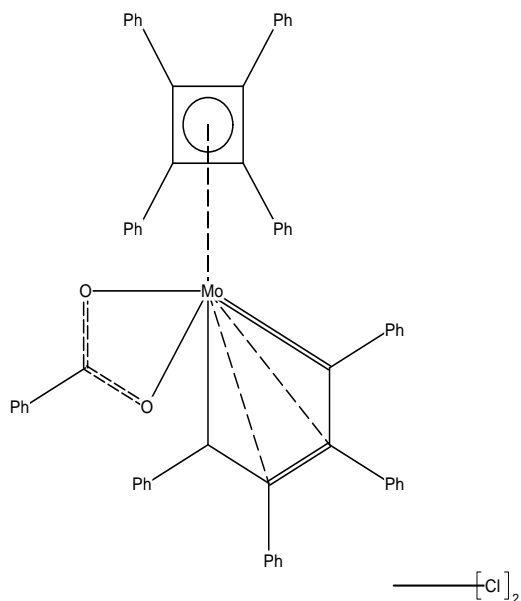
**Reference:** Su-Chin Chang, Wen-Yann Yeh, Gene-Hsiang Lee, Shie-Ming Peng (2002) *J.Chin.Chem.Soc.(Taipei)* **49**,325

**Formula:** C<sub>63</sub> H<sub>46</sub> Mo<sub>1</sub> O<sub>2</sub> C<sub>1</sub> H<sub>2</sub> Cl<sub>2</sub>

**Compound Name:** (η<sup>4</sup>-1,2,3,4-Tetraphenylcyclobutadiene)-(benzoato-O,O')-(η<sup>2</sup>-1,2,3,4-tetraphenylbut-2-en-1-yliden-4-yl)-molybdenum dichloromethane solvate

**Space Group:** P-1 **Cell:** a 12.454(0) b 13.442(0) c 16.493(0)  
**Space Group No.:** 2 **(Å,°)** α 84.65(0) β 69.79(0) γ 73.09(0)

**R-Factor (%):** 4.02 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.361



## PABPMO

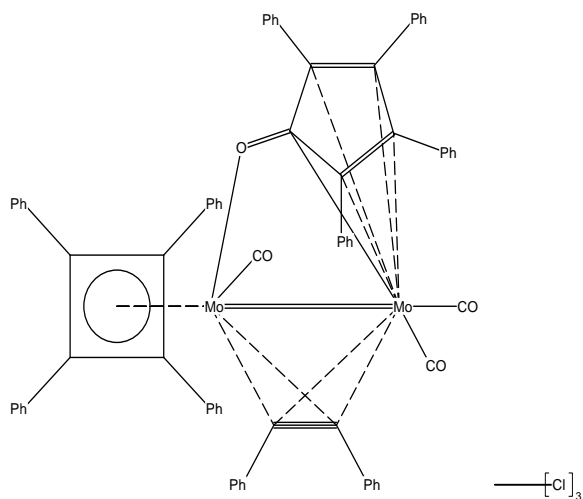
**Reference:** J.A.Potenza, R.J.Johnson, R.Chirico, A.Efraty (1977) *Inorg.Chem.* **16**,2354

**Formula:** C<sub>74</sub> H<sub>50</sub> Mo<sub>2</sub> O<sub>4</sub>.0.4(C<sub>1</sub> H<sub>1</sub> Cl<sub>3</sub>)

**Compound Name:** (Carbonyl-(η<sup>4</sup>-tetraphenylcyclobutadiene)molybdenum)-(μ<sub>2</sub>-diphenylacetylene)-(dicarbonyl-(η<sup>4</sup>-tetraphenylcyclopentadienone)-molybdenum) chloroform solvate

**Space Group:** P21/a **Cell:** a 23.960(20) b 22.140(30) c 12.490(20)  
**Space Group No.:** 14 **(Å,°)** α 90.00 β 110.24(1) γ 90.00

**R-Factor (%):** 11.10 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.328



# Search: search1 (Tue Feb 1 11:03:45 2005): Hits 9-10

## PCBMOC10

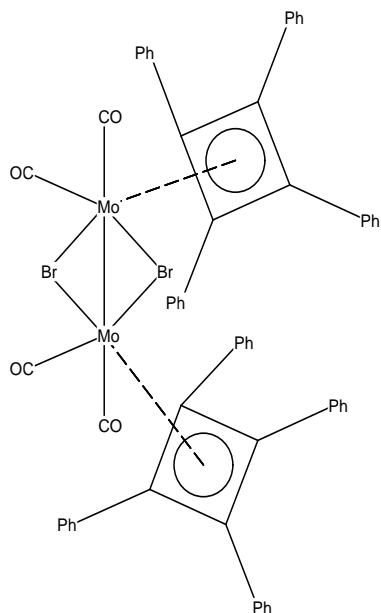
**Reference:** M.Mathew, G.J.Palenik (1973) *J.Organomet.Chem.* ,**61**, 301

**Formula:** C<sub>60</sub> H<sub>40</sub> Br<sub>2</sub> Mo<sub>2</sub> O<sub>4</sub>

**Compound Name:** Di- $\mu_2$ -bromo-bis( $\pi$ -tetraphenylcyclobutadiene)-tetracarbonyl-dimolybdenum

**Space Group:** P-1      **Cell:**    *a* 11.306(4)    *b* 13.681(4)    *c* 17.561(4)  
**Space Group No.:** 2      ( $\text{\AA}$ , $^\circ$ )     $\alpha$  105.58(1)     $\beta$  91.14(2)     $\gamma$  108.50(5)

**R-Factor (%):** 5.60      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.585



## TPCBMO

**Reference:** A.Efraty, J.A.Potenza, L.Zyontz, J.Daily, M.H.A.Huang, B.Toby (1978) *J.Organomet.Chem.* ,**145**,315

**Formula:** C<sub>58</sub> H<sub>40</sub> Mo<sub>1</sub> O<sub>2</sub>

**Compound Name:** Dicarbonyl-bis(tetraphenylcyclobutadiene) molybdenum

**Space Group:** P21/n      **Cell:**    *a* 20.150(20)    *b* 18.820(30)    *c* 11.030(10)  
**Space Group No.:** 14      ( $\text{\AA}$ , $^\circ$ )     $\alpha$  90.00     $\beta$  91.59(6)     $\gamma$  90.00

**R-Factor (%):** 4.10      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.374

