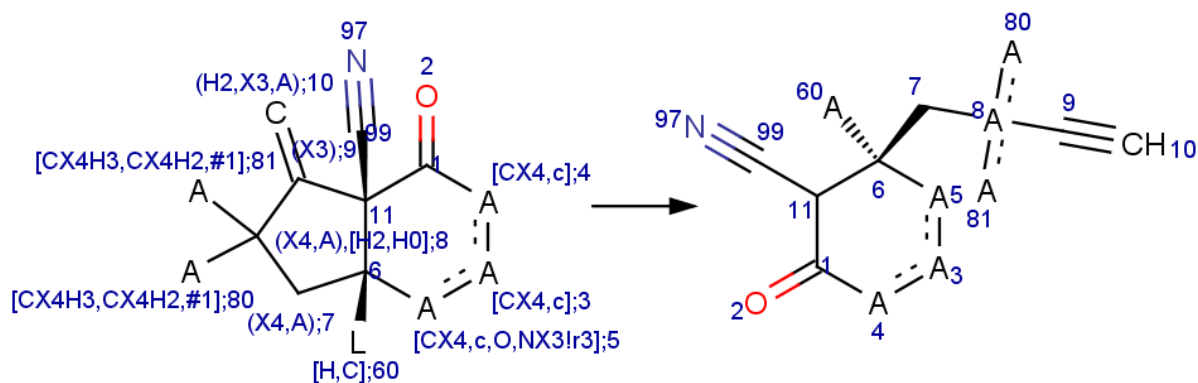




id : 31006881,

name : "Lewis acid-catalyzed conia-ene annulation",

reaction SMARTS :

```
"[#1,#6:60][C@@:6]12[CX4:7][CX4H2,CX4H0:8]([CX4H3,CX4H2,#1:80])([CX4H3,CX4H2,#1:81])[CX3:9](=[CX3H2:10])[C@@:11]1([C:1](=[O:2])[CX4,c:4][CX4,c:3][CX4,c,O,NX3lr3:5])[C:99]#[N:97]>>[C:10]#[C:9]#[*:8]([*:80])([*:81])[C:7][C@@:6]1([*:60])[*:5][*:3][*:4][C:1](=[O:2])[C:11]1[C:99]#[N:97]",
```

references: "10.1039/C1OB05591G",

typical reaction conditions : "ZnI2. Toluene. Reflux",

diastereoselective : false,

protections : [

"[#6][CH2][OH]", "[#6][SX2H]", "[nH]", "[#6]C([OH])=O", "[OH][CX4][CX4][OH]", "[c][OH]", "[OH][c][c][OH]", "[CX4,c][NH2]", "[#6]C([#6])=O", "[#6][CH]=O", "[OH][CX4]C[CX4][OH]", "[#6][CH]([#6])[OH]", "[CX4,c][NH][CX4,c]", "[#6]C([#6])([#6])[OH]"],

incompatibilities : [

"[CX4!H0][c]1[n][n][n][n]1", "[CX4,c][NX3][NH2]", "[C]=[CX3][CX4]O[S](=O)(=O)[#6]", "[#6,SiX4]O[CX4][NX3]", "[#6]C(=O)[NH]C([#6])=O", "[#6][BX3]([O,#6])[O,#6]", "[#6,N,O,P,S][NH]S([#6])(=O)=O", "ClC=N", "[#6][CR0](=[O])[O]C([#6])([#6])[#6]", "[#6][SX2][SX2][#6]", "[O,N,P,S,n,Si,Se]C(=O)[C](C#N)=C", "[#6]C(=S)[OH]", "[CX4H1]S(=O)(=O)[#6]", "[#6]S(=O)[Cl,Br,I]", "[CX4]1[CX4]2[CX4][CX4]12", "[#6]O[N+](O)=O", "[#6]C(=O)[NX3][NX3H2]", "[NX3!H0]=[CX3]([O,SX2])[NX3]", "n[CX4]O[#6,SiX4]", "[NX3][C]=[C]", "[Sn]C#C[*]", "[CX4]1[SX2][CX4]1", "[CX3]=[CX3][Sn]", "[CX4]1[CX3]=[CX3]1", "c[O][S](=O)(=O)[#6]", "[CX4,c][SX2][CX4][SX2][CX4,c]", "[#6]C(=O)N([OH0])[#6]", "N#C[CX4!H0]P=[O,SX1]", "[#6]=[N+]=[N-]", "[#6]O[SX3](=O)[#6]", "[CX3]=[CX3]S(=O)(=O)[O,#6]", "[#6][SeX2][#6]", "[CX3]=[CX3][O][C]=O", "[OH][CX4][NX3]",

"[CX3]([#6,#1])([#6,#1])=[NX2][#6]", "[#6][Mg][*]", "[#6]C(=O)[Cl,Br,I]", "N#C[CX4!H0]C#N",
 "N#C[C](C#N)=[C]", "S(=O)[CX4!H0]C#N", "[CX3]=[CX2]=O", "[CX4!H0]P=[O,SX1]",
 "[Sn][CX3]=[CX2]=[CX3]", "[CX3]=[CX3][O][S](=O)(=O)[#6]", "[C]#[C][CX4]O[S](=O)(=O)[#6]",
 "c[N+]#[N]", "[CX3]=[CX3][CX4]OP(=O)", "[OH][CX4][O]", "[CX4!H0][N+](=[O-])=O",
 "[#6][Zn][*]", "[#6]C(=O)[SX2H0]", "[#6][NX3][OH]", "[#6]C(=S)[OH0]",
 "[O,N,P,S,n,Si,Se]C(=O)[CX4!H0]C(=O)[O,N,P,S,n,Si,Se]", "[CX4H2][Cl,Br,I]",
 "[#6,O,N,P,S,Se,B]C(=[O,SX1])C#N", "[O-][N+](=O)[CX3]=[CX3]", "[#6][N+]#[C-]",
 "[CX4H1][Cl,Br,I]", "[c]1[n][n][n][n]1[CX4!H0]", "[#6][B-](F)(F)F", "[#6]C(=[SX1])[#6]",
 "[#6]C(=[S])[NH][#6]", "[CX3]=[CX3][OH]", "[CX3]=[CX3][CX4]OC(=O)[#6,N,O,S,Se]",
 "N#C[C]=[C]C#N", "[O,N,P,S,n,Si,Se]C(=O)[C](C(=O)[O,N,P,S,n,Si,Se])=[C]",
 "[#6]C(=O)ON1C(=O)[#6][#6]C1=O", "[CX3]=[CX2]=[CX3]P(=O)([O,#6])[O,#6]",
 "[CX3]=[CX3][CX4!H0]C(=O)[O,N,S,P,Se]", "[SiX4][CX3]=[CX2]=[CX3]",
 "[CX4H0][O][S](=O)(=O)[#6]", "[OH0][CX3](=O)[CX3]=[CX2]=[CX3]", "[#6]OO[#6]",
 "[Sn][CX4][CX3]=[CX3]", "[SiX4,SX2,Se,P][Cl,Br,I]", "[CX4][O][CX4][O][CX4]",
 "[CX4]1O[CX4]1", "n[CX4][OH]", "[CX4H2]S(=O)(=O)[#6]", "[#6][CH]=[SX1]",
 "[CX4]1[NX3][CX4]1", "[#6][BX3]([OH])[OH]", "[#6]C(=O)[NX3][OH]",
 "[CX3]=[CX2]=[CX3]S(=O)(=O)[O,#6]", "[CX3]=[CX2]=[CX3,CX2]",
 "[CX3]=[CX3]P(=O)([O,#6])[O,#6]", "[O,N,P,S,n,Si,Se]C(=O)[C]=[C]C(=O)[O,N,P,S,n,Si,Se]",
 "[O,N,P,S,n,Si,Se]C(=O)[C]=[C]C#N", "[CX3]([#6,#1])([#6,#1])=[NX2H]", "[OH][CX4]!@O",
 "[O-][N+](=O)[CX3]=[CX2]=[CX3]", "[#6]C(=O)[NH2]", "[#6,N,O,P,S,Se][O][C](=[O])[NH2]",
 "c=[SX1]", "[#6]C(=[O])OC(=[O])[#6]", "[Cl,Br,I]C#C", "P(=O)[OH]",
 "[CX3]=[CX3]1[CX4][CX4]1", "[#6]O[OH]", "[PX4]=[NH]", "[c][Sn]",
 "[#6]C(=[O])N([NH2])C(=[O])[#6]", "[O,N,P,S,n,Si,Se]C(=O)[CX4!H0]C#N",
 "[CX4]([OH0,PH0,BH0,SH0,Se])[Cl,Br,I]", "[CX3]([#6,#1])([#6,#1])=[NX2][OX2,NX3,S,P]",
 "[NX3][CX3](=[O,SX1])[NX3!H0]", "[#6][SX3](=O)[OH]", "[SiX4][CX4][CX3]=[CX3]",
 "[O,N,P,S,n,Si,Se]C(=O)[CX4!H0]P=[O,SX1]", "[n,s,o][cH][nr5]", "[CX4H1][O][S](=O)(=O)[#6]",
 "[NX3H,n,O,SX2,PX3H][CH](=[O])", "[#6,N,O,P,S,Se][O][C](=[O])[NH][#6,N,O,P,S,Se]",
 "[#6][NX2]=[NX2][#6]", "[#6][S](=O)(=O)[OH]", "[#6]C(=O)[NX3][NX3H][CX4,c]",
 "[n][c;r6](=[O])[n,c]", "[CX4,c][SX2][CX3]([SX2][CX4,c])=C", "[n][c;r6]([Cl,F])[n,c]",
 "[O,S,Se,P,NX3]C#C", "S(=O)[CX4!H0]C(=O)[O,N,P,S,n,Si,Se]", "[CX4H0][Cl,Br,I]",
 "[SX3]=[NH]", "[SiX4][O][CX3]=[CX3]", "C#C", "[#6]C(=O)[N]=[N+]=[N-]",
 "S(=O)[CX4!H0]P=[O,SX1]", "[#6][S](=O)(=O)[NH2]", "[#6][Li]", "[CX4H2][O][S](=O)(=O)[#6]",
 "[#6][N]=[N+]=[N-]", "[#6][PX3]([#6])[#6]", "[NX3!H0][CX3](=[#7])[NX3]", "[#6][SX2,O]C#N",
 "[#6]N=C=[O,S]", "[CX3]=[CX3][O][CX4,c]", "[#6]C(=[S])[NH2]", "[SX4]=[NH]",
 "[#6][SX3](=O)[#6]", "[#6]C(=[O])[NH][#6]", "[CX3]=[NX3+][O-]"

Associated unwanted motifs prone to side reactions

```
"[CH](C#N)([CX3r5,CX3r6]=O)*[AR0,aR1][AR0,aR1]C(=O)[OH0]",  
"[CH](C#N)([CX3r5,CX3r6]=O)*[AR0,aR1][AR0,aR1][AR0]C(=O)[OH0]",  
"[CH](C#N)([CX3r5,CX3r6]=O)*[AR0][AR0,aR1][AR0,aR1]C(=O)[OH0]",  
"[CH](C=O)([CX3r5,CX3r6]=O)*[AR0,aR1][AR0,aR1]C(=O)[OH0]",  
"[CH](C=O)([CX3r5,CX3r6]=O)*[AR0,aR1][AR0,aR1][AR0]C(=O)[OH0]",  
"[CH](C=O)([CX3r5,CX3r6]=O)*[AR0][AR0,aR1][AR0,aR1]C(=O)[OH0]",  
"[CH](C#N)([CX3r5,CX3r6]=O)*[AR0,aR1][AR0,aR1][AR0][AR0]C(=O)[OH0]",  
"[CH](C#N)([CX3r5,CX3r6]=O)*[AR0][AR0,aR1][AR0,aR1][AR0]C(=O)[OH0]",  
"[CH](C#N)([CX3r5,CX3r6]=O)*[AR0][AR0][AR0,aR1][AR0,aR1]C(=O)[OH0]",  
"[CH](C=O)([CX3r5,CX3r6]=O)*[AR0,aR1][AR0,aR1][AR0][AR0]C(=O)[OH0]",  
"[CH](C=O)([CX3r5,CX3r6]=O)*[AR0][AR0,aR1][AR0,aR1][AR0]C(=O)[OH0]",  
"[CH](C=O)([CX3r5,CX3r6]=O)*[AR0][AR0][AR0,aR1][AR0,aR1]C(=O)[OH0]" ]
```

Figure. General scheme and part of an expert-coded record describing one of Chematica's 100,000+ reaction rules, here a variant of the conia-ene cyclisation. The figure has the key fields of the Chematica's record describing scope and chemical nuances of the transformation as well as the associated motifs not allowed in potential synthons (since they are prone to side reactions).