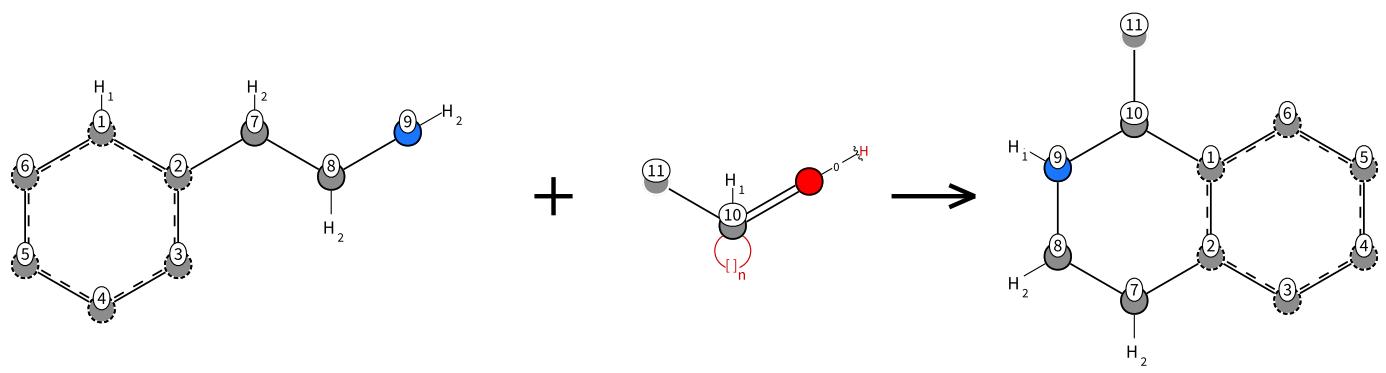
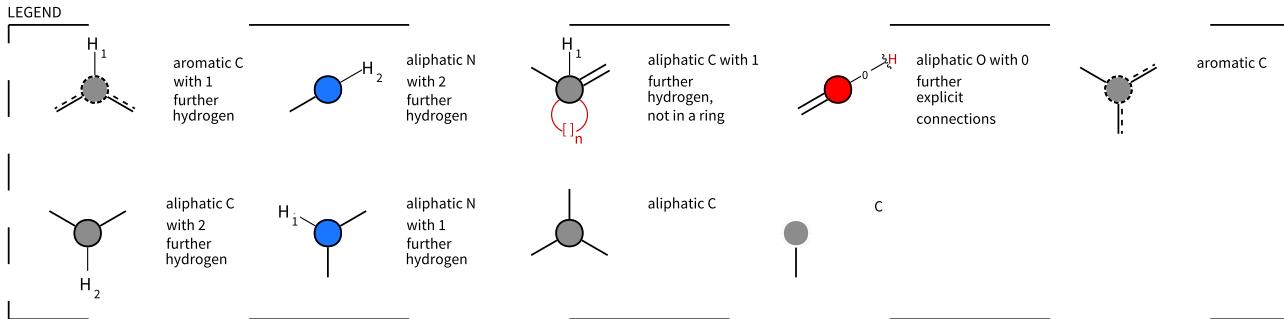


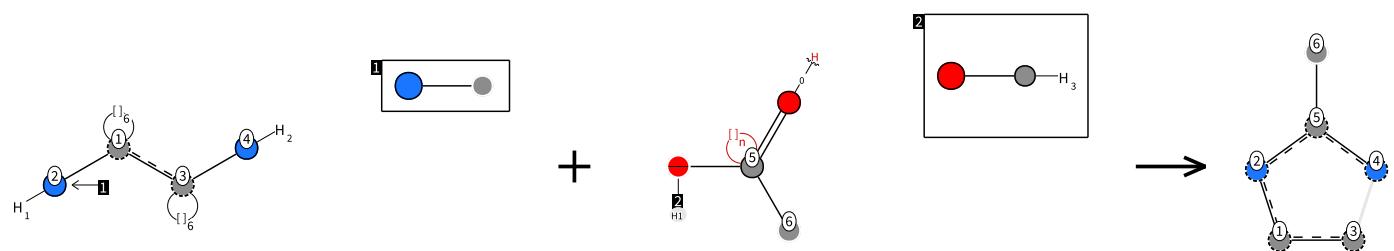
[cH1:1]1:[c:2](-[CH2:7]-[CH2:8]-[NH2:9]):[c:3]:[c:4]:[c:5]:[c:6]:1.[#6:11]-[CH1;R0:10]=[OD1]>>[c:1]12:[c:2](-[CH2:8]-[NH1:9]-[C:10]-2(-[#6:11])):[c:3]:[c:4]:[c:5]:[c:6]:1



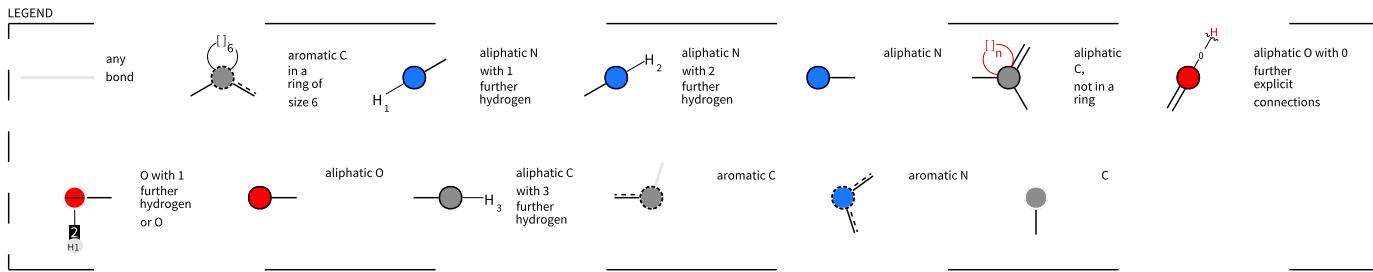
Picture created by the SMARTSviewer [https://smarts.plus/].
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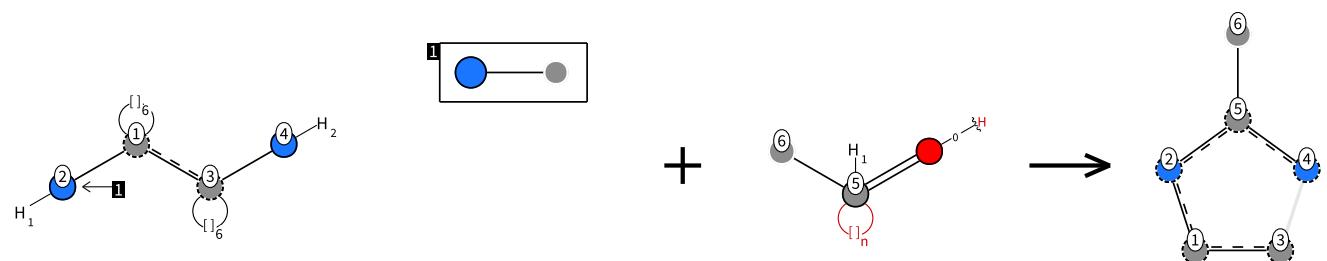
[c;r6:1]([NH1:\$N([#6]:2)];[c;r6:3]([-NH2:4]).[#6:6]-{C;R0:5}(=[OD1])-#8H1,\$(O-[CH3]))>>[c:3]2:[c:1];[n:2];[c:5](-[#6:6]):[n:4]@2



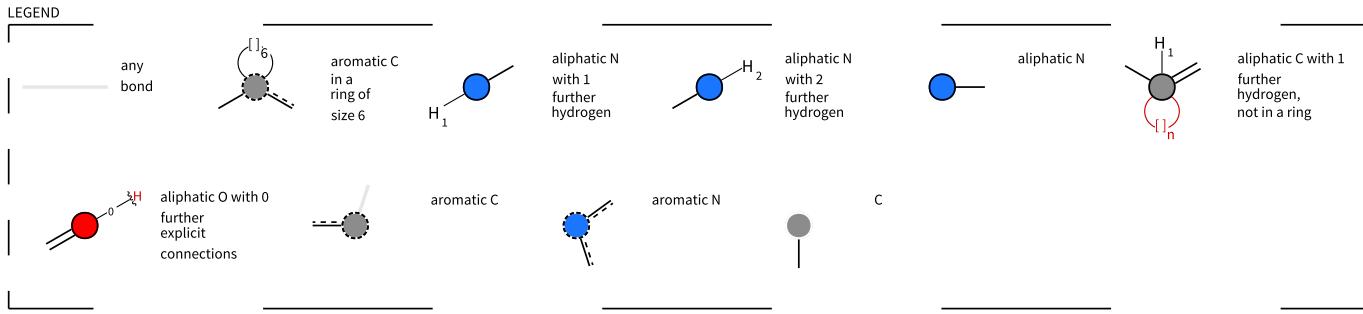
Picture created by the SMARTSviewer (<https://smarts.plus/>).
Copyright: ZBH - Center for Bioinformatics Hamburg.



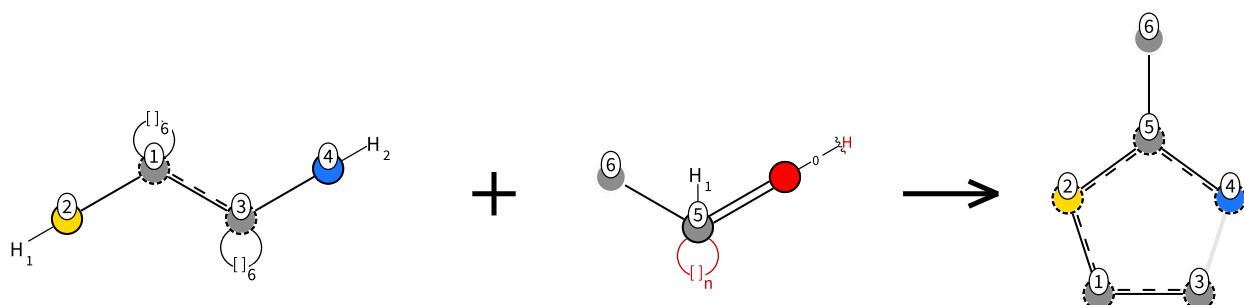
[c;r6:1]-[NH1;S(N-[#6]):2]:[c;r6:3]-[NH2:4].[#6]-[CH1;R0:5](=[OD1])>>[c:3]2:[c:1]:[n:2]:[c:5](-[#6:6]):[n:4]@2



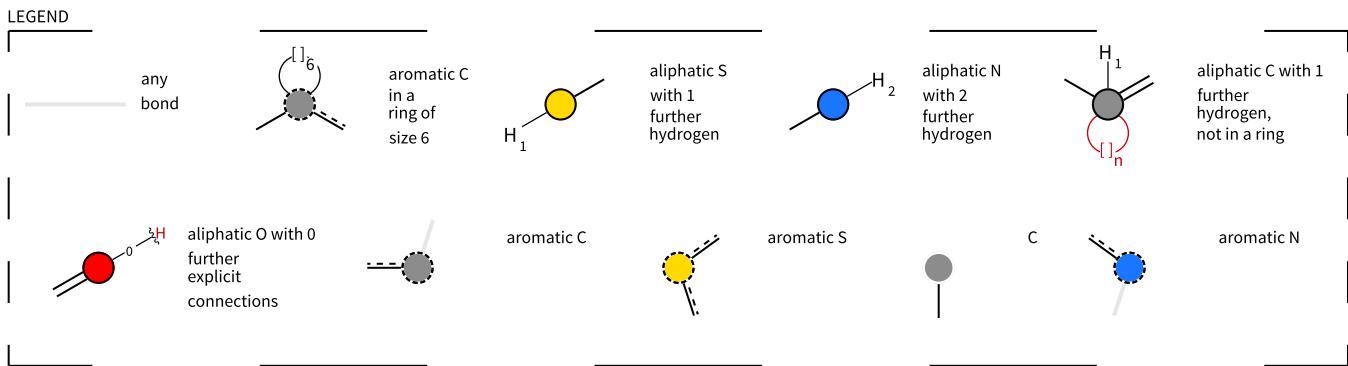
Picture created by the SMARTSviewer [<https://smarts.plus/>].
Copyright: ZBH - Center for Bioinformatics Hamburg.



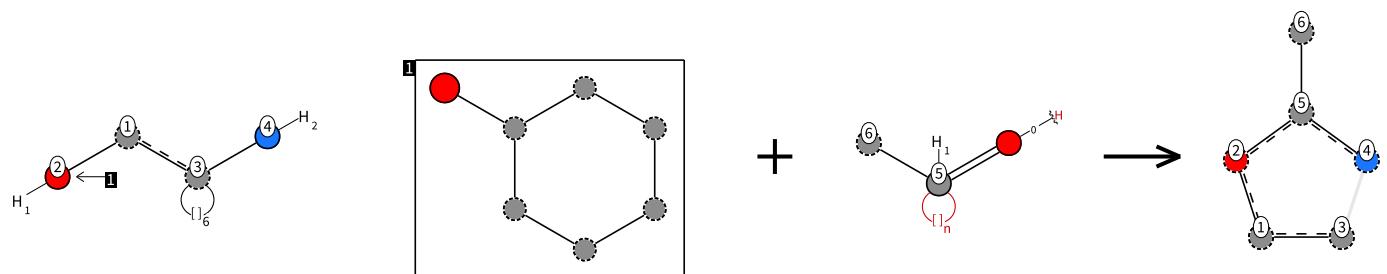
[c;r6:1](-[SH1:2]):[c;r6:3](-[NH2:4]).[#6:6]-[CH1;R0:5](=[OD1])>>[c:3]2:[c:1]:[s:2]:[c:5](-[#6:6]):[n:4]@2



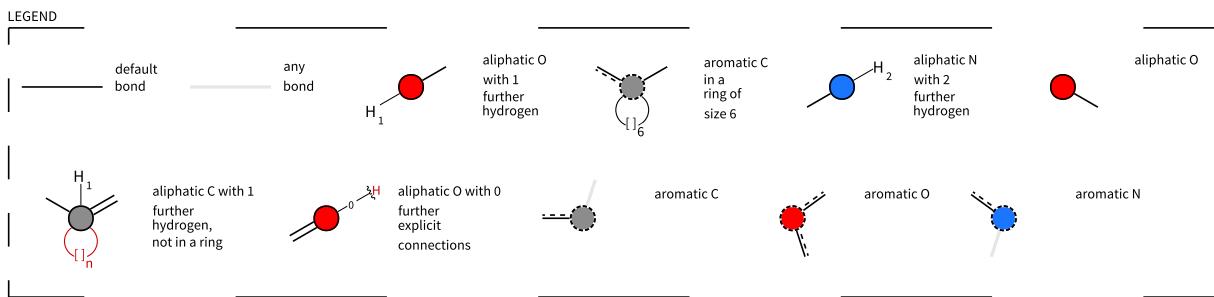
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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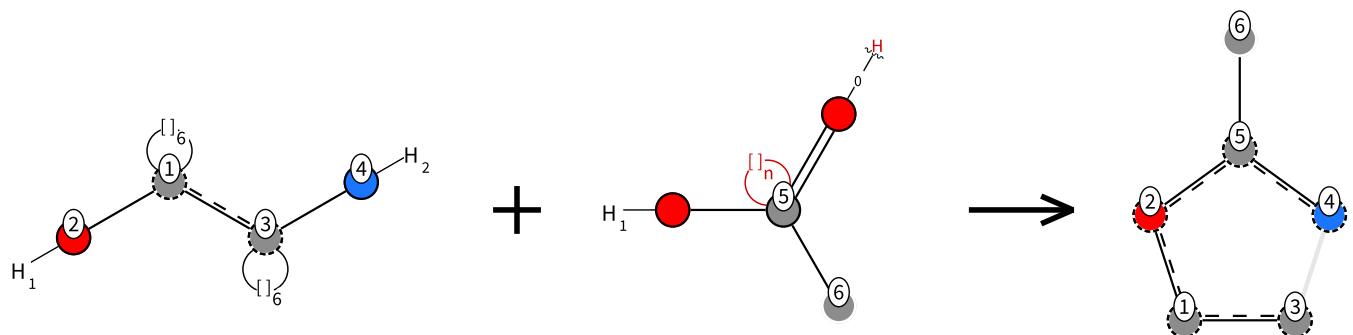
[c:1]-[OH1;\$(Oc1ccccc1);2];[c;r6:3]-[NH2:4].[c:6]-[CH1;R0:5](=[OD1])>>[c:3]2:[c:1];[o:2];[c:5](-[c:6]);[n:4]@2



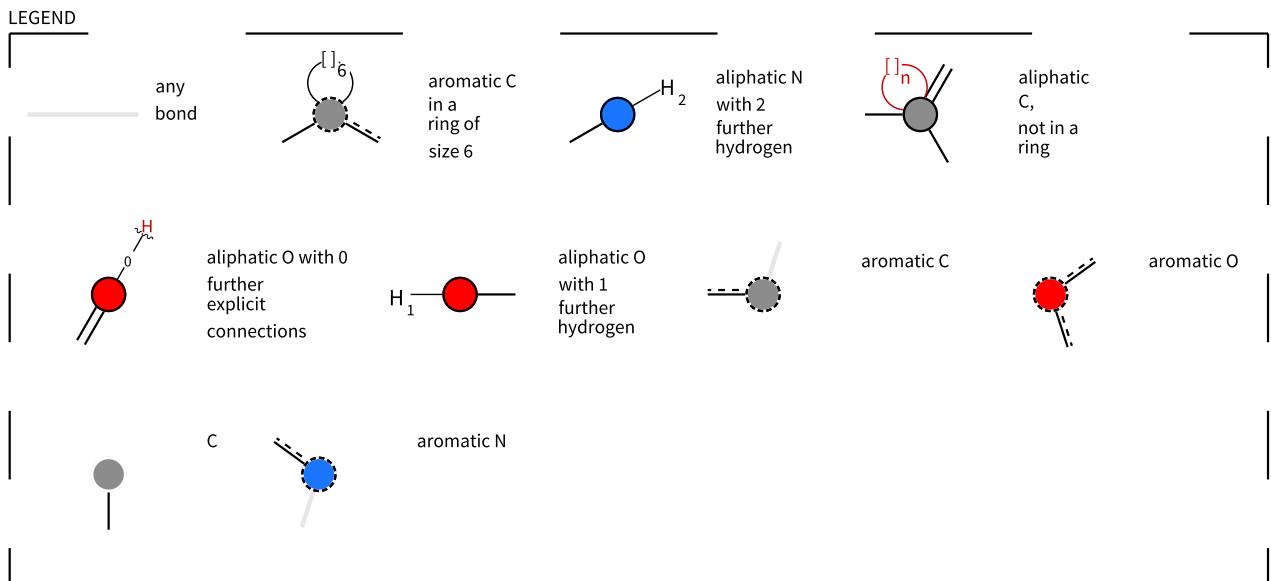
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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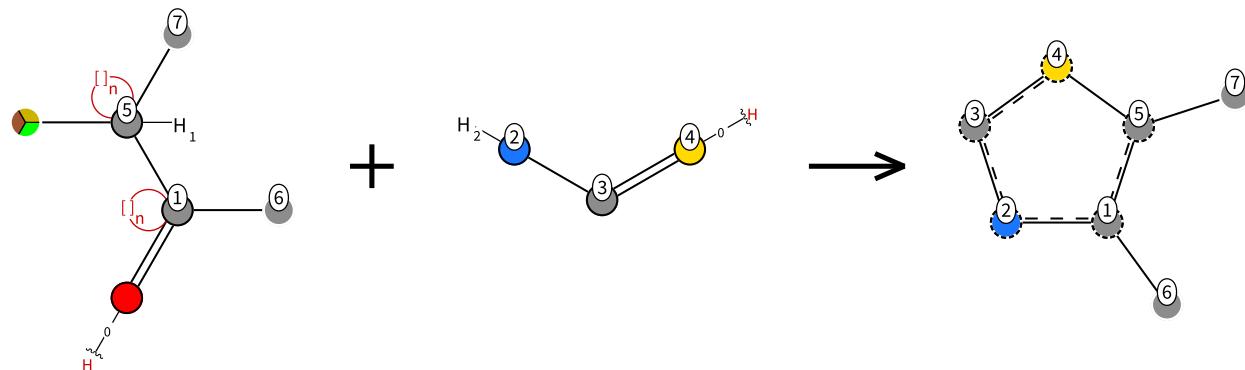
[c;r6:1](-[OH1:2]):[c;r6:3](-[NH2:4]).[#6:6]-[C;R0:5](=[OD1])-[-OH1]>>[c:3]2:[c:1]:[o:2]:[c:5](-[#6:6]):[n:4]@2



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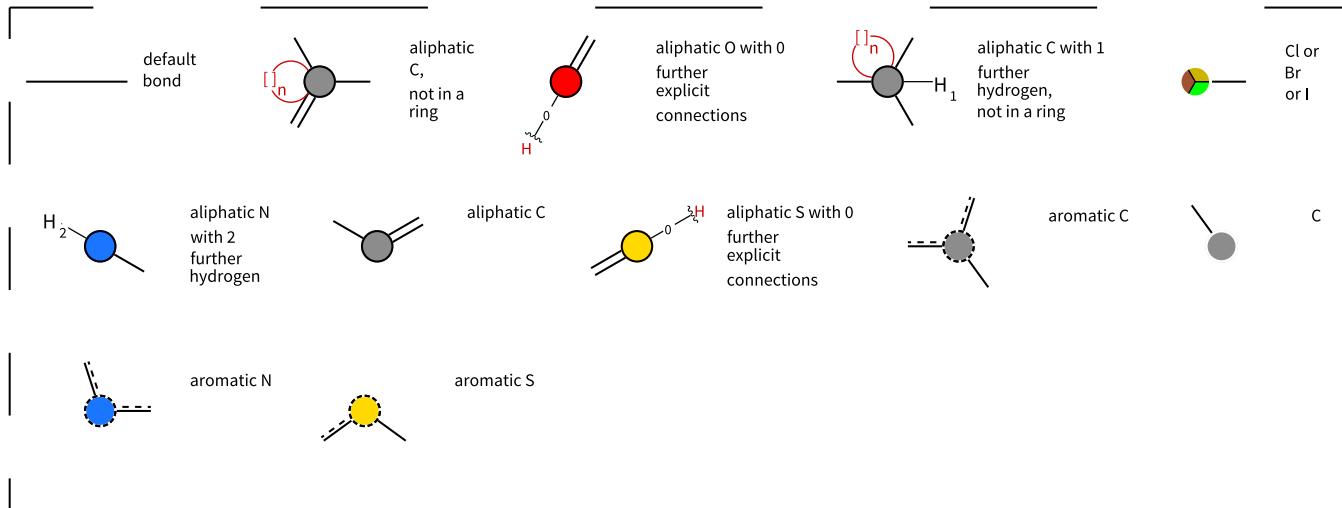


```
[#6:6]-[C;R0:1](=[OD1])-CH1;R0:5)(-[#6:7])-*;#17,#35,#53].[NH2:2]-[C:3]=[SD1:4]>>[c:1]2(-[#6:6]):[n:2]:[c:3]:[s:4][c:5]([#6:7]):
```

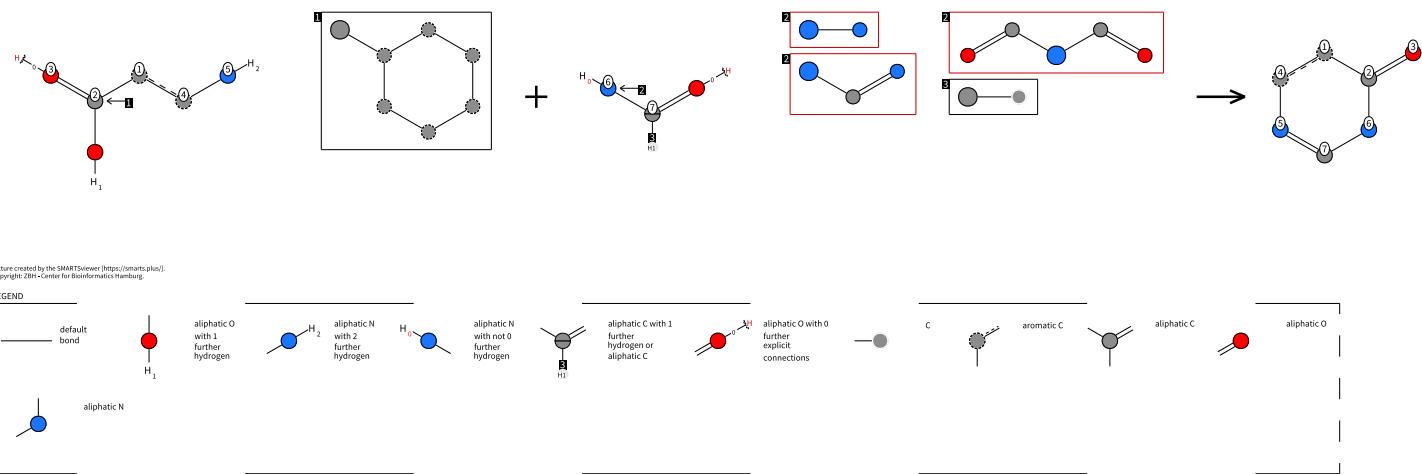


Picture created by the SMARTSviewer [<https://smarts.plus/>].
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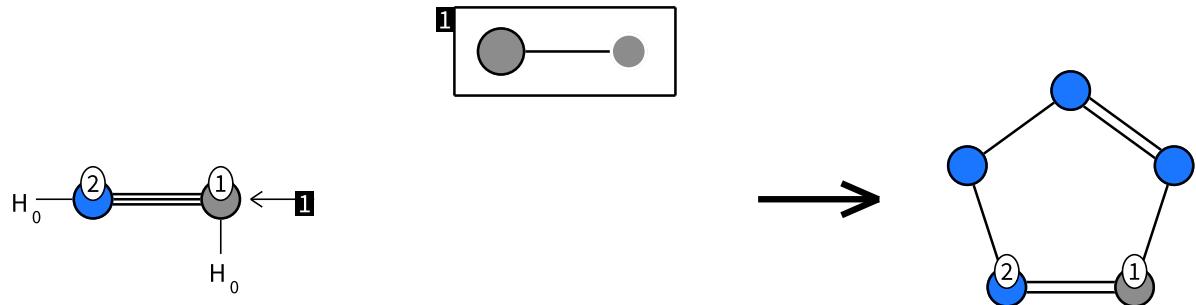
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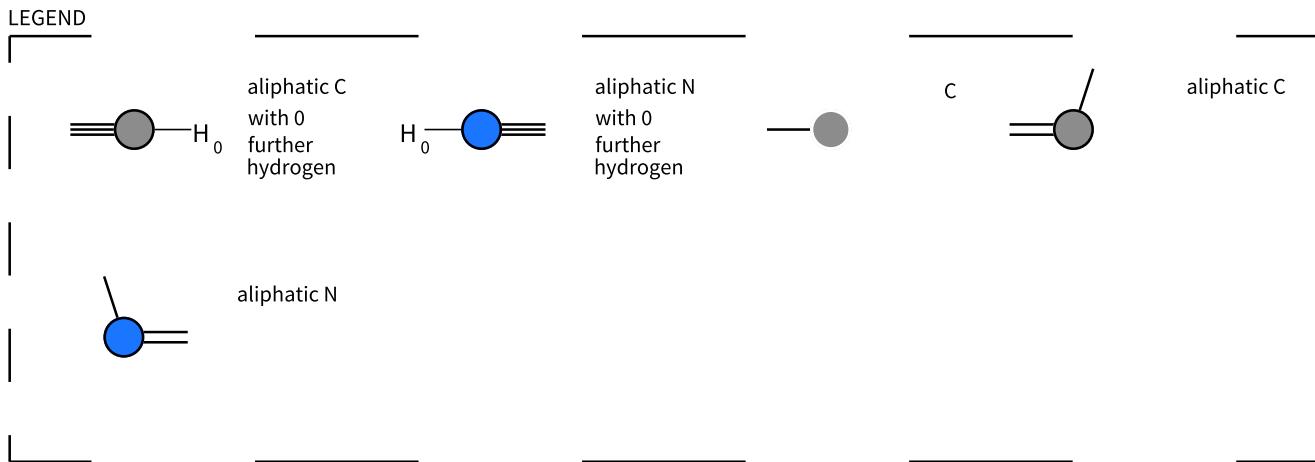
[c:1][{C;\$(C-C1CCCC1);2}{([OD1:3]);([OH1])}{(c:4)([NH2:5])}{[N];[H0];\$[Na+];\$[N<=N];\$[N<=O];\$[C=O];\$[C-H1,\$[C-H6]);?}{([OD1]>>[c:4]{2:[c:1]-[C:2]}{=[O:3]}{[N:6]-[C:7]=[N:5]-2}



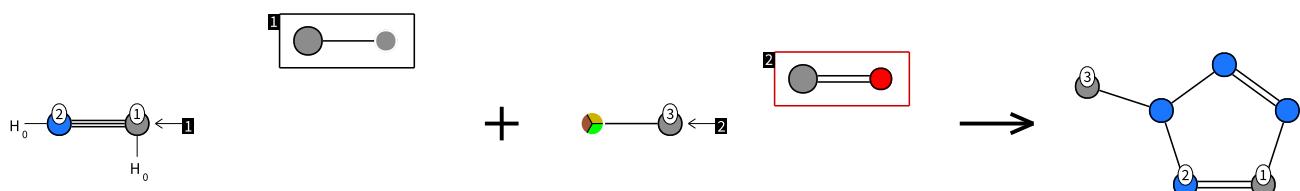
[CH0;\$(C-[#6]):1]#[NH0:2]>>[C:1]1=[N:2]-N-N=N-1



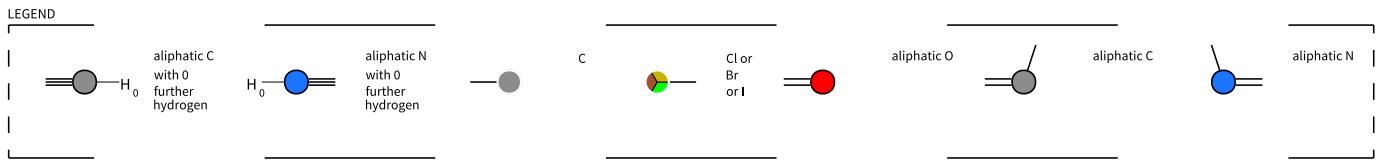
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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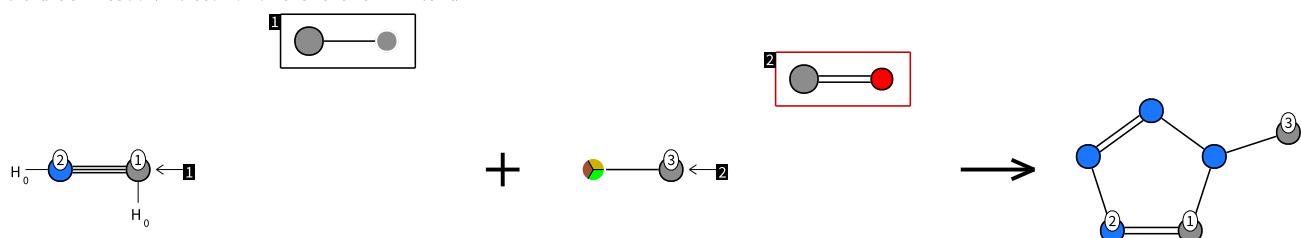
[CHO;\$(C-[#6]):1]#[NH0:2].[C;A;!\$(C=O):3]-[*:#17,#35,#53]>[C:1]1=[N:2]-N(-[C:3])-N=N-1



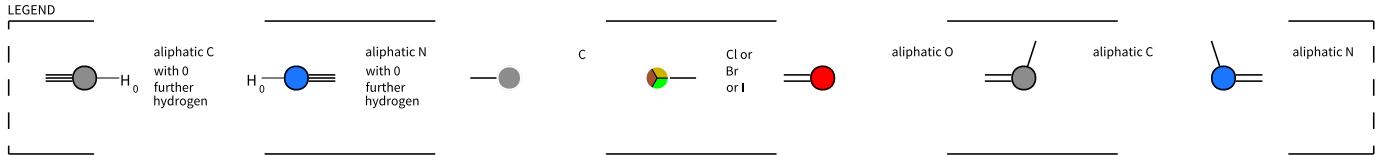
Picture created by SMARTSviewer (<https://smarts.plus/>).
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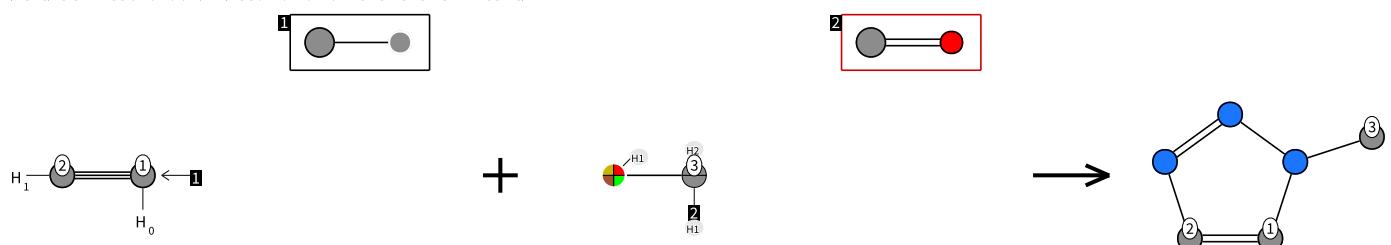
[CHO;\$(C-[#6]):1]#[NHO:2].[C;A;!\$(C=O):3]-[*:#17,#35,#53]>>[C:1]1=[N:2]-N=N-N-1(-[C:3])



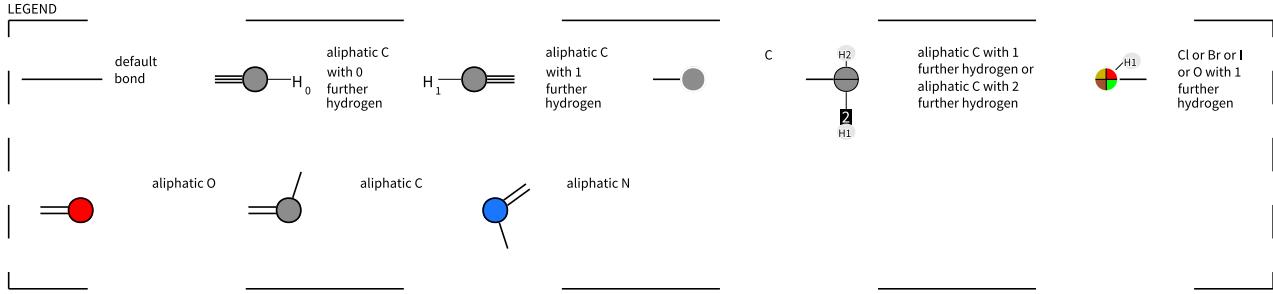
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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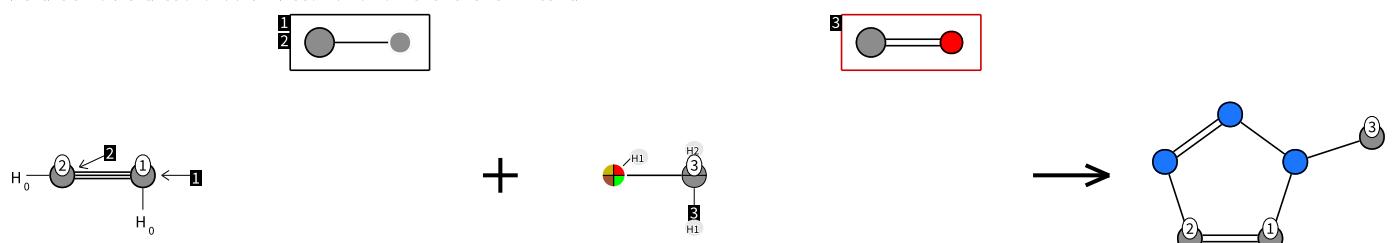
[CHO;\$(C-[#6]:1)#[CH1:2].[C;H2;A;!\$(C=O):3]-*;#17,#35,#53,OH1]>>[C:1]1=[C:2]-N=NN-[C:3]-1



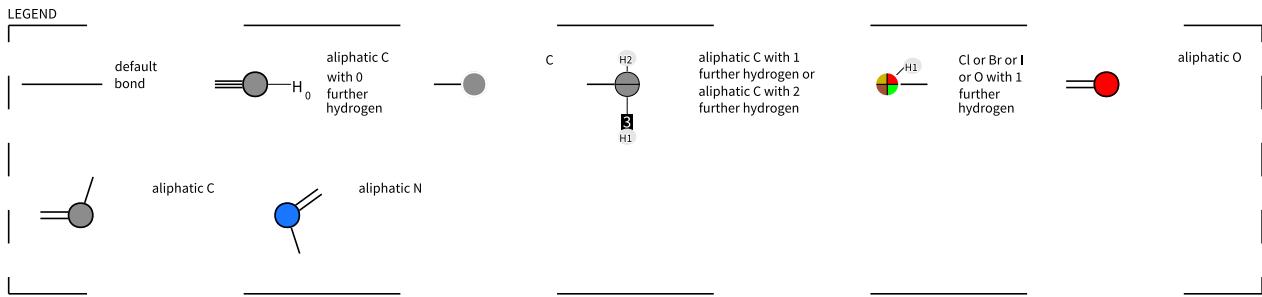
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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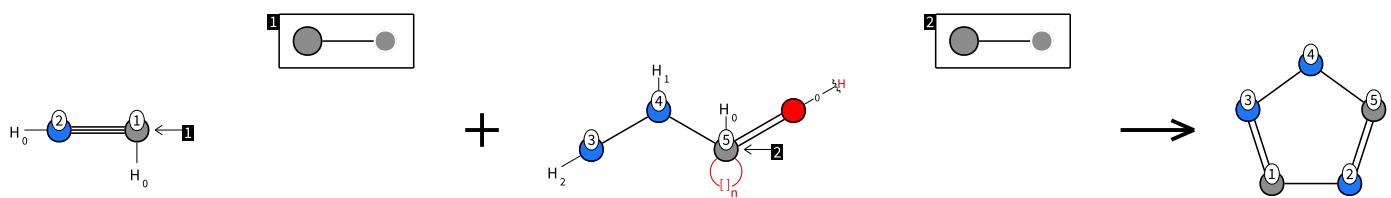
[CHO;\$(C-[#6]):1]#[CHO;\$(C-[#6]):2].[C;H1,H2;A;\$(C=O);3]-[';#17,#35,#53,OH1]>>[C:1]1=[C:2]-N=NN(-[C:3])-1



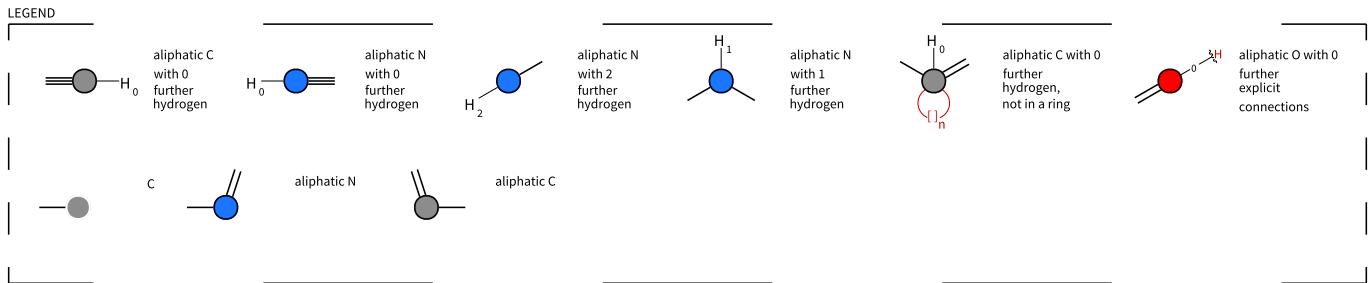
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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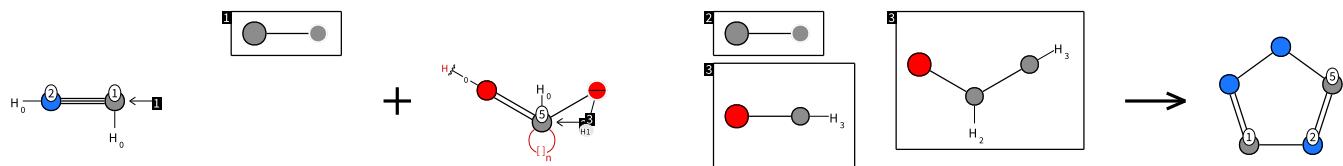
[CHO;\$(C-[#6]):1]#[NHO:2].[NH1:4]-[CH0;\$(C-[#6]);R0:5]=[OD1]>>[N:2]1-[C:1]=[N:3]-[N:4]-[C:5]=1



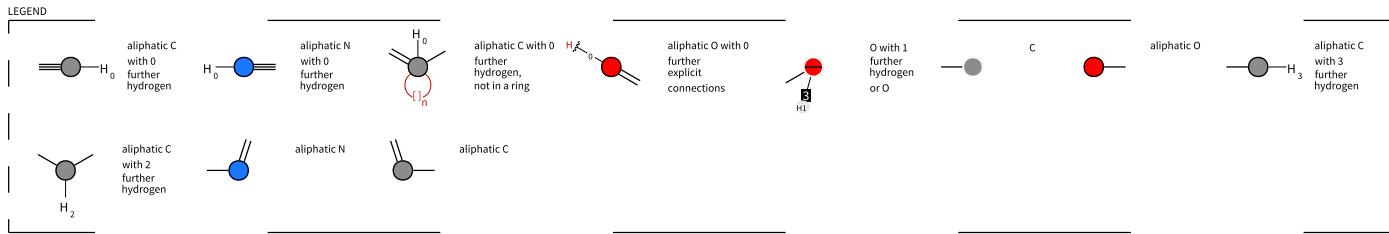
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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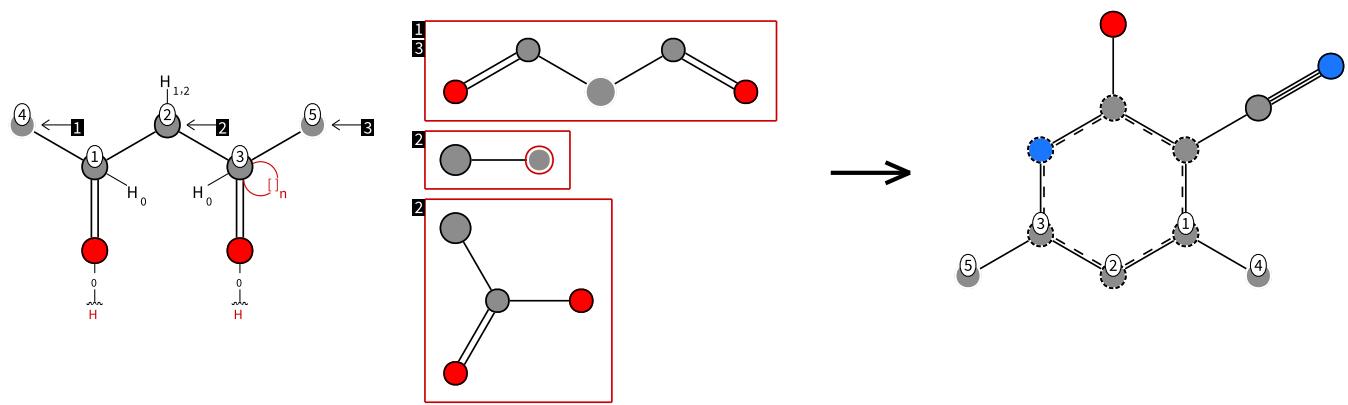
[CH0;\$C-[#6]:1]#[NH0:2].[CH0;\$C-[#6];R0:5]=[OD1]-[#8;H1,\$(O-[CH3]),\$(O-[CH2]-[CH3])]>>[N:2]1-[C:1]=N-N-[C:5]=1



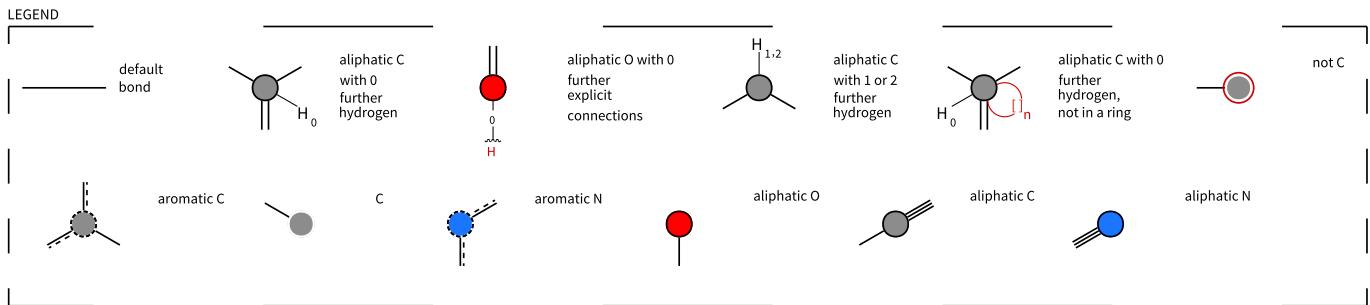
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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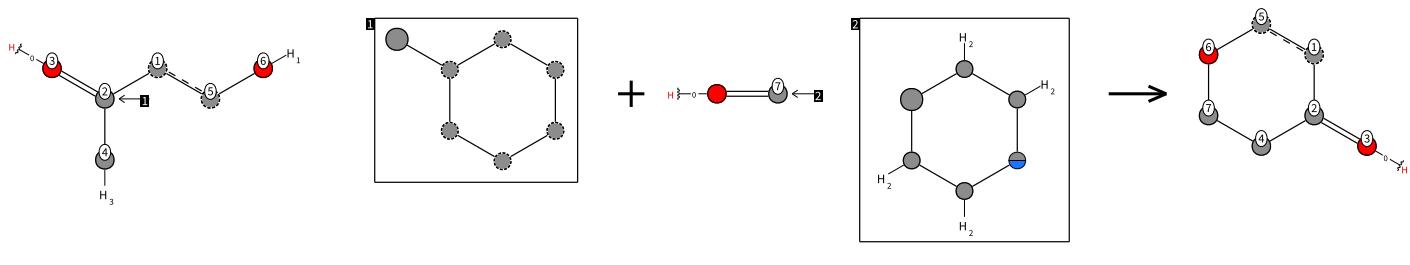
[#6;!\$([#6](=C=O)-C=O):4]-[CH0:1](=[OD1])-C;H1&!\$(C-*;[#6])&!\$(C-C(=O)O),H2:2]-[CH0;R0:3](=[OD1])-[#6;!\$([#6](=C=O)-C=O):5]>>[c:1]1(-[#6:4]):[c:2]:[c:3](-[#6:5]):n;c(-O)c(-C#N):1



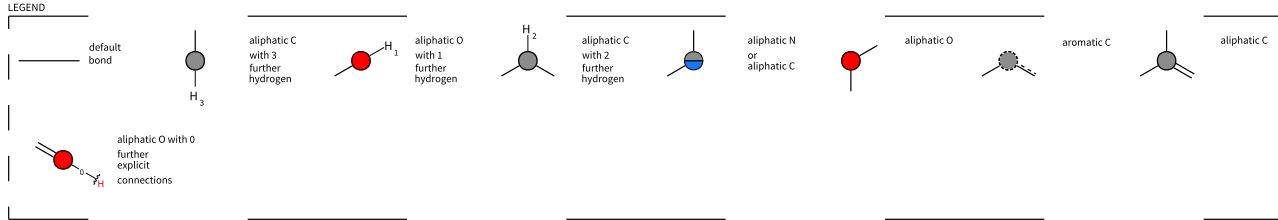
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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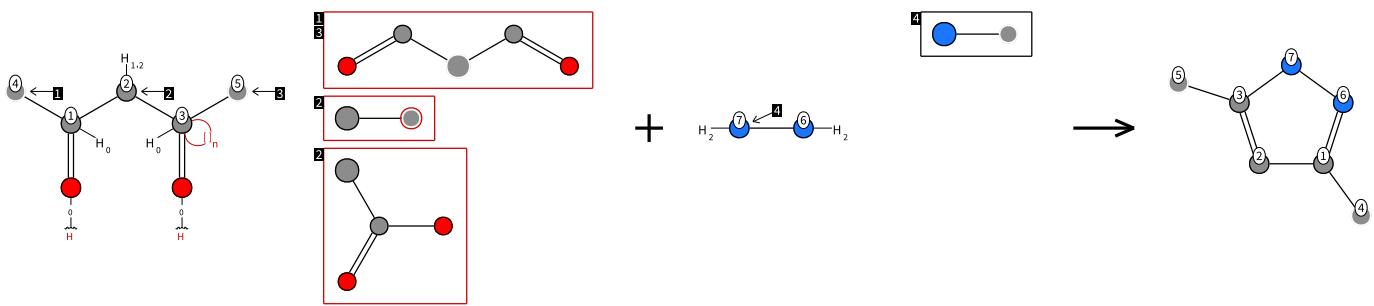
[c:1](-[C;\$(C-c1ccccc1)2]([=OD1:3]-[CH3:4]):[c:5](-[OH1:6]).[C;\$(C1-[CH2]-[CH2]-[N,C]-[CH2]-[CH2]-1);7]([=OD1])>>[O:6]1-[c:5]:[C:1]-[C:2]-[=OD1:3]-[C:4]-[C:7]-1



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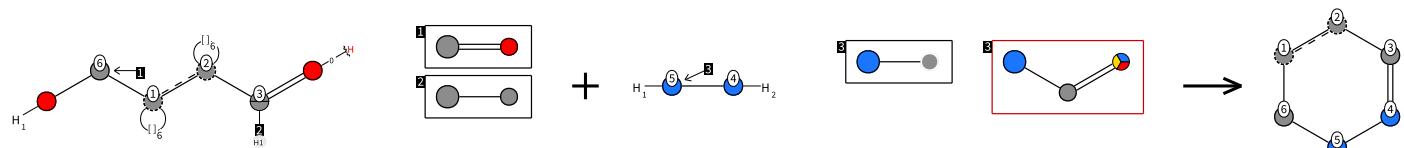
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[#6;5|[#6;(-C=O)-C=O]:4]-[CH(=O):1|([=OD1])-;[CH-1&S(C(-[*];#6)&S(C(-C(=O)O);H2;2]-[CH(=O);R0;3]:|([=OD1])-;#6;5|[#6;(-C=O)-C=O]:5];[NH2;6]-[N;1H0;S(N-[#6];H2;2]>:[C;1]1|([-#6;4]-;[C;2]=;[C;3](=-#6;5);[N;7]-[N;6]=1]
```



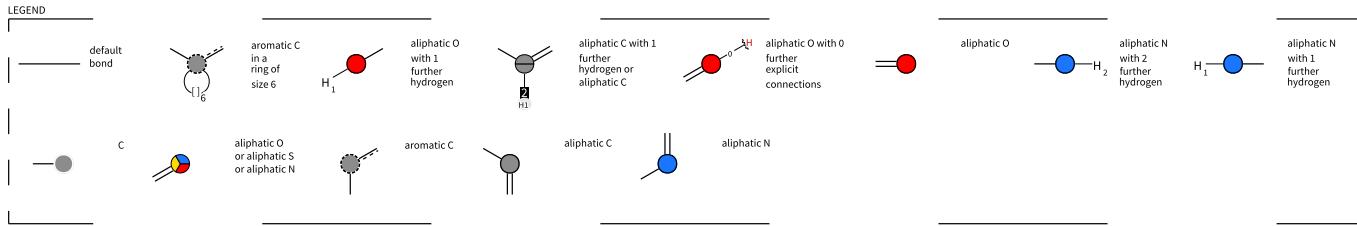
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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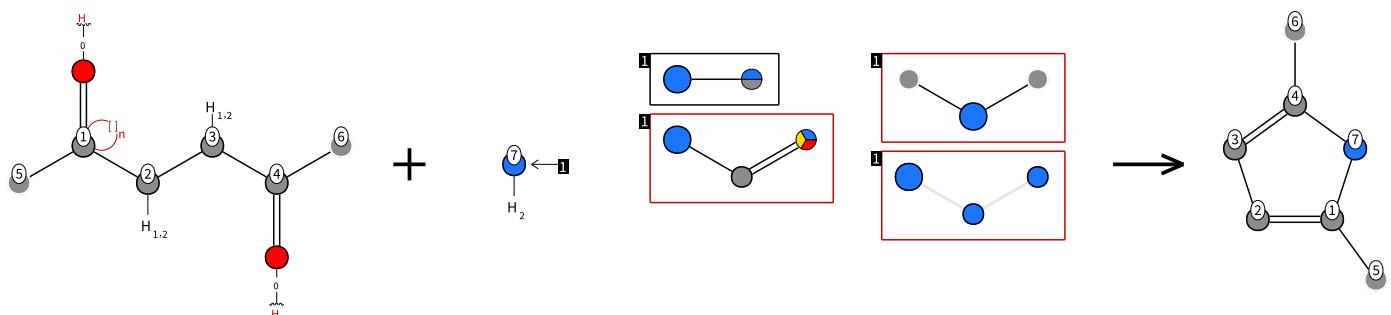
[c;r6:1]-[C;\$(C=O):6]-[OH1]):[c;r6:2]-[C;H1,\$(C-C):3]=[OD1].[NH2:4]-[NH1;\$(N-[#6]);\$(NC=[O,S,N]):5]>>[c:1]1:[c:2]-[C:3]=[N:4]-[N:5]-[C:6]-1



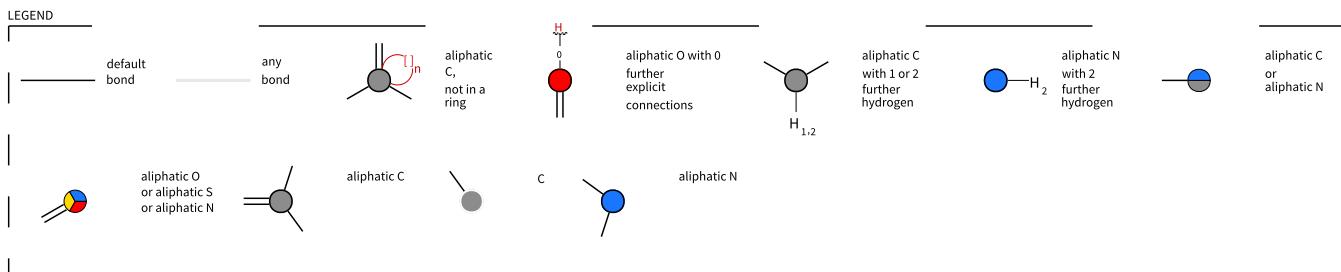
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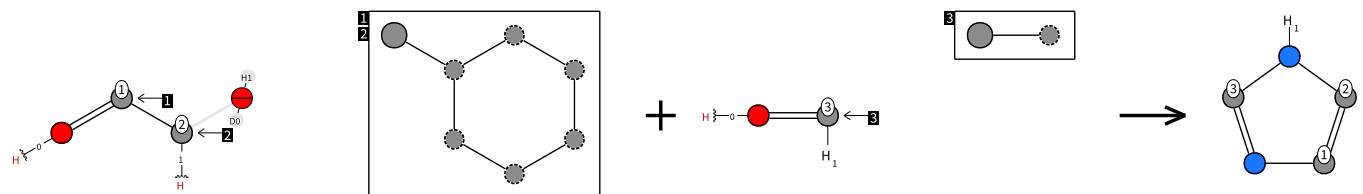
[#6:5]-{C;R0:1}(=[OD1])-{C;H1,H2:2}-[C;H1,H2:3]-{C:4}(=[OD1])-[#6:6].[NH2;\$(N-[C,N]);!\$(NC=[O,S,N]);!\$(N([#6])(#6));!\$(N-N-N);7]>>[C:1]1(.[#6:5])=[C:2]-{C:3}=[C:4](.-[#6:6])-{N:7}-1



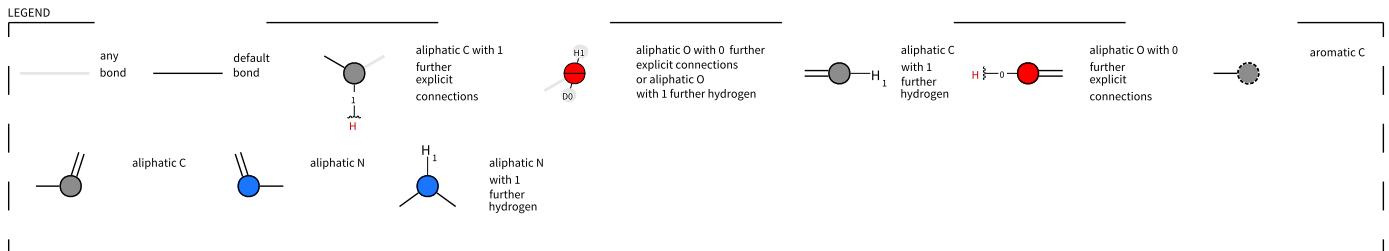
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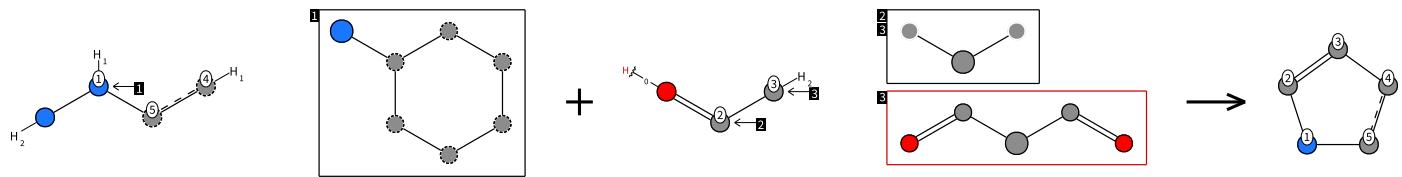
[C;\$(C-c1ccccc1):1]![=OD1]-[C;D3;\$(C-c1ccccc1):2]-[O;D1,H1].[CH1;\$(C-c):3]=[OD1]>>[C:1]1-N=[C:3]-[NH1]-[C:2]=1



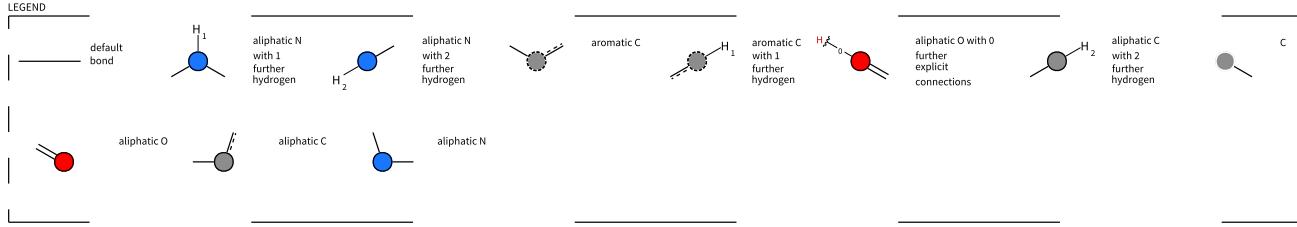
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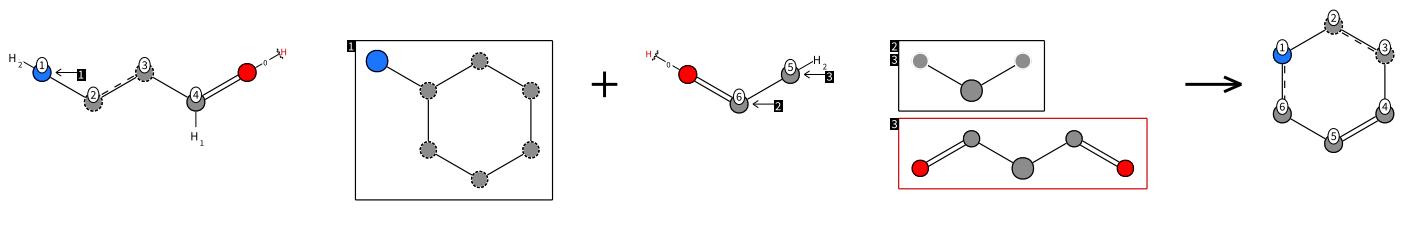
[NH1;\$(N-c1ccccc1):1]-[NH2])-c:5]:[CH1:4].[C;\$(C([#6]):[6]):2](=[OD1])-[CH2;\$(C([#6]):[6]):\$C(C=O)C=O:3]>>[C:5]1-[N:1]-[C:2]=[C:3]-[C:4]:1



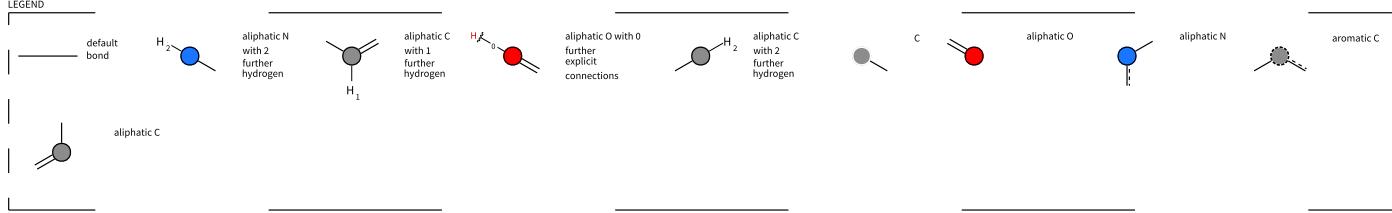
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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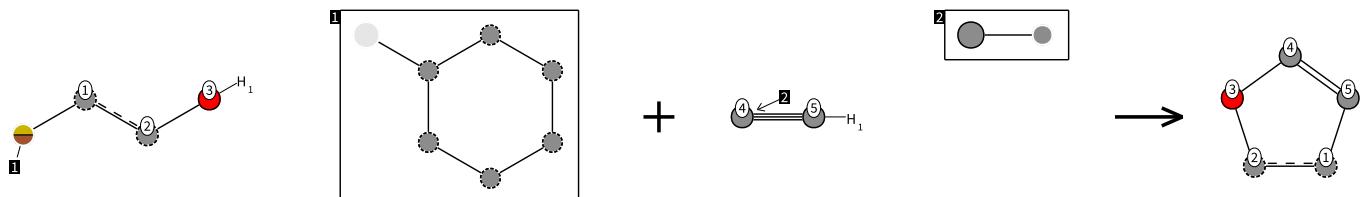
[NH2;\$(N<1cccccc1);1]-[c:2]-[c:3]-[CH1:4]=[OD1].[C;\$(C([#6])#6)-[OD1])-[CH2;\$(C([#6])#6);\$(C(C=O)C=O);5]>>[N:1]-[c:2]-[c:3]-[C:4]=[C:5]-[C:6];1



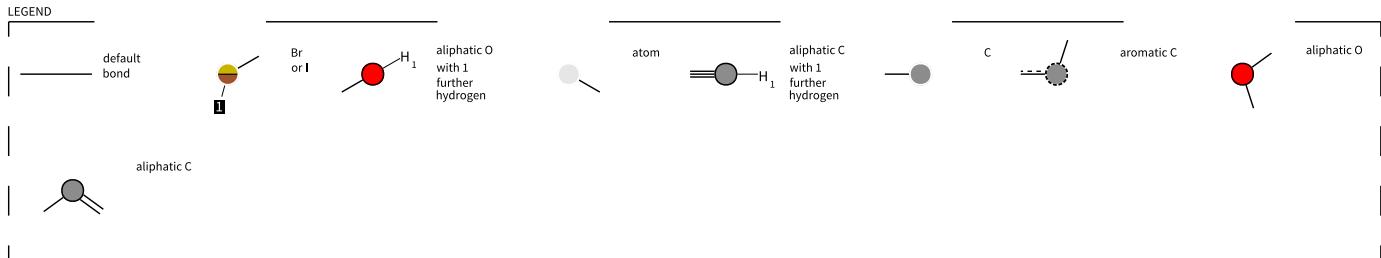
Picture created by the SMARTSviewer [https://smarts.plus/].
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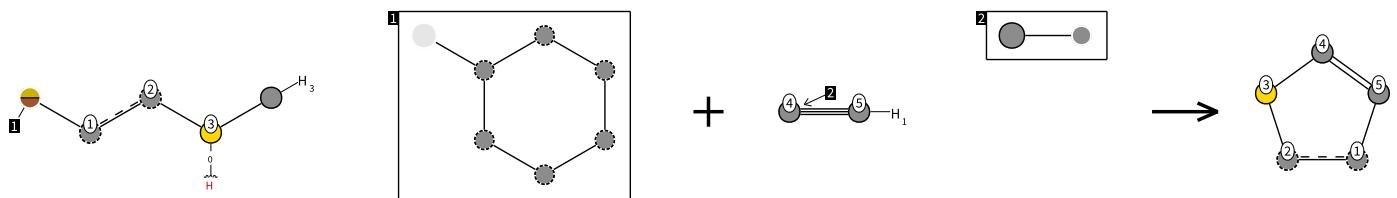
[*;Br;{("c1ccccc1)}-[c:1]:{c:2}:{OH1:3].[CH1:5]#[C;{C-#6}]:4]>>[c:1]1:{c:2}:{O:3}:[C:4]=[C:5]-1



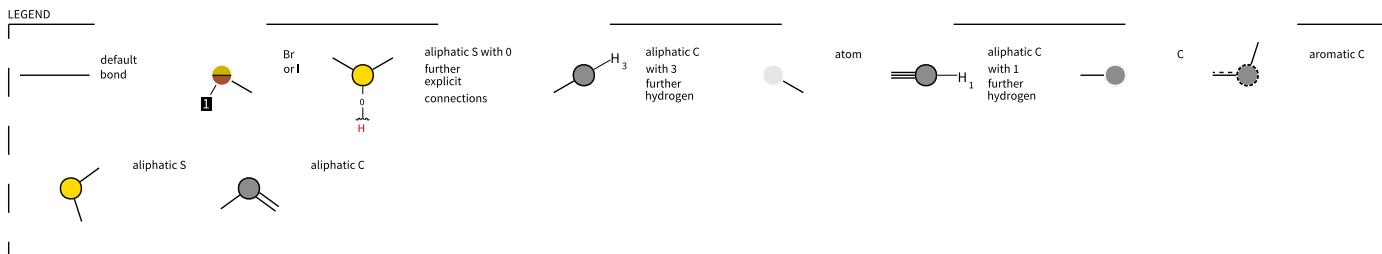
Picture created by SMARTSviewer [https://smarts.plus/].
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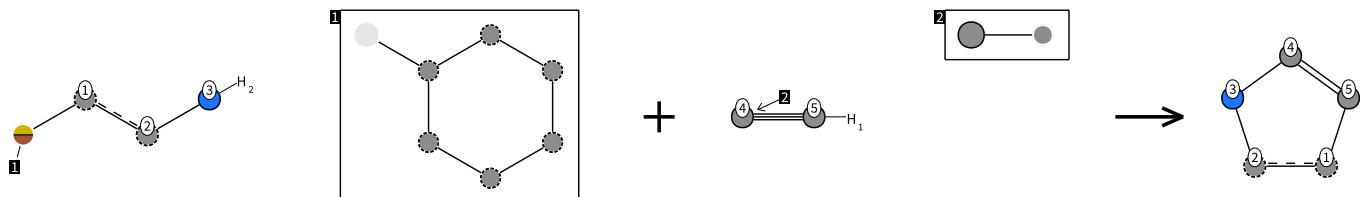
[*:Br]&[*cccccc1]-[c:1]:[c:2]-[SD2:3]-[CH3].[CH1:5]#[C:\$([C-#6]):4]>>[c:1]1:[c:2]-[S:3]-[C:4]=[C:5]-1



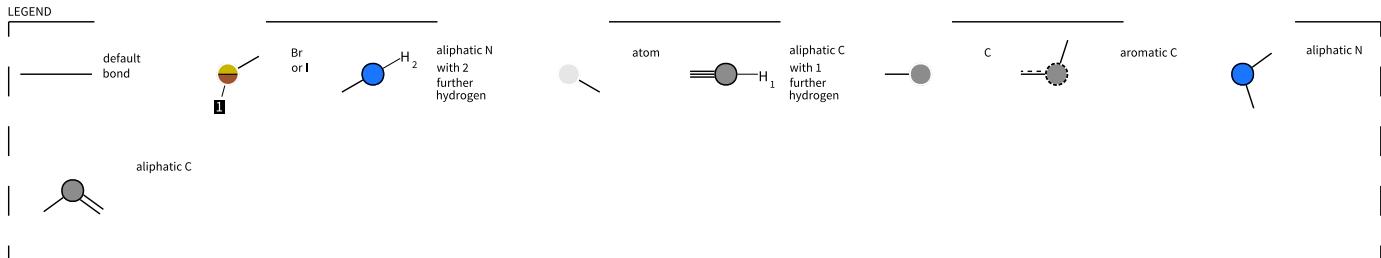
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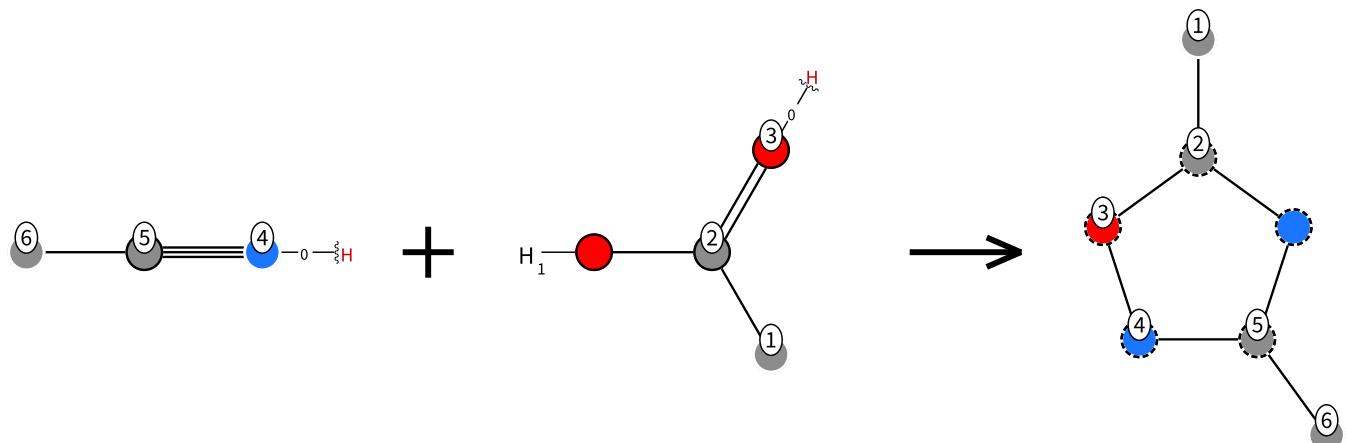
[*;Br;\$(c1ccccc1)]-[c:1]:[c:2]-[NH2:3].[CH1:5]#[C;C-#6]:4>>[c:1]1:[c:2]-[N:3]-[C:4]=[C:5]-1



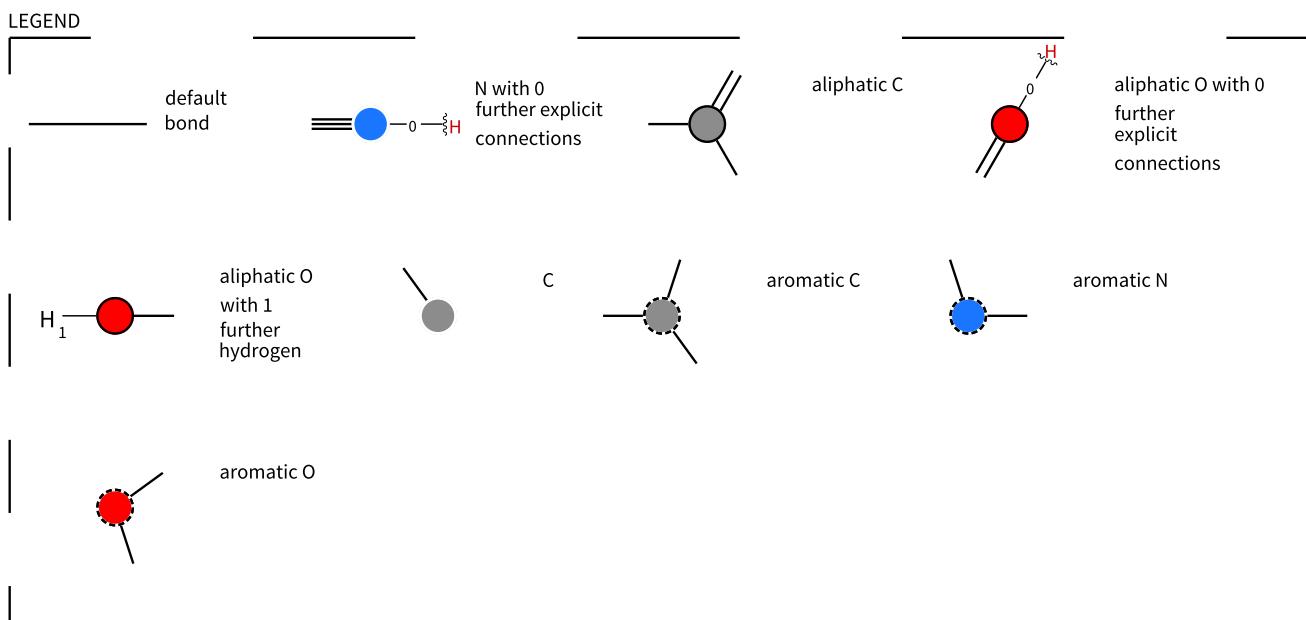
Picture created by SMARTSviewer [https://smarts.plus/].
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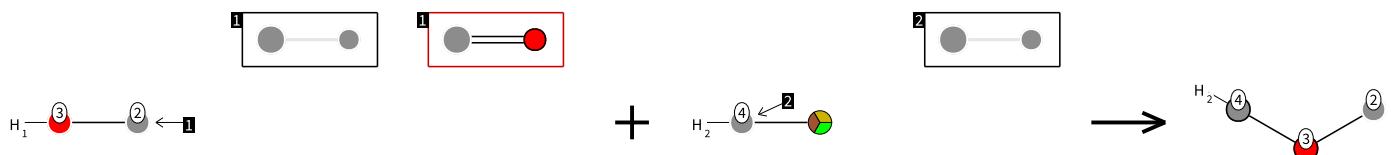
[#6:6][C:5]#[#7;D1:4].[#6:1][C:2](=[OD1:3])[OH1]>>[#6:6][c:5]1[n:4][o:3][c:2]([#6:1])n1



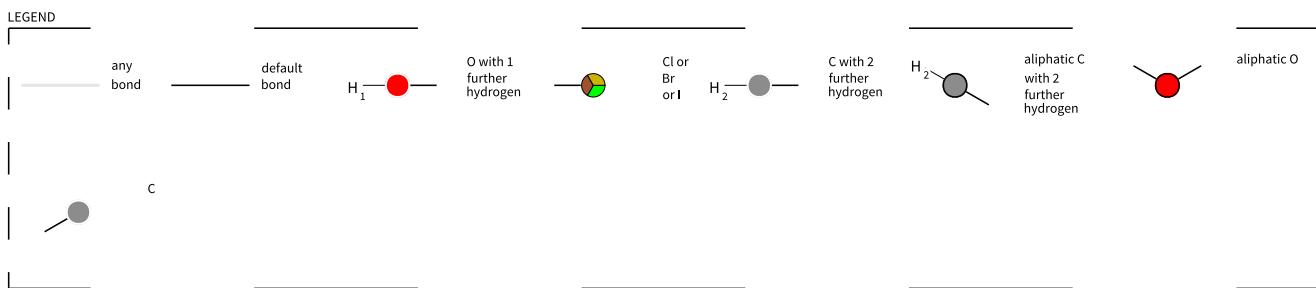
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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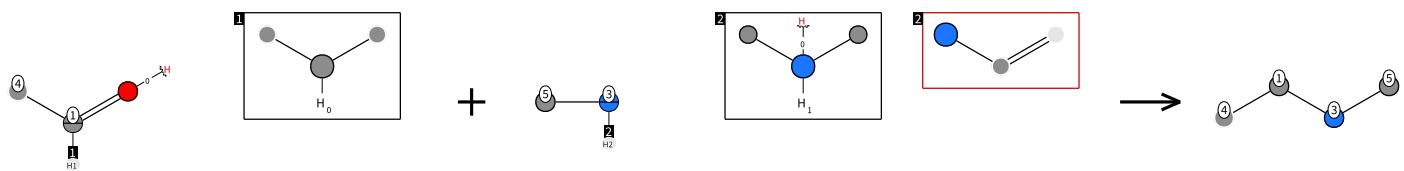
[#6;\$([#6]-[#6]);\$([#6]=O);2][#8;H1:3].[Cl,Br,I][#6;H2;\$([#6]-[#6]):4]>>[CH2:4][O:3][#6;2]



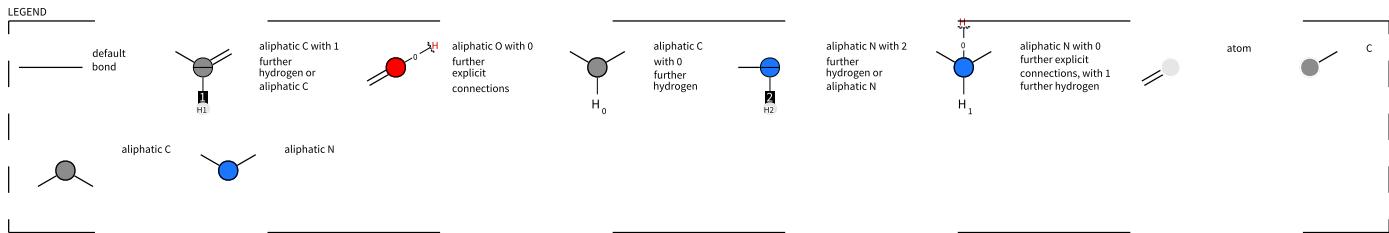
Picture created by the SMARTSviewer [https://smarts.plus/].
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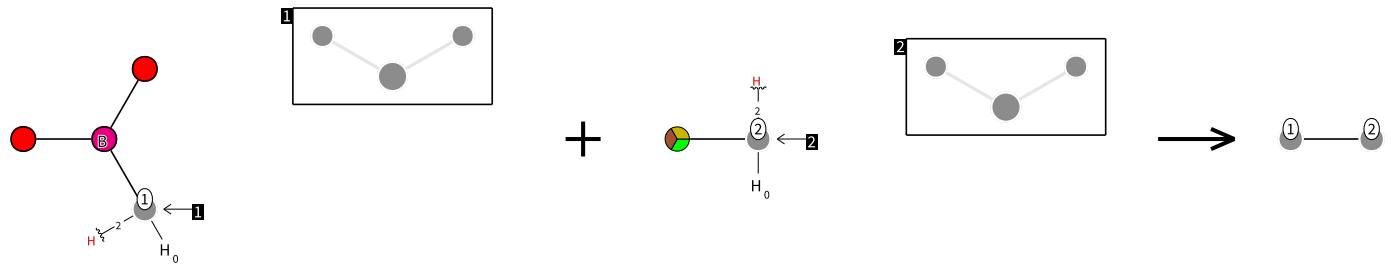
[#6:4]-{C;H1,\$([CH0]-[#6]):1}=[OD1].[N;H2,\$([NH1;D2][C;C];\$[N-#6]=*)]:3-[C:5]>>[#6:4][C:1]-[N:3]-[C:5]



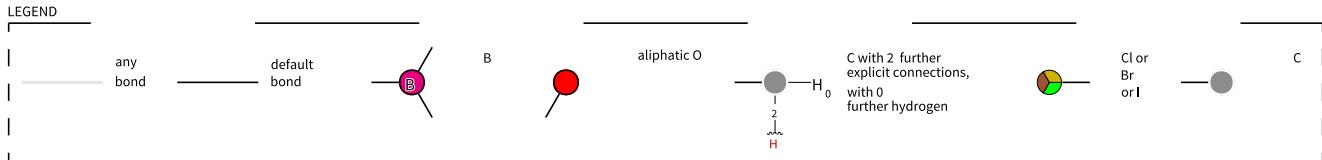
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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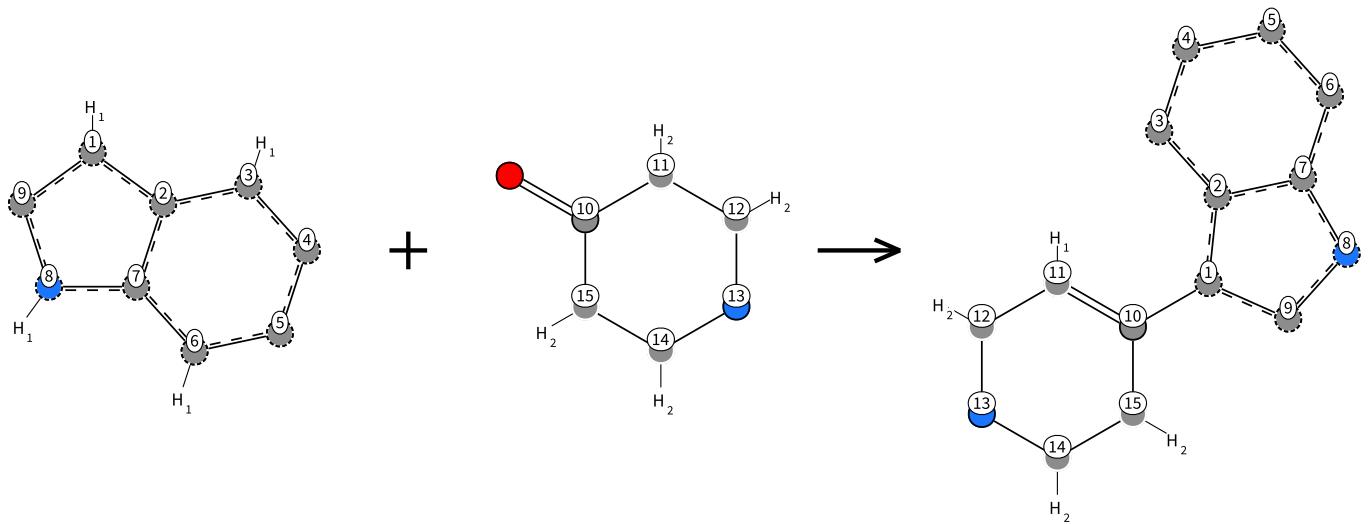
[#6;H0;D3;\$([#6](-[#6])-[#6]:1]B(O)O.[#6;H0;D3;\$([#6](-[#6])-[#6]:2][Cl,Br,I]>>[#6:2][#6:1]



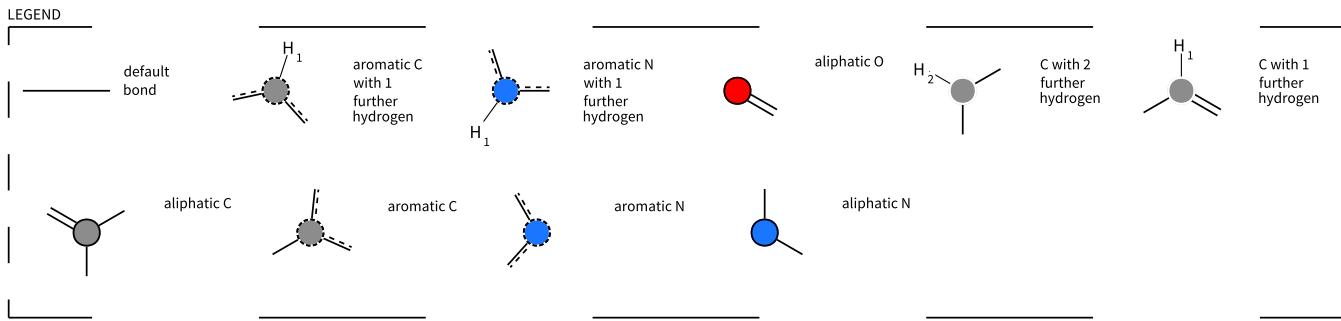
Picture created by SMARTSviewer [<https://smarts.plus/>].
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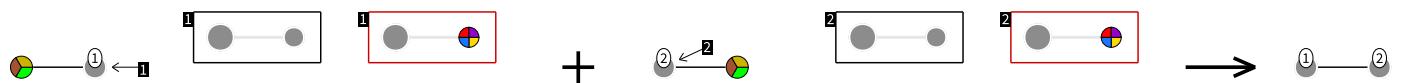
[c;H1:3]1:[c:4]:[c:5]:[c;H1:6]:[c:7]2:[nH:8]:[c:9]:[c;H1:1]:[c:2]:1:O=[C:10]1[#6;H2:11][#6;H2:12][N:13][#6;H2:14][#6;H2:15]1>>[#6;H2:12]3[#6;H1:11]=[C:10]([c:1]1:[c:9]:[n:8]:[c:7]2:[c:6]:[c:5]:[c:4]:[c:3]:[c:2]:1:2)[#6;H2:15][#6;H2:14][N:13]3



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[#6;\$([#6]~[#6]);!\$([#6]~[S,N,O,P]):1][Cl,Br,I].[Cl,Br,I][#6;\$([#6]~[#6]);!\$([#6]~[S,N,O,P]):2]>>[#6:2][#6:1]

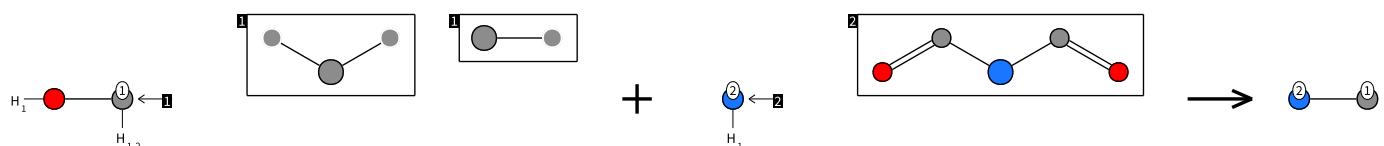


Picture created by the SMARTSviewer [https://smarts.plus/].
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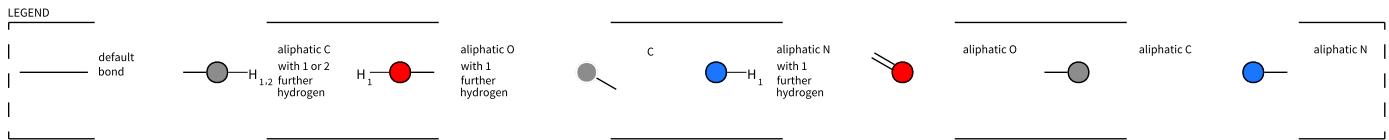
LEGEND

	any bond
—	default bond
—	Cl or Br or I
—	aliphatic S or aliphatic N or aliphatic O or aliphatic P
—	C

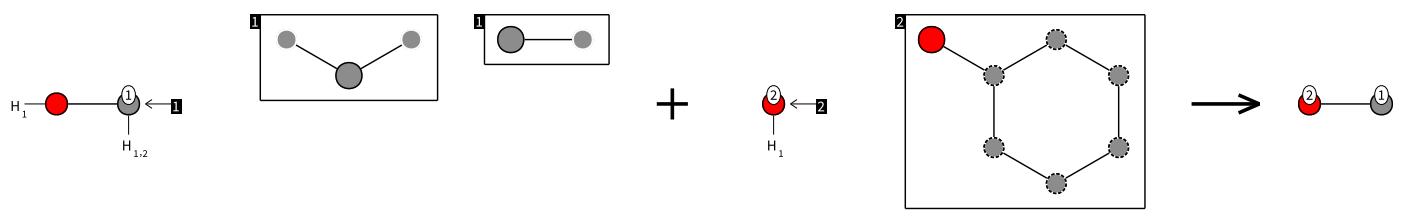
[C;H1&&(C([#6])[#6]),H2&&(C[#6]:1)[OH1].[NH1];\$[N(C=O)C=O];2]>>[C:1][N:2]



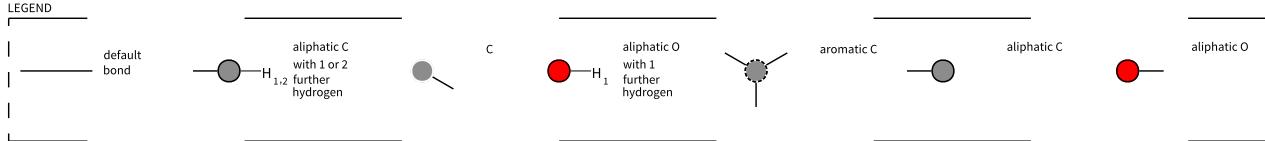
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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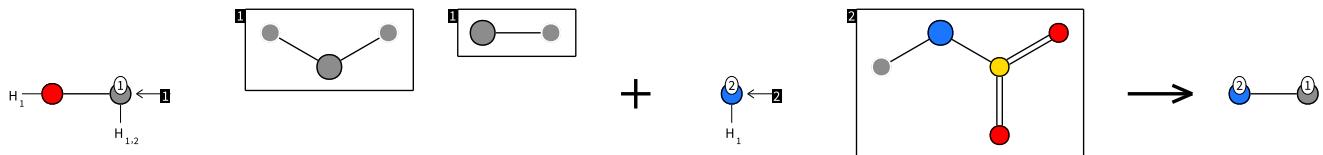
[C;H1&\$([C][#6]),H2&\$([C][#6]):1][OH1].[OH1];\$([Oc1ccccc1]:2)>>[C:1][O:2]



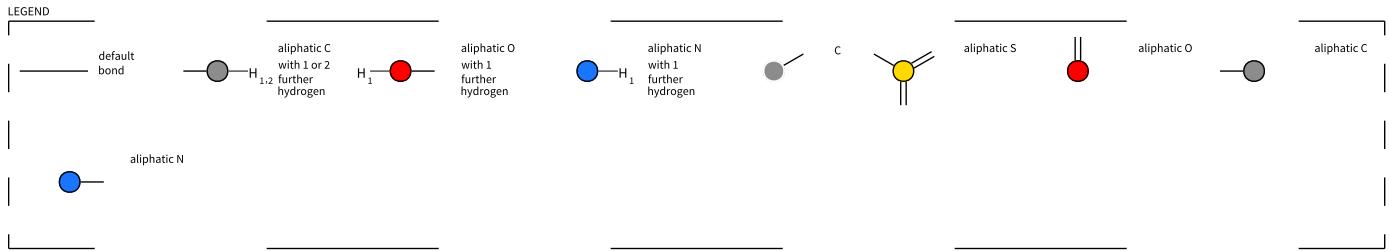
Picture created by the SMARTSviewer [https://smarts.plus/].
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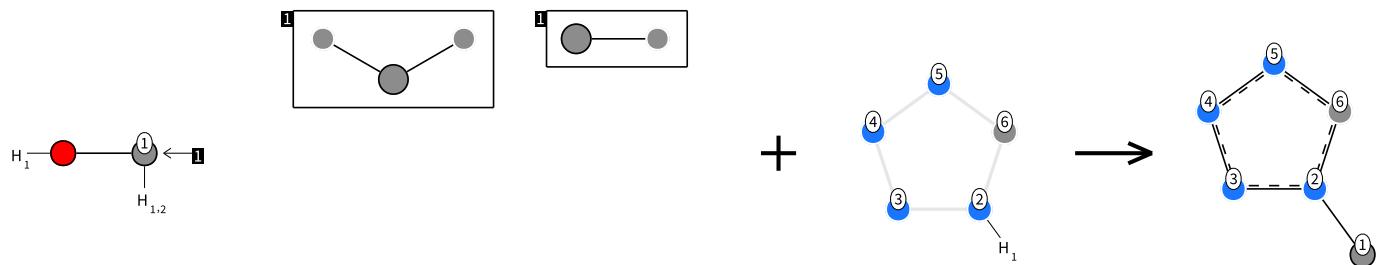
[C;H1&\$([C][#6]),H2\$([C][#6];1)[OH1].[NH1;\$([N][#6])S(=O);2]>>[C:1][N:2]



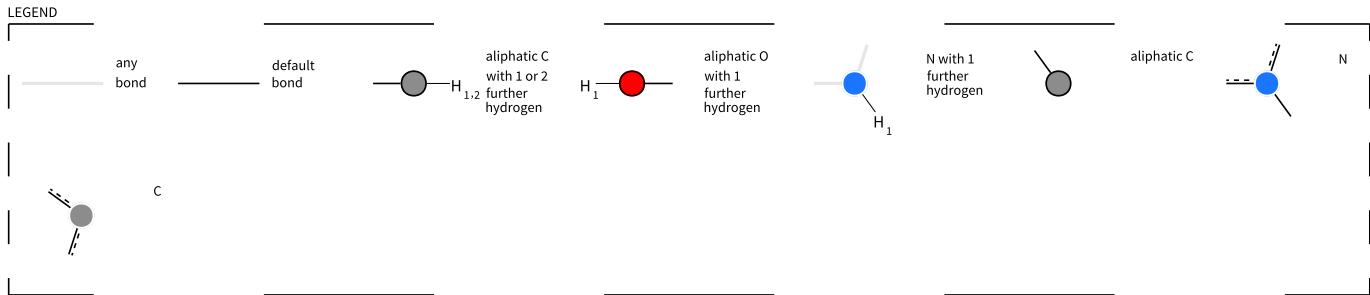
Picture created by the SMARTSviewer (<https://smarts-plus/>).
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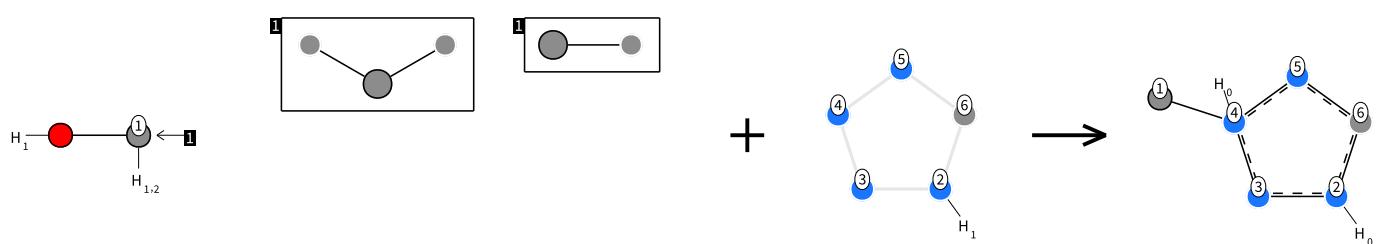
[C;H1&\$C([#6])[#6]),H2&\$C([#6]):1][OH1].[#7H1:2]1-[#7:3]-[#7:4]-[#7:5]-[#6:6]-1>>[C:1][#7:2]1:[#7:3];[#7:4];[#7:5];[#6:6];1



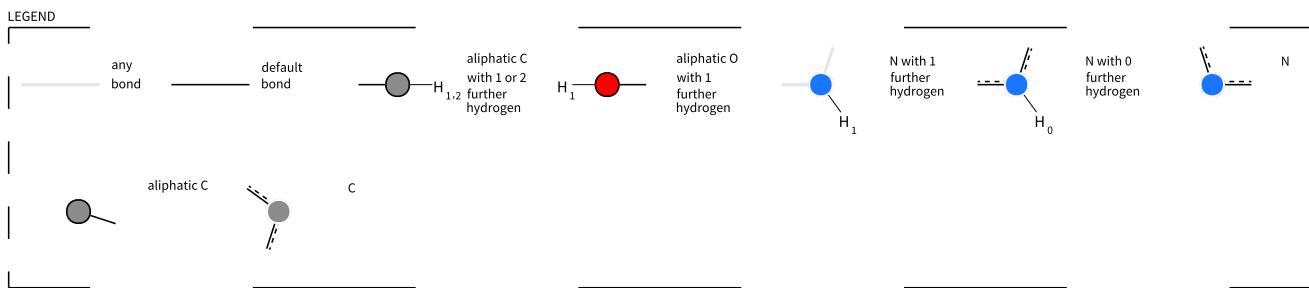
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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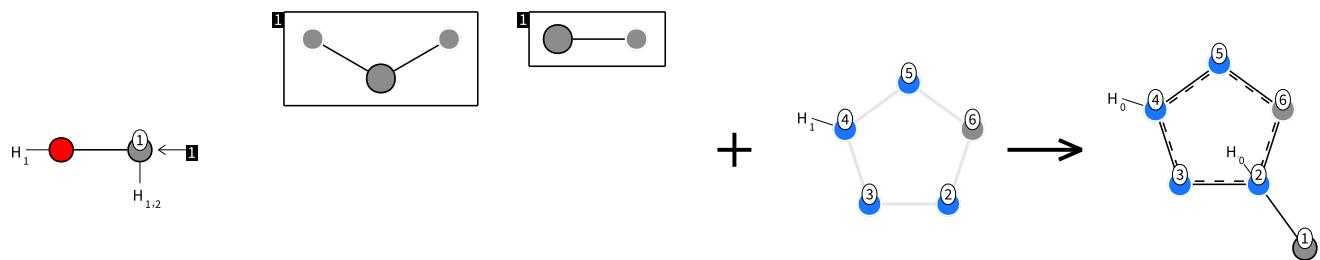
[C;H1&\$([C][#6]),H2&\$([C][#6]):1][OH1].[#7H1:2]1-[#7:3]-[#7:4]-[#6:6]-1>>[#7H0:2]1:[#7:3];[#7H0:4](C:1);[#7:5];[#6:6]:1



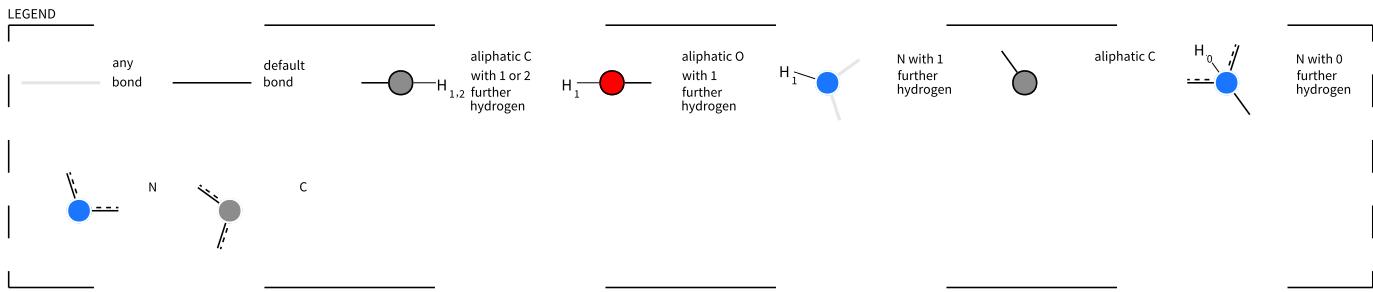
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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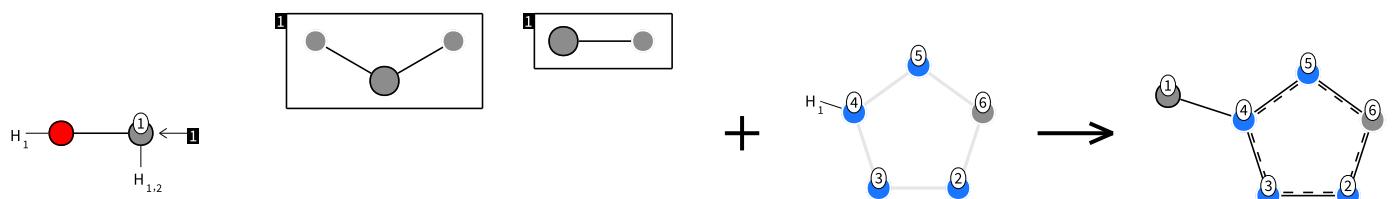
[C;H1&\$([C][#6]),H2&\$([C][#6]):1][OH1].[#7:2]1~[#7:3]~[#7H1:4]~[#7:5]~[#6:6]~1>>[C:1][#7H0:2]1:[#7:3];[#7H0:4];[#7:5];[#6:6];1



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[C;H1&\$([C([#6])#6]),H2&\$([C[#6]):1][OH1],[#7:2]1-[#7:3]-[#7H1:4]-[#7:5]-[#6:6]-1>>[#7:2]1:[#7:3];[#7:4]([C:1]);[#7:5];[#6:6];1

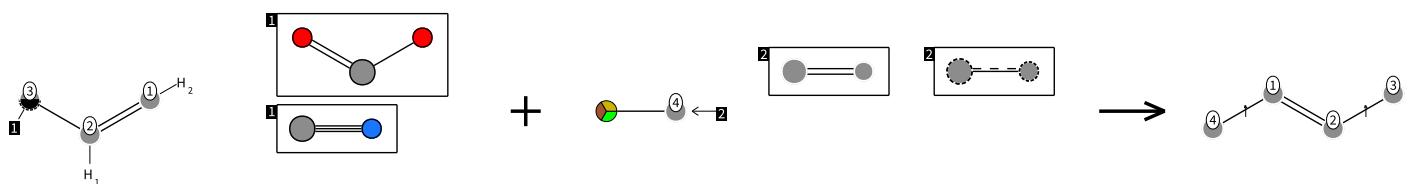


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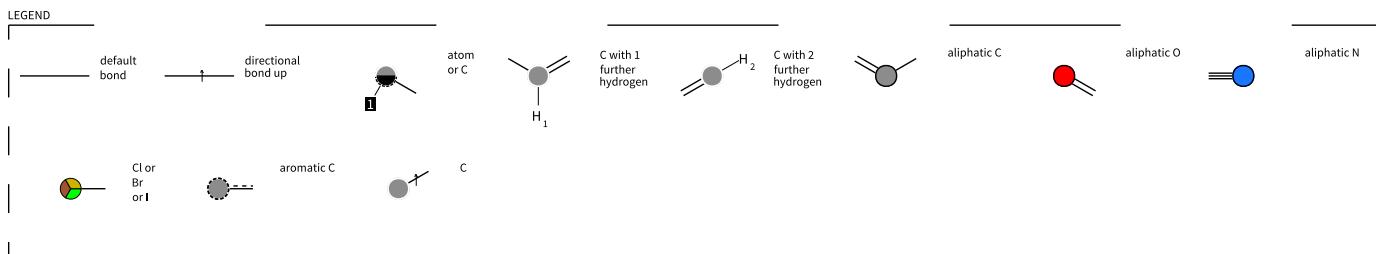
LEGEND

any bond	default bond	aliphatic C with 1 or 2 further hydrogen	aliphatic O with 1 further hydrogen	N with 1 further hydrogen	N	aliphatic C

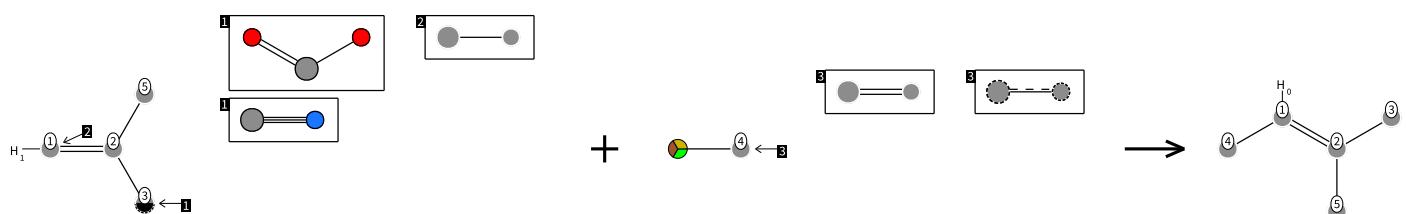
[#6;c,\$(Cl=O)O,\$(C#N);3][#6;H2:1].[#6;\$(#6=[#6]),\$(c:c);4][Cl,Br,I]>>[#6:4]/[#6:1]=[#6:2]/[#6:3]



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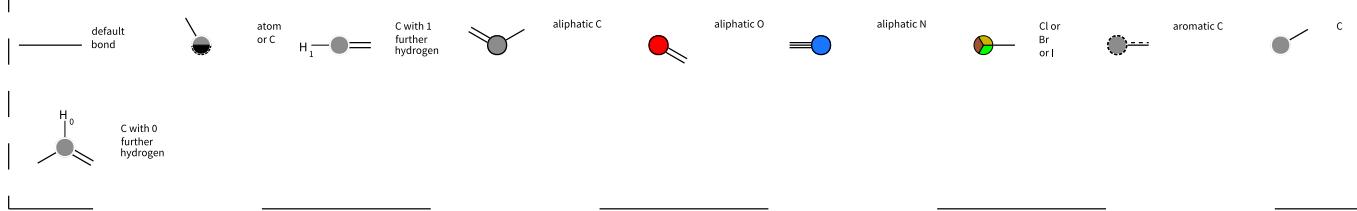


[#6;c,\$(C(=O)O),\$(C#N):3][#6:2]([#6:5])=[#6;H1;S([#6][#6]):1].[#6;\$(#[#6]=[#6]),\$(c:c):4][Cl,Br,I]>>[#6:4][#6;H0:1]=[#6:2]([#6:5])([#6:3])

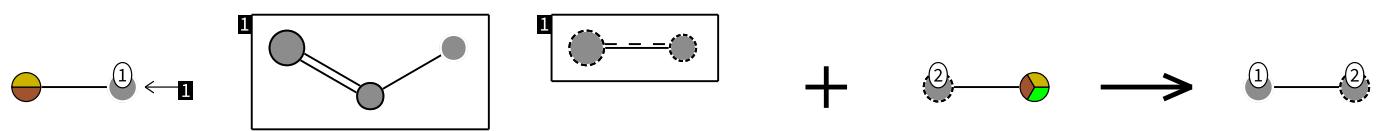


Picture created by the SMARTSviewer [<https://smarts.plus/>].
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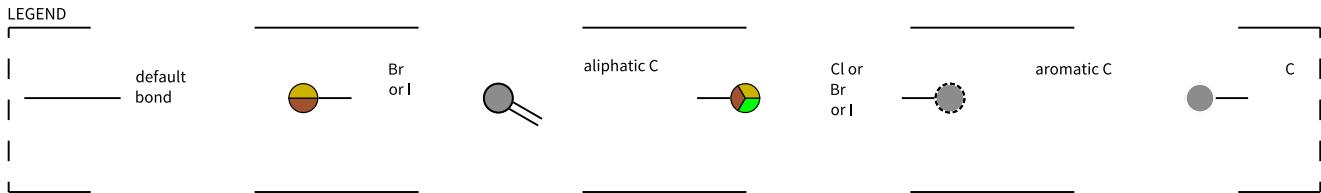
LEGEND



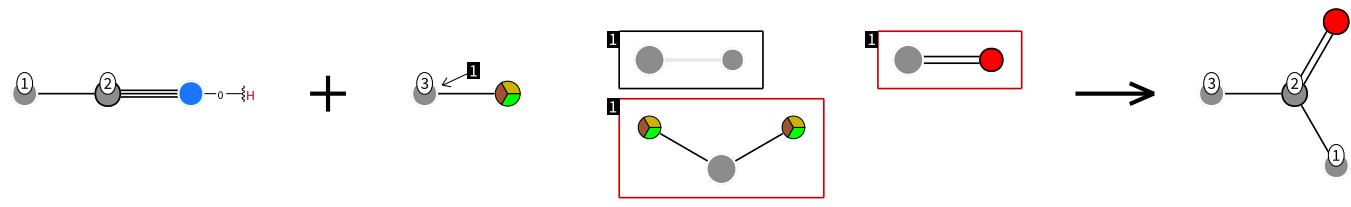
[#6;\$(C=C-[#6]),\$(c:c):1][Br,I].[Cl,Br,I][c:2]>>[c:2][#6:1]



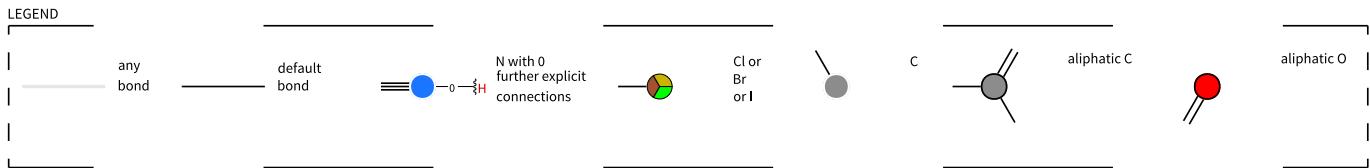
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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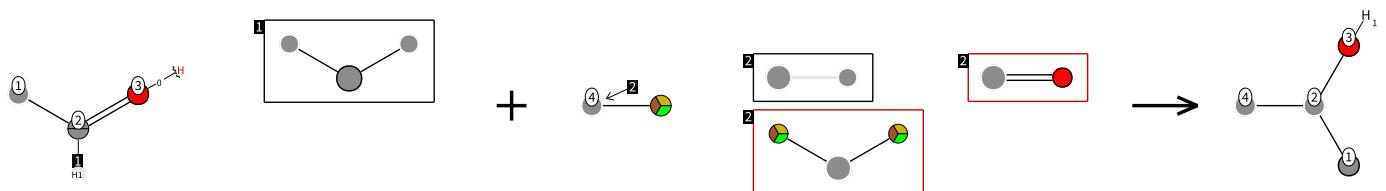
[#6:1][C:2]#[#7:D1].[Cl,Br,I][#6;\${([#6]-[#6]);!\$([#6]([Cl,Br,I])[Cl,Br,I]);!\$([#6]=O);3}>>[#6:1][C:2](=O){#6:3]



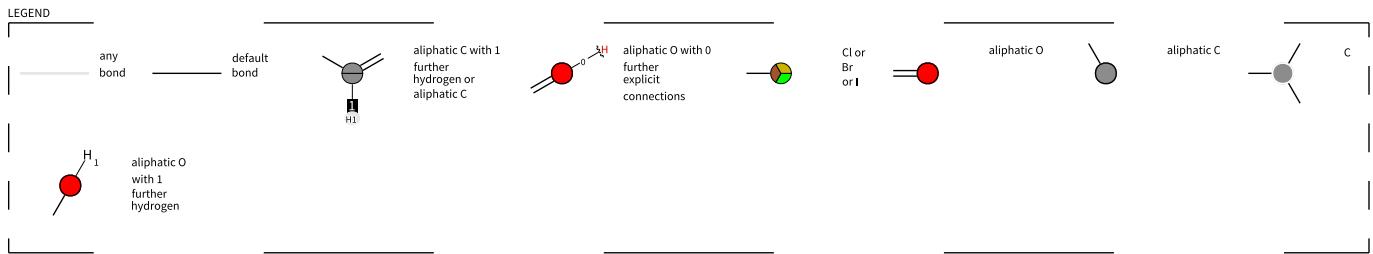
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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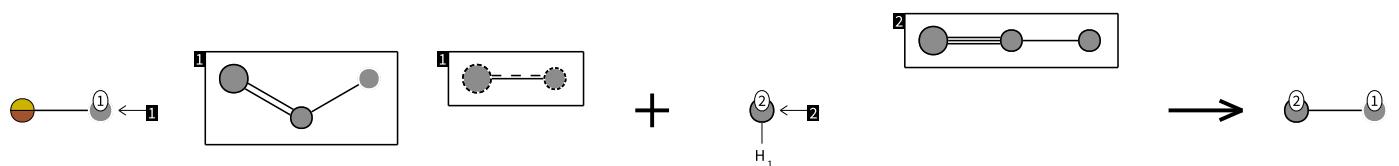
[#6:1][C;H1,\$([C](#6)[#6]):2]=[OD1:3].[Cl,Br,I][#6;\$([#6]-[#6]):\$([#6][[Cl,Br,I]][Cl,Br,I]);\$([#6]=O):4]>>[C:1][#6:2][OH1:3][#6:4]



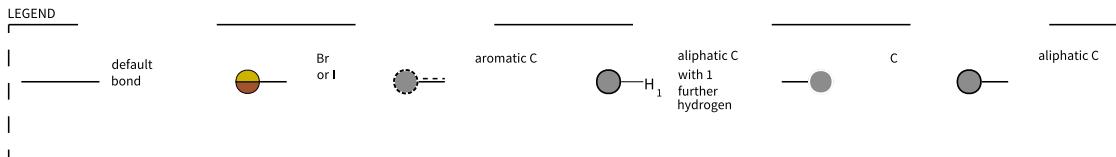
Picture created by the SMARTSviewer [https://smarts.plus/].
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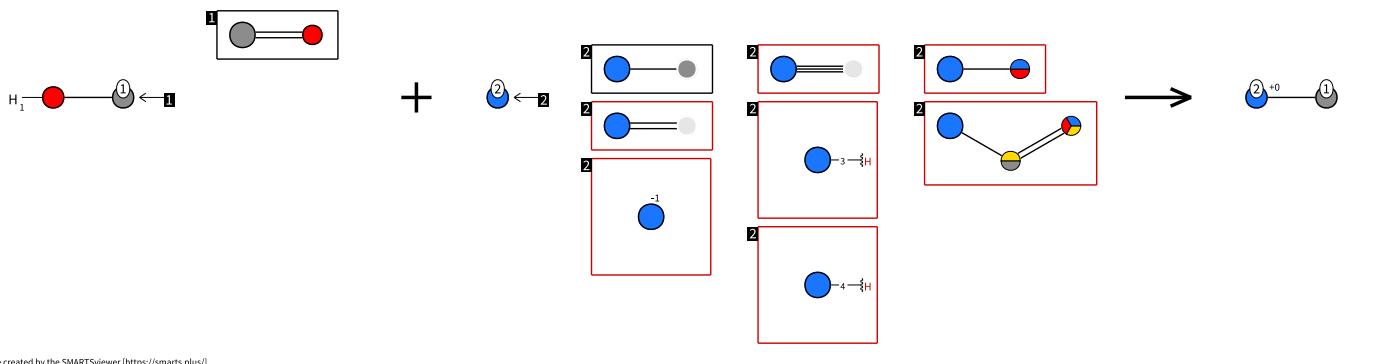
[#6;\$(C=C-{#6}),\$(c:c):1][Br,I].[CH1;\$(C#CC):2]>>[#6:1][C:2]



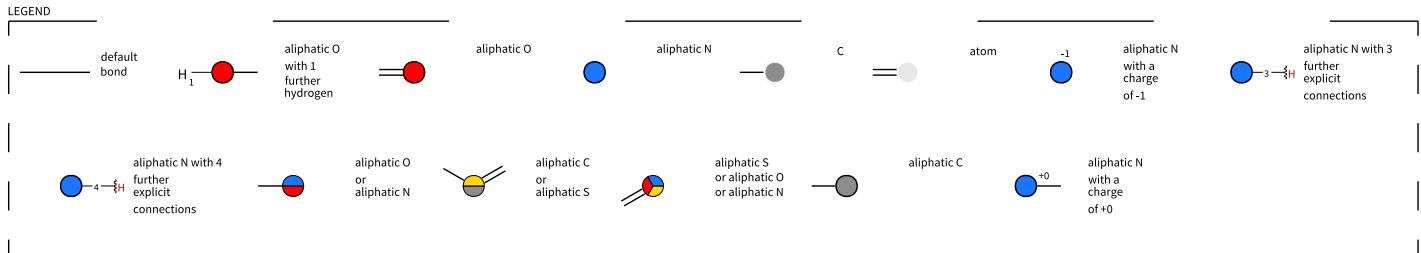
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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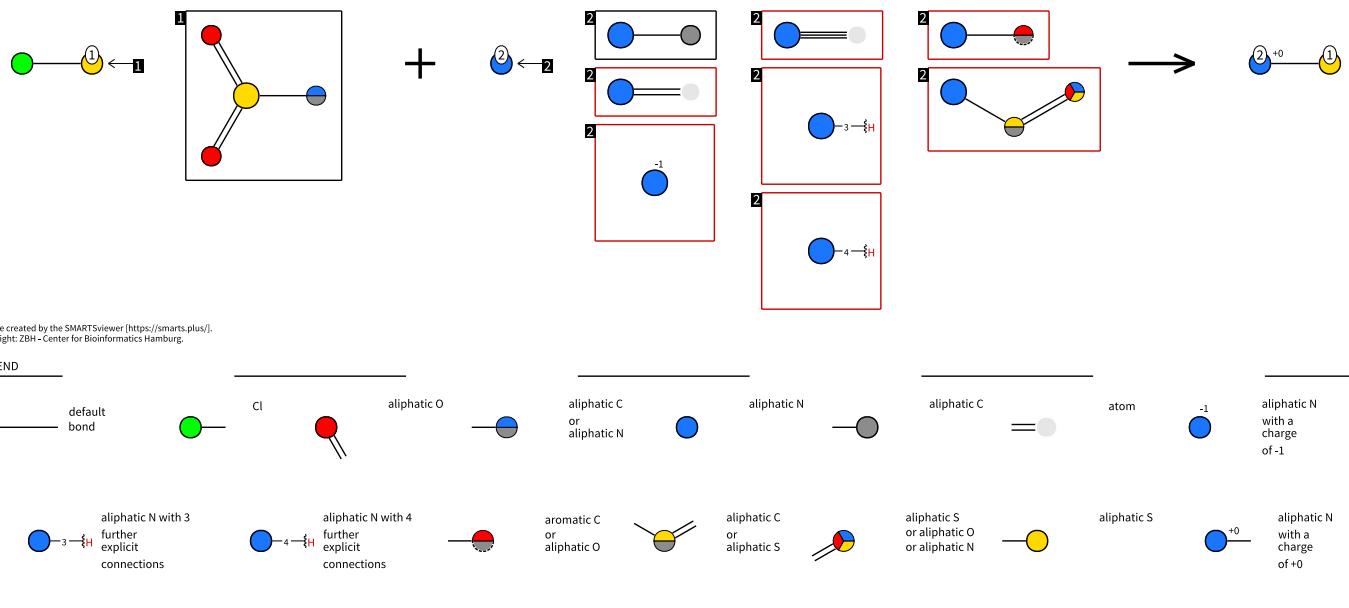
[C;\$(C=O):1][OH1].[N;\$(N[#6]):!\$N(*):!\$([N-]):!\$N(*):!\$([ND3]):!\$([ND4]):!\$([N(O,N)):!\$([N(C,S)=[S,O,N]):2]>[C:1][N+0:2]



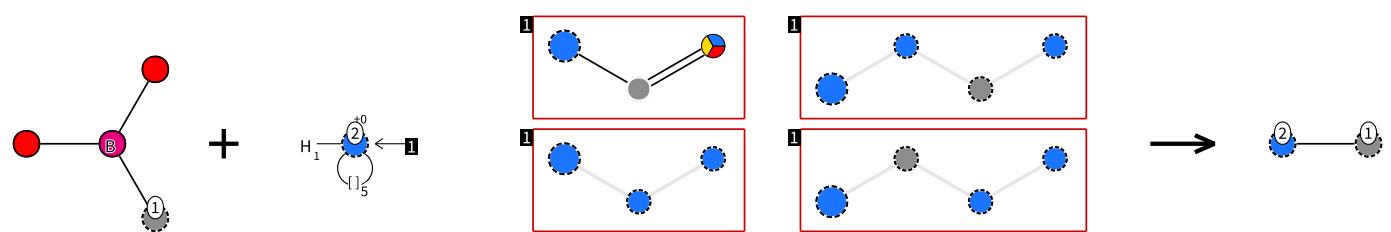
Picture created by the SMARTSviewer [<https://smarts.plus/>].
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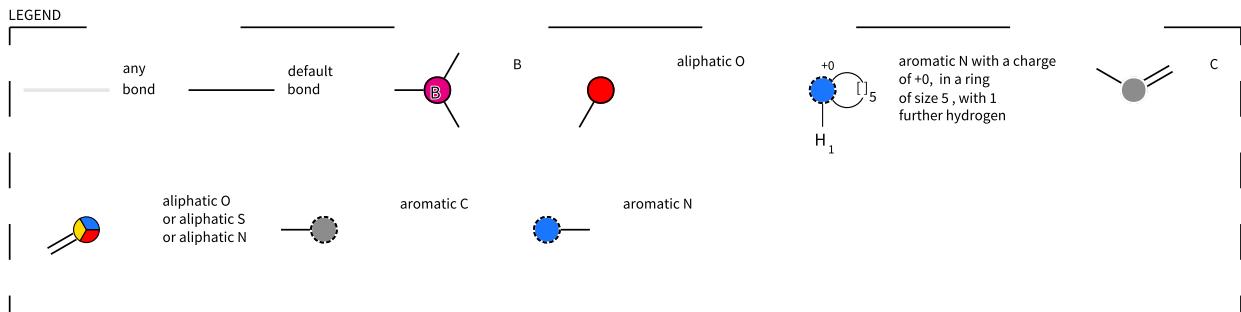
[S:\$(\$(S(=O)(=O)(C,N)):1][Cl].[N;\$(NC);\$(N=*)];\$(N-));\$(NH*);\$(ND3));\$(ND4));\$(Nc,O));\$(N(C,S)=[S,O,N]):2]>>[S:1][N+0:2]



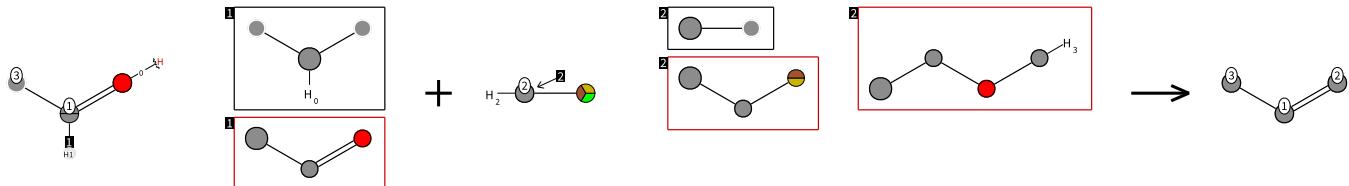
[c:1]B(O)O.[nH1;+0;5;!\$([#6]=[O,S,N]);!\$(n~n~n);!\$(n~n~c~n);!\$(n~c~n~n):2]>>[c:1][n:2]



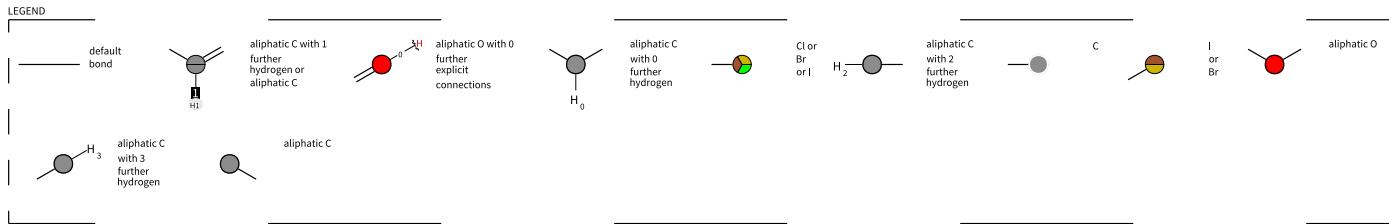
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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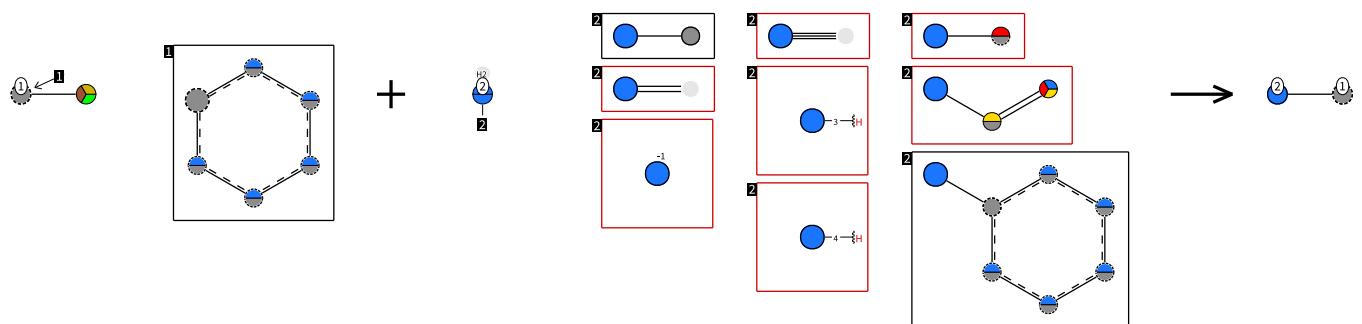


[#6:3]-[C;H1,\$([CHO](-[#6])[#6]);]\$([CC=O]:1)=[OD1].[Cl,Br,I][C;H2;\$([C-:#6]);]\$([CC[I,Br]):2]\$([CCO[CH3]):2]>>[C:3][C:1]=[C:2]

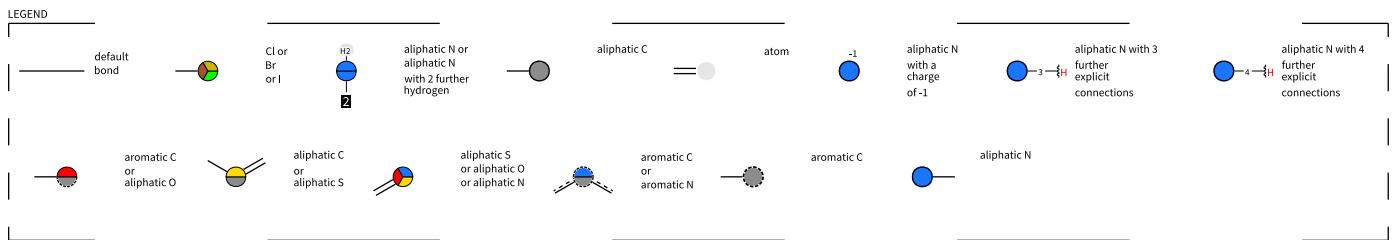


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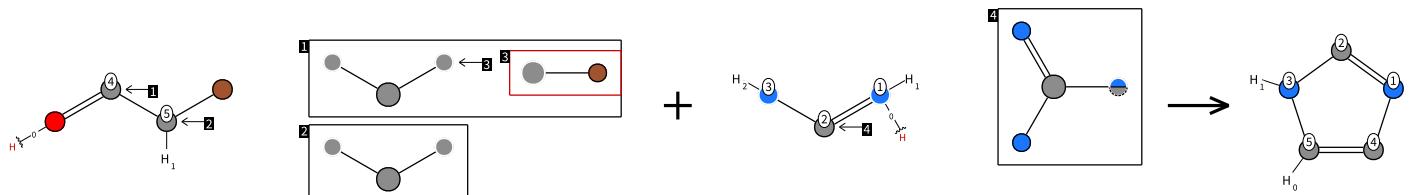




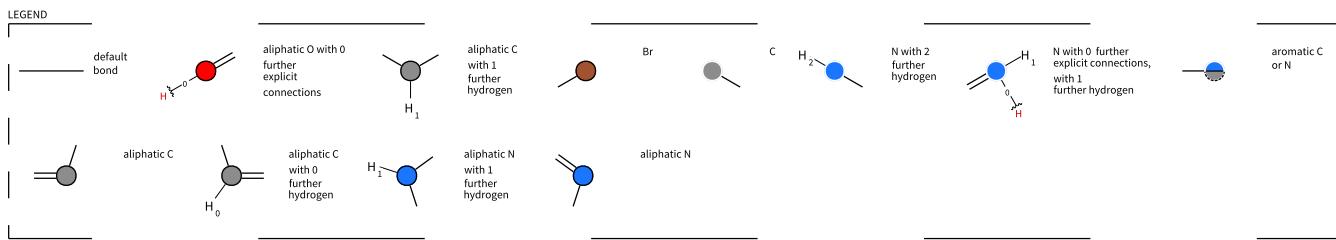
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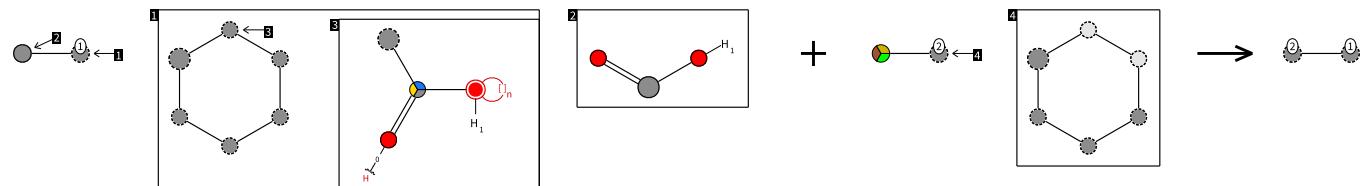
[C;\$(C([#6])[#6;!\$([#6]Br)])]:4]=[OD1]][CH;\$C([#6])[#6]):5]Br.[#7;H2:3][C;\$(C(=N)(N)[c,#7]):2]=[#7;H1;D1:1]>>[C:4]1=[CH0:5][NH:3][C:2]=[N:1]1



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```
[c;$c1[c;$c(C,S,N)(=[OD1])[*;R0;!OH1]]cccc1:1][C;$C(=O)[O;H1]).[c;$c1aacc1:2][Cl,Br,I]>>[c:1][c:2]
```



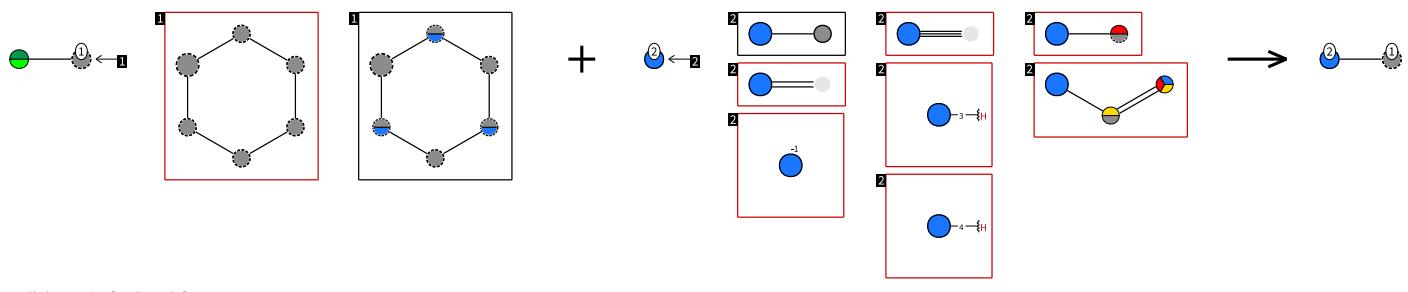
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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LEGEND

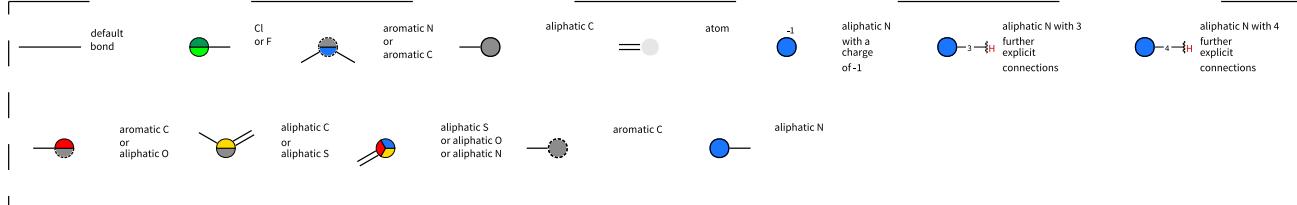
 default bond	 aliphatic C	 aliphatic C or aliphatic S or aliphatic N	 aliphatic O with 0 further explicit connections	 not O with 1 further hydrogen, not in a ring	 aliphatic O	 aliphatic O with 1 further hydrogen	 Cl or Br or I	 aromatic atom
---	--	--	--	---	--	--	--	--

```
[c;$(c1cccccc1);$([c1[n,c)c[n,c)c[n,c]1]:1)[Cl,F].[N;$([NC);!$([N=*);!$([N-]);!$([N#*);!$([ND3)];!$([ND4));!$([N(c,O));!$([N(C,S]=[S,O,N]):2]>>[c:1][N:2]
```

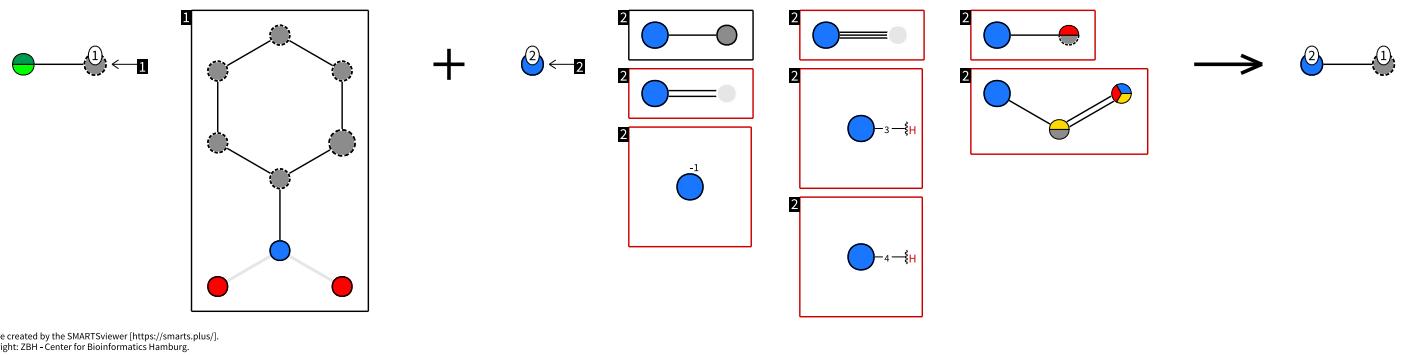


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LEGEND



[c;\$(c1c(N(-O)~O)cccc1):1][Cl,F].[N;\$(NC);!\$(N=*);!\$(N-);!\$(NH*);!\$(ND3));!\$(ND4)];!\$(N(c,O));!\$(N(C,S)=[S,O,N]);2]>[c:1][N:2]

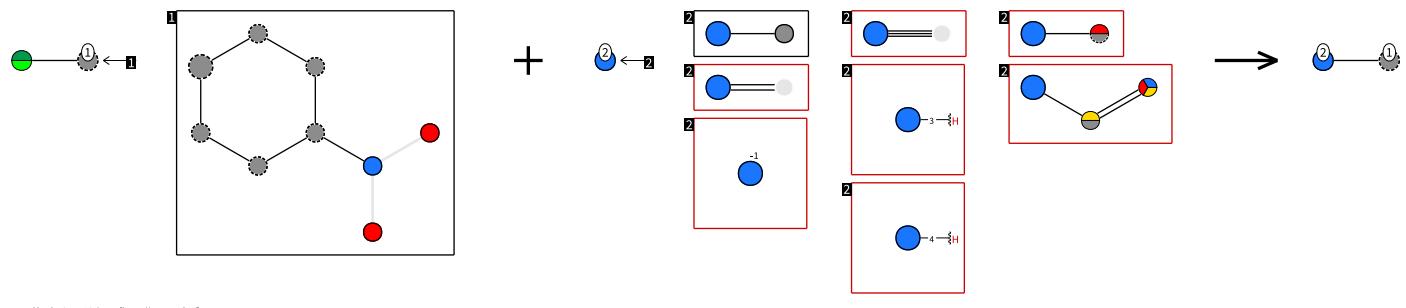


Picture created by the SMARTSviewer (<https://smarts.plus/>).
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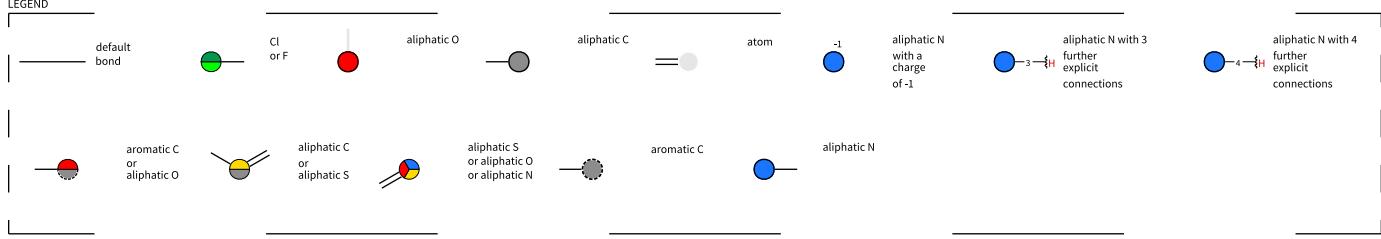
LEGEND

default bond	—
Cl or F	green circle
aliphatic O	red circle
aliphatic C	grey circle
atom	white circle
aliphatic N with a charge of -1	blue circle with -1 superscript
aliphatic N with 3 further explicit connections	blue circle with 3 H atoms
aliphatic N with 4 further explicit connections	blue circle with 4 H atoms
aromatic C or aliphatic O	grey circle with a double bond
aliphatic C or aliphatic S	yellow circle with a double bond
aliphatic S or aliphatic O or aliphatic N	yellow circle with a single bond
aromatic C	grey circle with a single bond
aliphatic N	blue circle with a single bond

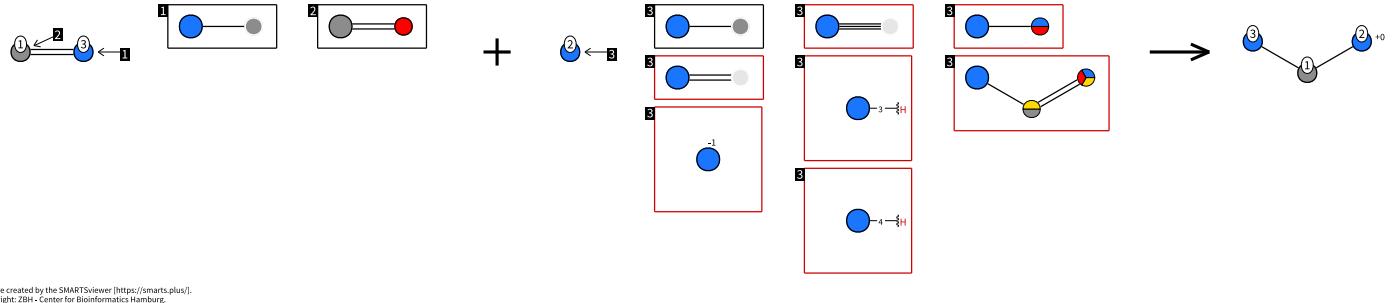
[c;\$(c1ccc(N(~O)~O)cc1):1||Cl,F].[N;S(NC);!S(N=');!S([N-]);!S(NH^+);!S([ND3]);!S([ND4]);!S(N(c,O));!S(N(C,S)=[S,O,N]):2]>>[c:1][N:2]



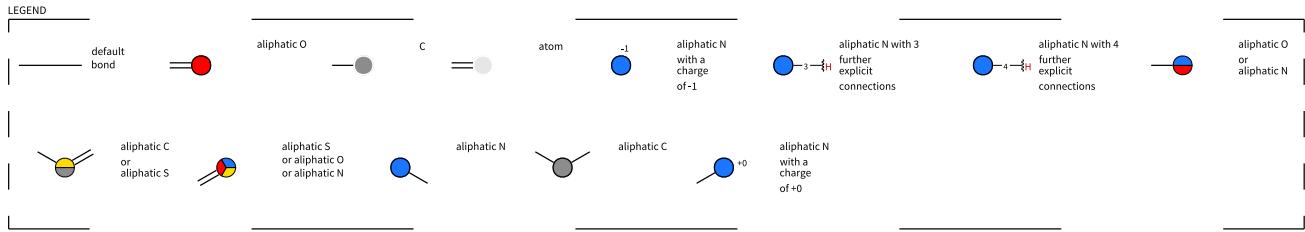
Picture created by the SMARTSviewer (<https://smarts.plus/>).
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[N;\$(N-[#6]):3]=[C;\$(C=O):1].[N;\$(N[#6]):\$[N=)];\$([N-]);\$[N#");\$([ND3]);\$([ND4]);\$[N(O,N)];!\$[N(C,S)=[S,O,N]];2]>[N:3]-[C:1]-[N+0:2]



Picture created by the SMARTSviewer [https://smarts.plus/].
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[N;\$(N-[#6]):3]=[C;\$(C=S):1].[N;\$(N[#6]);\$(N=");\$(N-);\$(N#)];\$(ND3)];\$(ND4)];\$(N(O,N));\$(N(C,S)=[S,O,N]):2]>>[N:3]-[C:1]-[N:0:2]

