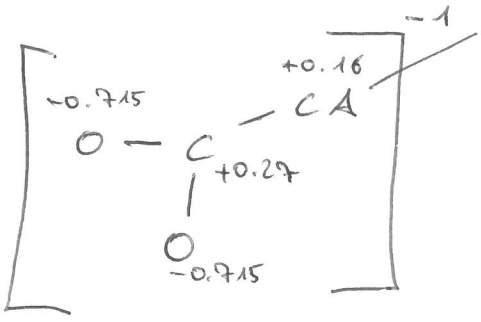
54A8 - terminal modifications

C-terminal:

•) COO^- :

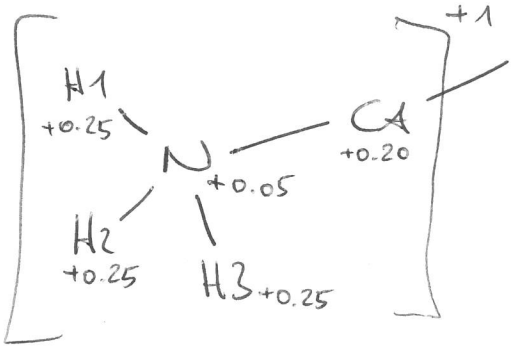


celtosyngroup as in ASP;
charge to 54A7:
- charge charge;
- 4 instead of 3 charges charge compared to COOH;

not affected by charge: COOH, AMD, CME;

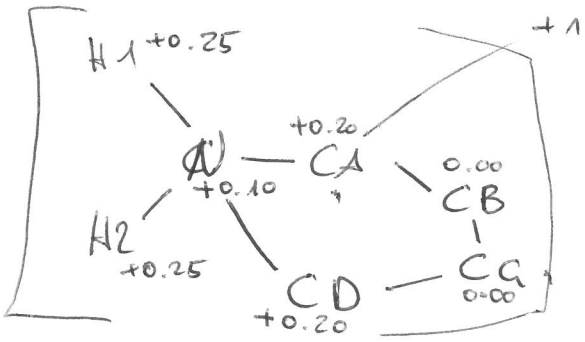
N-terminal:

•) $NH3^+$:
(same for GLY - NH3+)



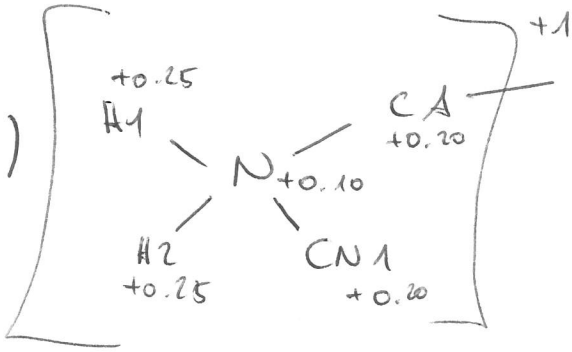
charge to 54A7:
- charge charge;

•) NPRO :
(PRO-NH2+)



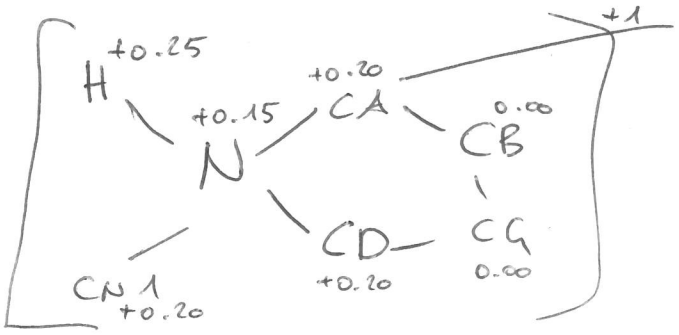
charge to 54A7:
- charge charge;

•) 1NM+ :
(same for GLY-1NM+)



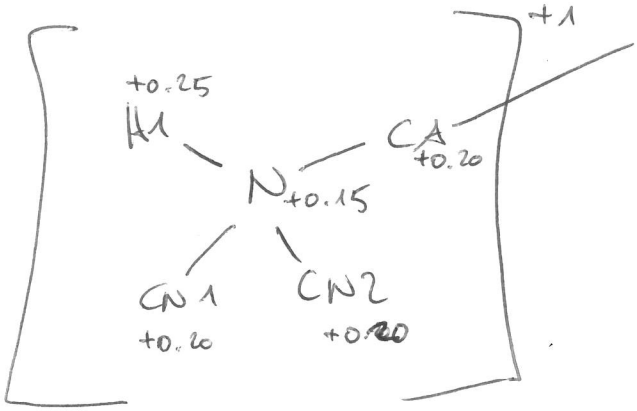
parameters for KMC;

•) PRO-1NM+:



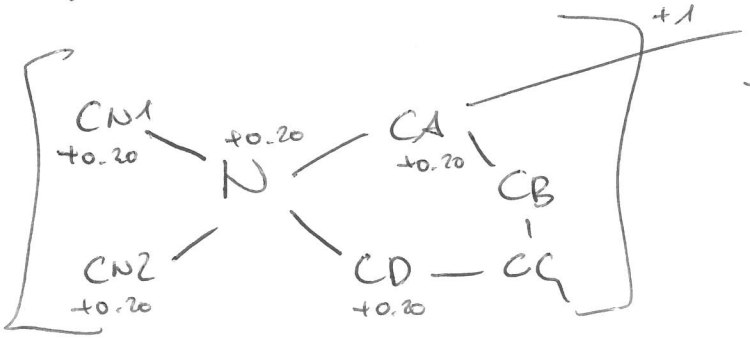
Set H to +0.25, keep CN1 and CA/CD constant and adapt N;

•) 2NM+:
(same for GLY-2NM+)



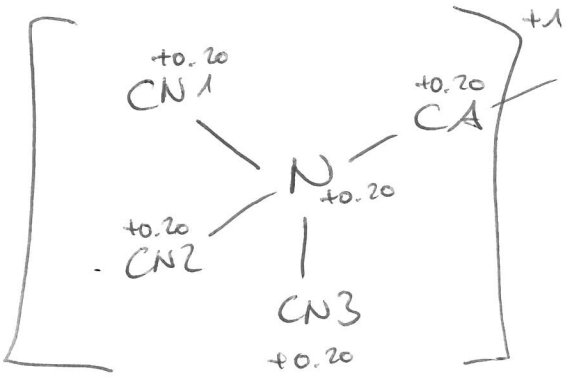
Set H1 to +0.25 and keep the carbons at +0.20, adapt N;

•) ~~PRO~~-2NM+:



keep: is considered like the new (5448) version of K3C;

•) 3NM+:
(same for GLY-3NM+)



keep: is considered like the new (5448) version of K3C;