Electron Donor-Acceptor Complex-Initiated C-H Trifluoromethylation and Perfluoroalkylation of Enamides and Quinoxalinones

Yaqi Song,[a] Tian-Yu Sun,[c] Xiao-Feng Xia [a,b,*] and Dawei Wang [a,*]

[a]Key Laboratory of Synthetic and Biological Colloids, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, Wuxi, Jiangsu, 214122, China. E-mail: xiaxf@jiangnan.edu.cn; wangdw@jiangnan.edu.cn

[b]School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, 453007, China.

[c]Key Laboratory of Computational Chemistry and Drug Design, State Key Laboratory of Chemical Oncogenomics, Shenzhen Key Laboratory of Chemical Genomics, School of Chemical Biology and Biotechnology, Peking University Shenzhen Graduate School, Shenzhen, Guangdong, PR China, 518055 E-mail: Tian-Yu_Sun@pku.edu.cn

Computational details

All density functional theory (DFT) calculations were conducted with the Gaussian 16 program.[1] Geometry optimization was performed with M06-2X[2]/def2SVP[3] level with Grimme's D3 dispersion correction[4]. Frequency analysis was conducted at the same theoretical level to identify the stationary point as an energy minimum. The single point energies were calculated by M06-2X-D3/def2TZVP[5] level with the SMD solvation model[6] (dichloroethane). The CYLview20 software[7] was utilized to draw the 3D visualization.

Reference

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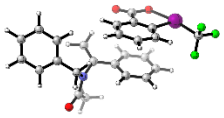
Cartesian Coordinates



C	-1.56589400	2.44259500	-0.19812100
C	-0.70871900	2.31565300	0.89426500
C	0.58572400	1.82986400	0.71552500
C	1.03590800	1.44698900	-0.55602500
C	0.16671400	1.58097100	-1.64847700
C	-1.12412100	2.07049100	-1.46983900
H	-2.57475400	2.83555000	-0.05696800
H	-1.04770300	2.60208500	1.89134600
H	1.25939400	1.74516200	1.57066700
H	0.50522900	1.29922500	-2.64648500
H	-1.78449200	2.16522300	-2.33377600
C	2.40616400	0.89568400	-0.73279000
N	3.37132700	1.26900100	0.25313000
C	2.72582100	0.02517300	-1.70055400
H	3.75164600	-0.33662600	-1.79077500
H	1.96405400	-0.36907300	-2.37751700
C	3.73656800	0.27573700	1.26225700
H	2.82007300	-0.25899700	1.55323300
H	4.11465900	0.83382900	2.12912700
C	3.99340700	2.49752200	0.27569300
C	3.55838800	3.48425900	-0.78572100
H	3.69017400	3.05716700	-1.78916400
H	2.49456400	3.73540300	-0.67050700
H	4.16844400	4.38601400	-0.67541000
O	4.84603100	2.76180200	1.09952500
C	4.77768500	-0.71044100	0.78634100
C	6.09078900	-0.27932700	0.55687500
C	4.44474000	-2.04221700	0.53074100
C	7.04665900	-1.16990800	0.07476500
H	6.34564800	0.76326700	0.76184600
C	5.40235700	-2.93671300	0.05047200
H	3.41916700	-2.38115900	0.69902600
C	6.70492900	-2.50012300	-0.18009900
H	8.06737500	-0.82639400	-0.10092200
H	5.12777600	-3.97379900	-0.14810100
H	7.45605500	-3.19540400	-0.55798100
C	-1.83315100	-0.97052300	1.83145100
C	-1.90261200	-0.96815400	0.44460200
C	-0.85928300	-1.34974000	-0.37960400
C	0.32783100	-1.78102600	0.21687300

C	0.43513800	-1.81073900	1.60387100
C	-0.63413800	-1.39838600	2.40276900
H	-2.65960300	-0.66409600	2.46840600
H	1.14443500	-2.08042600	-0.44354700
H	1.35446300	-2.16098000	2.07612200
H	-0.54508100	-1.41702000	3.48968800
O	-2.19810700	-0.96783300	-2.27521800
I	-3.63541200	-0.43353100	-0.67238800
C	-4.74581400	0.13285400	1.16828100
F	-4.94191000	-0.87153000	2.01290900
F	-5.92998300	0.57328900	0.75966700
F	-4.14071300	1.11348200	1.83082200
C	-1.00480200	-1.28875200	-1.89195700
O	-0.05320200	-1.51302100	-2.60478000

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C	-0.00050700	0.61671300	2.42905300
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C	-1.79218900	1.78160200	1.27465800
C	-2.71775200	0.90336900	1.85945700
C	-2.30033800	-0.11146100	2.70309000
H	-0.58746900	-1.05533000	3.62967900
H	1.05568500	0.47339400	2.64659400
H	-3.76751900	1.05304400	1.60423000
H	-3.02449700	-0.79716000	3.14356700
C	-1.41735400	3.52232700	-0.16219500
C	0.04951000	3.49025800	0.06444500
H	-1.75319400	4.27277200	-0.88437800
N	-2.26588800	2.75306400	0.40566100
O	0.81667100	4.24932700	-0.48876500
N	0.47307200	2.55248200	0.99874500
C	1.89781700	2.54452200	1.33125300
H	2.26100100	3.55443500	1.10465200
H	2.00525400	2.36876000	2.40965200
C	2.68975000	1.52913400	0.53602500
C	2.75936600	1.64719900	-0.85917000
C	3.33712100	0.46155200	1.16331000
C	3.45438800	0.69883100	-1.60774800

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C	4.02254100	-0.49640200	0.41299100
H	3.30473000	0.37112700	2.25245600
C	4.08070900	-0.37882000	-0.97587300
H	3.49708400	0.79802500	-2.69338000
H	4.51162900	-1.33288500	0.91408600
H	4.61731200	-1.12397400	-1.56540100
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C	-1.55567600	-1.22422300	-0.66191100
C	-2.17812700	-0.19072900	-1.34372400
C	-3.57213700	-0.16665100	-1.38624500
C	-4.30187000	-1.16705000	-0.75075100
C	-3.64263000	-2.19648100	-0.07522100
H	-1.75124200	-3.04749300	0.51668300
H	-4.04218100	0.66186300	-1.91880500
H	-5.39205100	-1.14911300	-0.77838600
H	-4.21556800	-2.97983700	0.42298400
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I	0.56404100	-1.04584500	-0.70762000
C	0.83394200	-2.97789200	0.35930800
F	0.35653700	-2.94906900	1.60168800
F	2.14552300	-3.18473900	0.42795100
F	0.28181000	-4.01283800	-0.26220500
C	-1.36364500	0.92020300	-1.98837800
O	-1.90433600	1.77362400	-2.64791600