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# Crystal Structure and DFT calculations of (6*E*)-6-({[2–methoxy-5- (trifluoromethyl) phenyl] amino} methylidene)-4–nitrocyclohexa-2,4–dien–1-one

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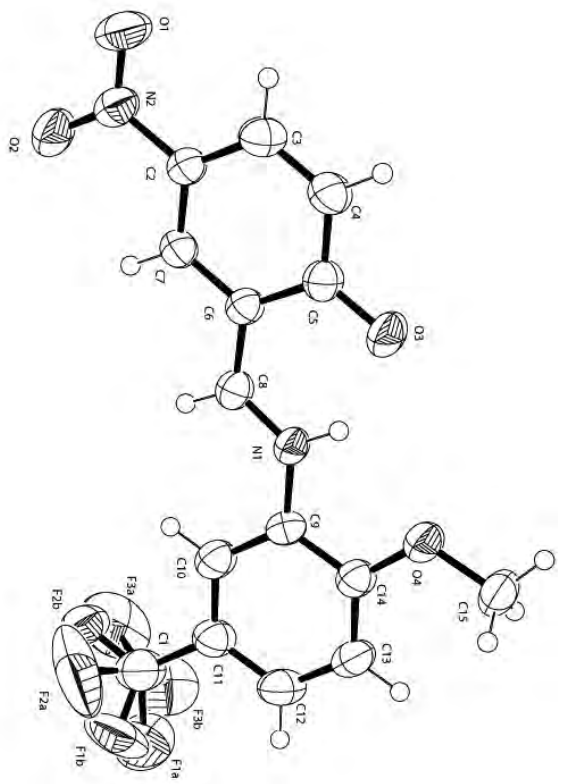
The crystal structure of (6*E*)-6-({[2-methoxy-5-(trifluoromethyl)phenyl]amino}methylidene)-4-nitrocyclohexa-2,4-dien-1-one ($C_{15}H_{11}F_3N_2O_4$) has been determined by means of single-crystal X-ray diffraction methods. The title compound $C_{15}H_{11}F_3N_2O_4$ is a Schiff base that adopts the ketol-amine tautomeric form in the solid state. Whole molecule is nearly planar with dihedral angle 6.19(10)$^o$ between the aromatic rings. The title compound crystallizes in the trigonal space group R-3 with the unit cell parameters: a=33.0238(17), b=33.0238(17), c= 7.1144(4)Å, α=90, b=90, γ=120 ($^o$), V= 6757.1(8)Å$^3$, Z=18. The molecular structure is stabilized by two N-H…O type intramolecular H bond , two C-H··O type intermolecular hydrogen bonds and a N-O…π and five π-π interactions. X-ray measurements was carried out on a STOE IPDS II diffractometer with Mo$K_\alpha$ radiation. The molecular structure was solved by direct method using SHELXS-97 and refinement by full-matrix least-squares on F$^2$ using SHELXL-14 program. An ortep-3 view of the molecule of title compound is shown in Fig.1.

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