Is there a quadruple Fe-C bond in $FeC(CO)_3$

Supplementary information

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The optimized structures and SCF energies of $FeC(CO)_3$ at the various levels of theory discussed in the paper are reported in the following. Energies in atomic units, coordinates in Angstrom.

B3LYP (SCF Energy: -1641.94773209)

Fe	0.000000	0.000000	0.135917
C	0.000000	1.813098	-0.235035
C	-1.570189	-0.906549	-0.235035
C	1.570189	-0.906549	-0.235035
O	0.000000	2.940042	-0.386495
O	-2.546151	-1.470021	-0.386495
O	2.546151	-1.470021	-0.386495
C	0.000000	0.000000	1.662110

M062X (SCF Energy: -1641.62310179)

Fe	-0.000000	-0.000000	0.151833
C	-0.000000	1.846191	-0.245841
C	-1.598848	-0.923095	-0.245841
C	1.598848	-0.923095	-0.245841
O	-0.000000	2.965208	-0.383550
O	-2.567945	-1.482604	-0.383550
O	2.567945	-1.482604	-0.383550
C	-0.000000	-0.000000	1.633761

MN15 (SCF Energy: -1641.64499366)

Fe	0.000000	0.000000	0.139720
C	0.000000	1.811301	-0.239026
C	-1.568633	-0.905650	-0.239026
C	1.568633	-0.905650	-0.239026
O	0.000000	2.938619	-0.382345
O	-2.544919	-1.469310	-0.382345
O	2.544919	-1.469310	-0.382345
C	0.000000	0.000000	1.641007

PBE0 (SCF Energy: -1641.24482796)

Fe	0.000000	0.000000	0.103491
C	0.000000	1.798980	-0.226052
C	-1.557962	-0.899490	-0.226052
C	1.557962	-0.899490	-0.226052
O	0.000000	2.927557	-0.347050
O	-2.535339	-1.463779	-0.347050
O	2.535339	-1.463779	-0.347050
C	0.000000	0.000000	1.617896

ωB97X-D (SCF Energy: -1641.77947185)

Fe	0.000000	0.000000	0.130281
C	0.000000	1.810000	-0.233751
C	-1.567506	-0.905000	-0.233751
C	1.567506	-0.905000	-0.233751
O	0.000000	2.933661	-0.375846
O	-2.540625	-1.466830	-0.375846
O	2.540625	-1.466830	-0.375846
C	0.000000	0.000000	1.640086

Hartree-Fock (SCF Energy: -1638.31921499)

Fe	0.000000	0.000000	0.328940
C	0.000000	1.874088	-0.327537
C	-1.623007	-0.937044	-0.327537
C	1.623007	-0.937044	-0.327537
O	0.000000	2.950635	-0.565095
O	-2.555324	-1.475317	-0.565095
O	2.555324	-1.475317	-0.565095
C	0.000000	0.000000	1.817584

MP2 (MP2 Energy: -1640.3382338949)

Fe	-0.000000	-0.000000	0.023327
C	-0.000000	-0.000000	1.677074
C	0.000000	1.733905	-0.248897
C	1.501606	-0.866953	-0.248897
O	-1.501606	-0.866953	-0.248897
O	0.000000	2.892545	-0.257867
O	-2.505017	-1.446273	-0.257867
C	2.505017	-1.446273	-0.257867

CCSD (CCSD energy: -1640.0612990777)

Fe	0.14989685	0.00000000	-0.00000000
C	1.68897376	0.00000000	-0.00000000
C	-0.25803213	0.91780077	-1.58967756
C	-0.25803213	-1.83560154	0.00000000
C	-0.25803213	0.91780077	1.58967756
O	-0.40352408	1.47980302	-2.56309402
O	-0.40352408	-2.95960605	0.00000000
O	-0.40352408	1.47980302	2.56309402

CCSD(T) (CCSD(T) energy: --1640.1862953122)

Fe	0.15881791	0.00000000	-0.00000000
C	1.71824933	0.00000000	-0.00000000
C	-0.25384445	0.90880224	-1.57409165
C	-0.25384445	-1.81760447	0.00000000
C	-0.25384445	0.90880224	1.57409165
O	-0.42438617	1.47424174	-2.55346159
O	-0.42438617	-2.94848347	0.00000000
O	-0.42438617	1.47424174	2.55346159

CASSCF (CASSCF energy: -1638.5923250507)

Fe	0.14314723	0.00000000	-0.00000000
C	1.71577019	0.00000000	-0.00000000
C	-0.26372588	0.95608019	-1.65597946
C	-0.26372588	-1.91216038	0.00000000
C	-0.26372588	0.95608019	1.65597946
O	-0.39808574	1.50912771	-2.61388587
O	-0.39808574	-3.01825542	0.00000000
O	-0.39808574	1.50912771	2.61388587