The supplementary information for

A theoretical study on the adsorption of 5-fluorouracil on B_{40}, $B_{39}M$, and $M@B_{40}$ (M = Mg, Al, Si, Mn, Cu, and Zn) nanocages: Implications for drug delivery

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1. Tables

Table S1 The relatively energies (kcal/mol) of $Mn@B_{40}$ and $B_{39}Mn$ clusters with various spin multiplicities at the B3LYP-D3/6-31G(d)&SDD level.

	Spin Multiplicities						
	singlet	doublet	triplet	quartet	quintet	sextet	septet
$Mn@B_{40}$		26.91		**0.00**		8.97	
$B_{39}Mn$	74.47		43.20		**0.00**		25.96

Table S2 The relatively large second order perturbation energies (E^2, in kcal/mol) for the critical donor-acceptor NBO interactions of the most stable 5-Fu@B_{40}, 5-Fu@[M@B_{40}] and 5-Fu@B_{39}M (M = Mg, Al, Si, Mn, Cu, and Zn) complexes at the SMD-M06-2X-D3/6-311+G(d, p)&SDD level.

Complex	Donor NBO (i)	Acceptor NBO (j)	E^2
5-Fu@B_{40}	BD (C6-O2)	LP*(B25)	32.20
	LP (O2)	LP*(B25)	359.57
	CR (O2)	LP*(B25)	16.47
5-Fu@[Mg@B_{40}]	BD (C7-O1)	LP*(B36)	36.28
	LP (O1)	LP*(B36)	368.35
	CR (O1)	LP*(B36)	17.58
5-Fu@[Al@B_{40}]	BD (C7-O1)	LP*(B26)	18.36
	LP (O1)	LP*(B26)	188.53
	CR (O1)	LP*(B26)	9.63
5-Fu@[Si@B_{40}]	BD (C6-O2)	LP*(B35)	32.20
	LP (O2)	LP*(B35)	359.30
	CR (O2)	LP*(B35)	16.53
5-Fu@[Mn@B_{40}]	BD (C6-O2)	BD*(B1-B7)	71.43
	LP (O2)	LP*(B7)	344.90
	CR (O2)	BD*(B6-B7)	3.30
5-Fu@[Cu@B_{40}]	BD (C7-O1)	LP*(B25)	23.69
	LP (O1)	LP*(B25)	221.49
	CR (O1)	LP*(B25)	11.73
5-Fu@[Zn@B_{40}]	BD (C6-O2)	LP*(B17)	32.77
	LP (O2)	LP*(B17)	350.32
	CR (O2)	LP*(B17)	16.44
5-Fu@B_{39}Mg	BD (C6-O2)	LP*(Mg52)	6.16
	LP (O2)	LP*(Mg52)	27.57
	CR (O2)	LP*(Mg52)	4.04
5-Fu@B_{39}Al	BD (C6-O2)	LP*(Al40)	14.40
	LP (O2)	LP*(Al40)	79.96

	CR (O2)	LP*(Al40)	10.64
5-Fu@$B_{39}Si$	BD (C6-O2)	LP*(B17)	17.63
	LP (O2)	LP*(B17)	190.68
	CR (O2)	LP*(B17)	9.18
5-Fu@$B_{39}Mn$	BD (C6-O2)	LP*(Mn52)	4.27
	LP (O2)	LP*(Mn52)	27.01
	CR (O2)	LP*(Mn52)	3.42
5-Fu@$B_{39}Cu$	BD (C6-O2)	LP*(Cu52)	2.87
	LP (O2)	LP*(Cu52)	27.40
	CR (O2)	LP*(Cu52)	2.53
5-Fu@$B_{39}Zn$	BD (C6-O2)	LP*(Zn52)	2.46
	LP (O2)	LP*(Zn52)	8.89
	CR (O2)	LP*(Zn52)	2.22

“BD”≈ 2-center bond; “CR”≈1-center core pair; “LP”≈1-center valence lone pair

2. Figures

Figure. S1 The ESP plots in conjunction with the extreme values for $M@B_{40}$ (M = Mg, Al, Si, Mn, Cu, and Zn) cages. The yellow and cyan balls correspond to the maximum and minimum point of electrostatic potential, respectively.

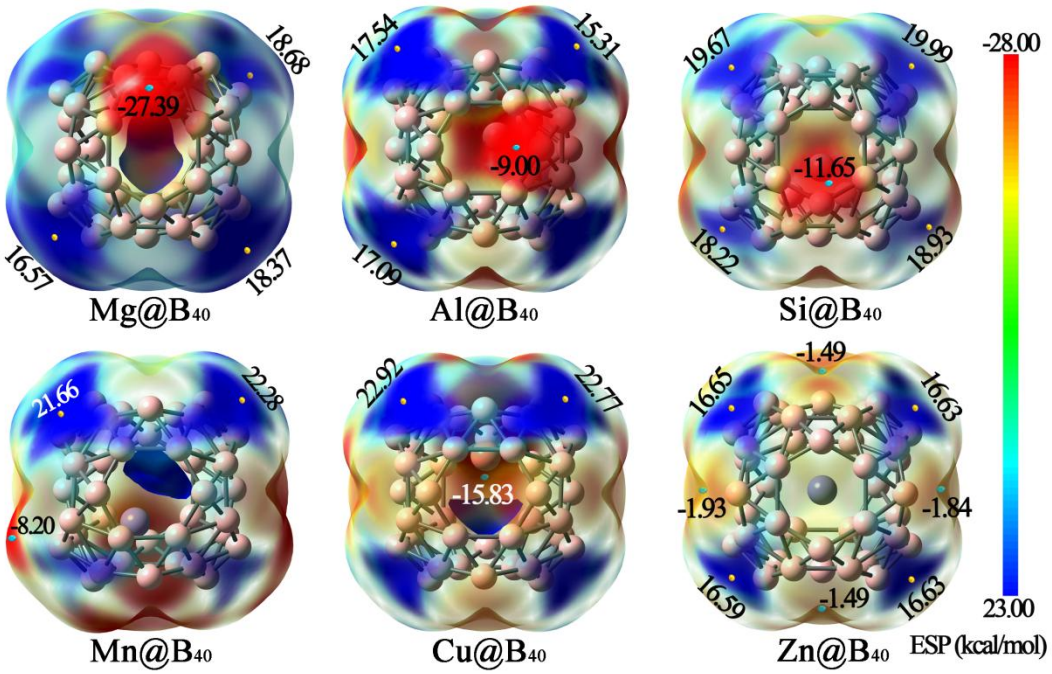


Figure. S2 LMOs related to the B-O bonds in 5-Fu@[M@B_{40}] (M = Mg, Al, Si, Mn, Cu, and Zn) complexes. The contributions of linked atoms to LMO are also given next to them.

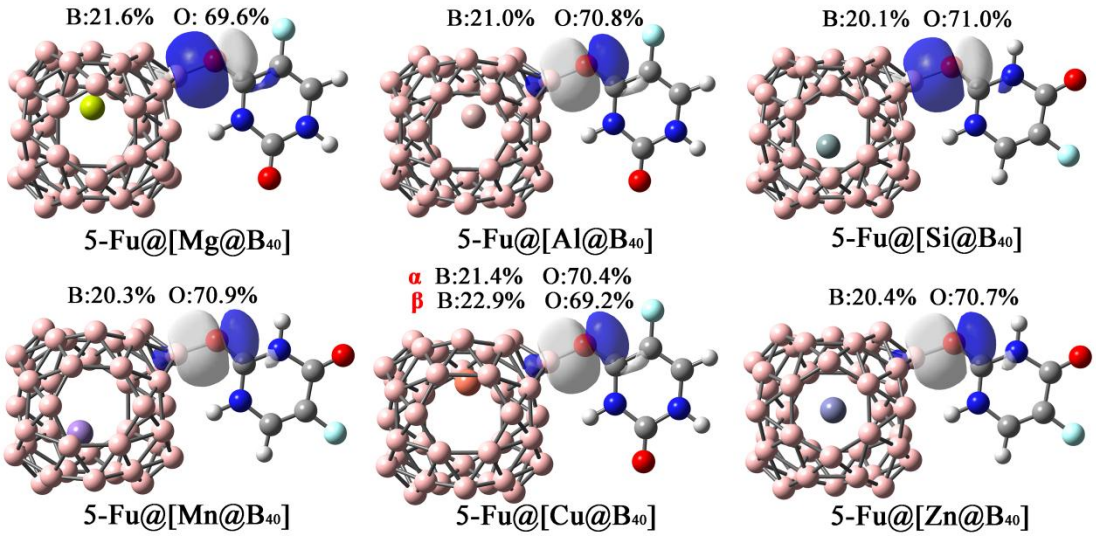


Figure. S3 ELF plots for 5-Fu@[M@B_{40}] (M = Mg, Al, Si, Mn, Cu, and Zn).

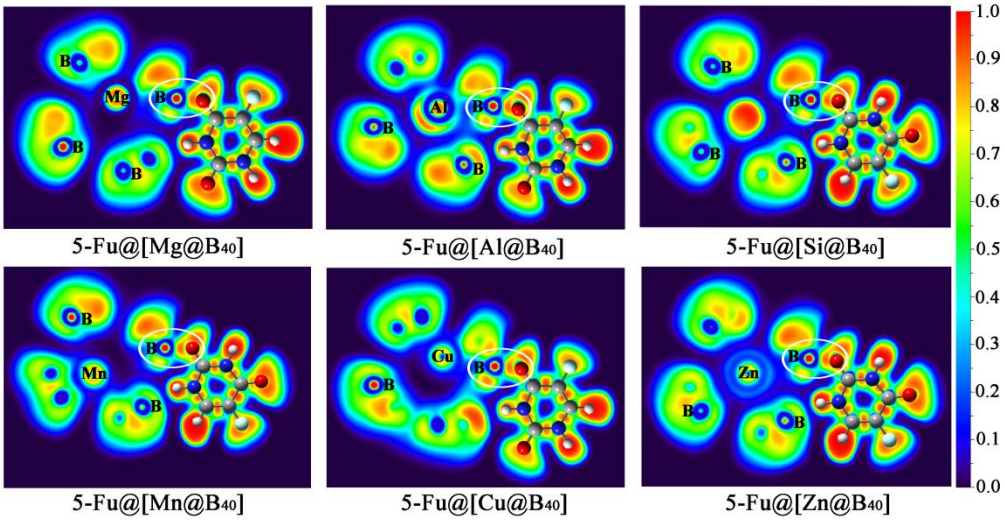


Figure. S4 The HOMO and LUMO orbitals of 5-Fu@[M@B_{40}] (M = Mg, Al, Si, Mn, Cu, and Zn) complexes with isovalue of 0.02 a.u.

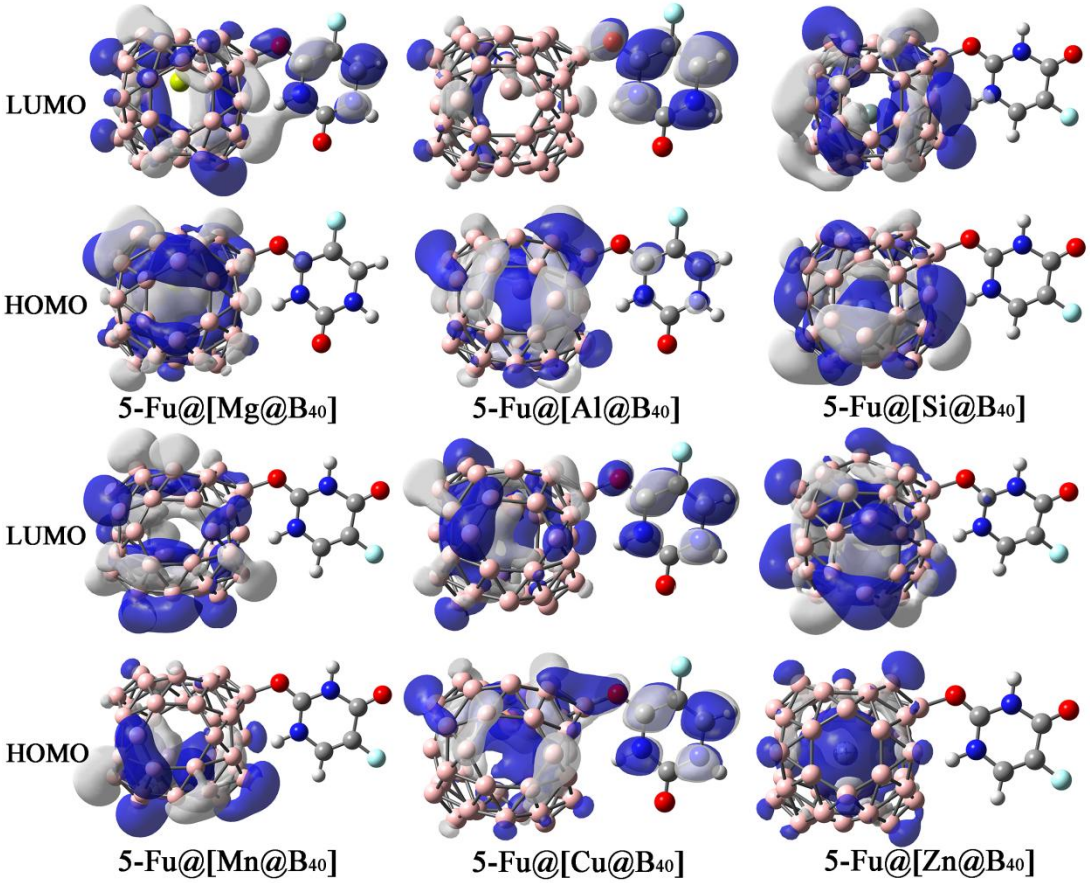


Figure. S5 The ESP plots inconjunction with the extreme values for $B_{39}M$ (M = Mg, Al, Si, Mn, Cu, and Zn) cages. The yellow and cyan balls correspond to the maximum and minimum point of electrostatic potential, respectively.

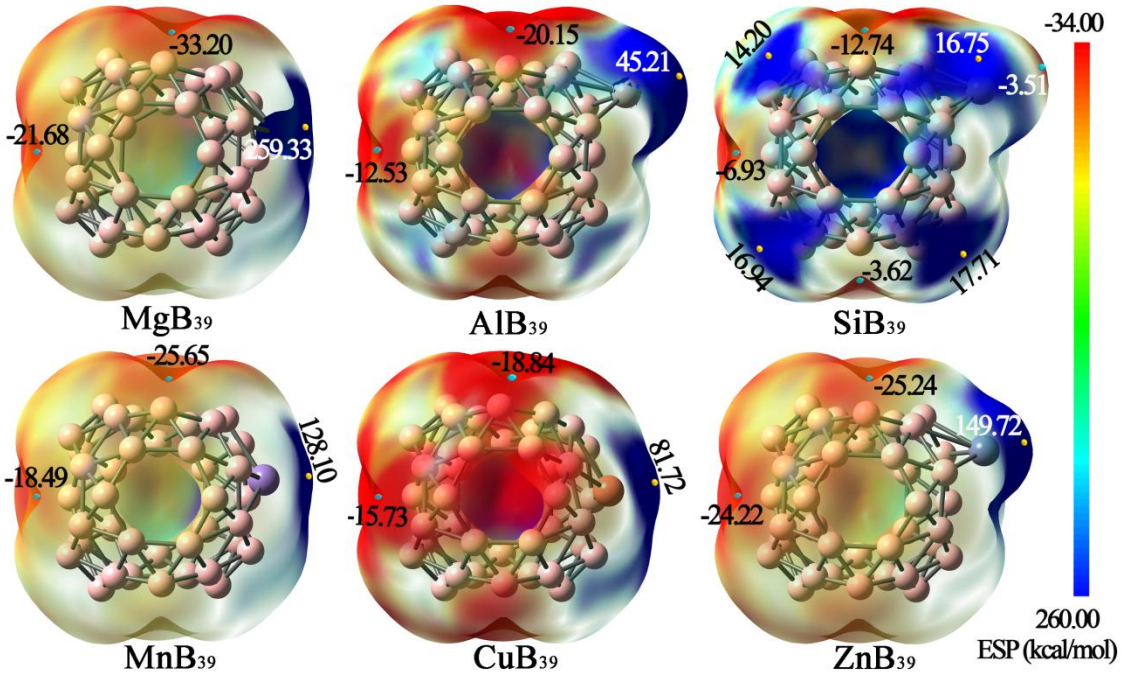


Figure. S6 LMOs related to the M-O bondsin 5-Fu@B_{39}M (M = Mg, Al, Mn, Cu, and Zn) complexes. The contributions of linked atoms to LMO are also given next to them.

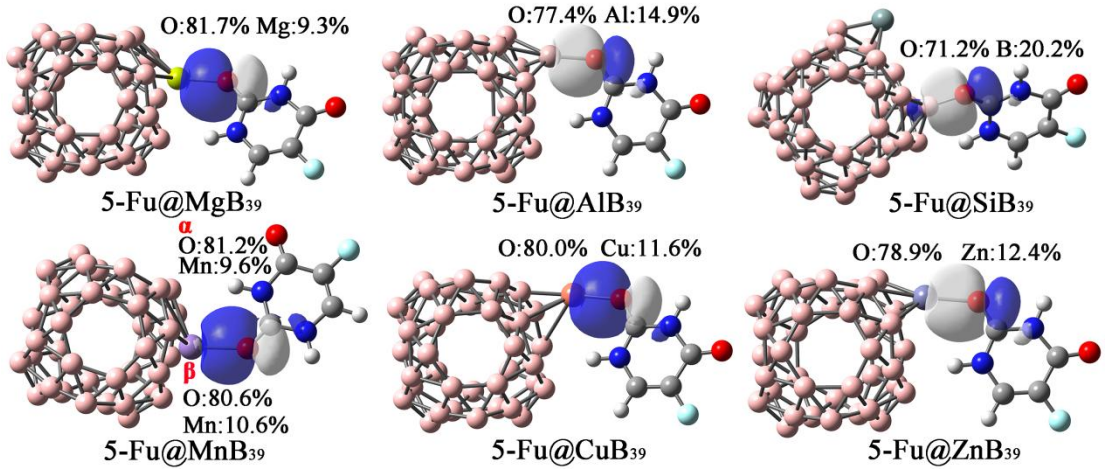


Figure. S7 ELF plots for 5-Fu@B_{39}M (M = Mg, Al, Mn, Cu, and Zn).

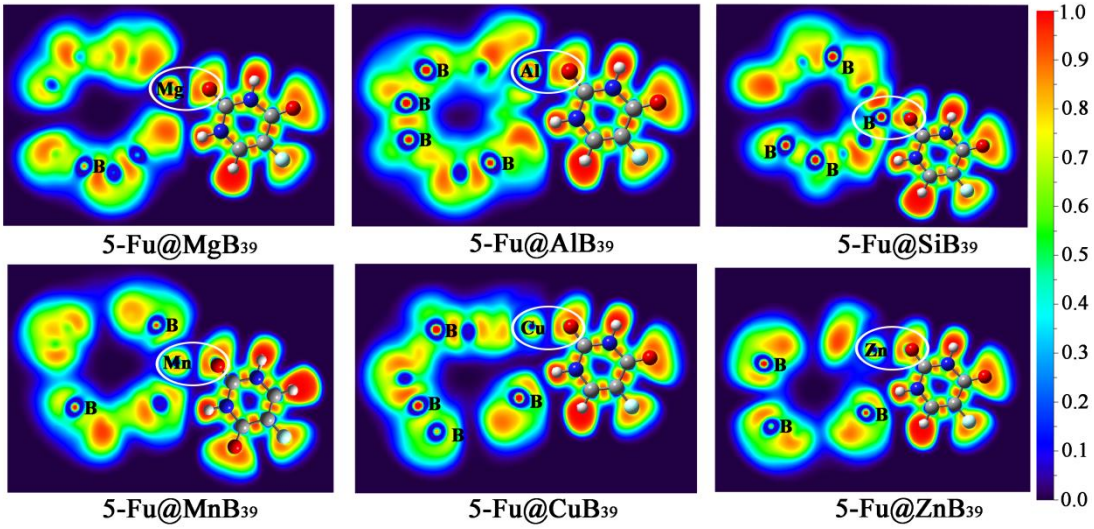
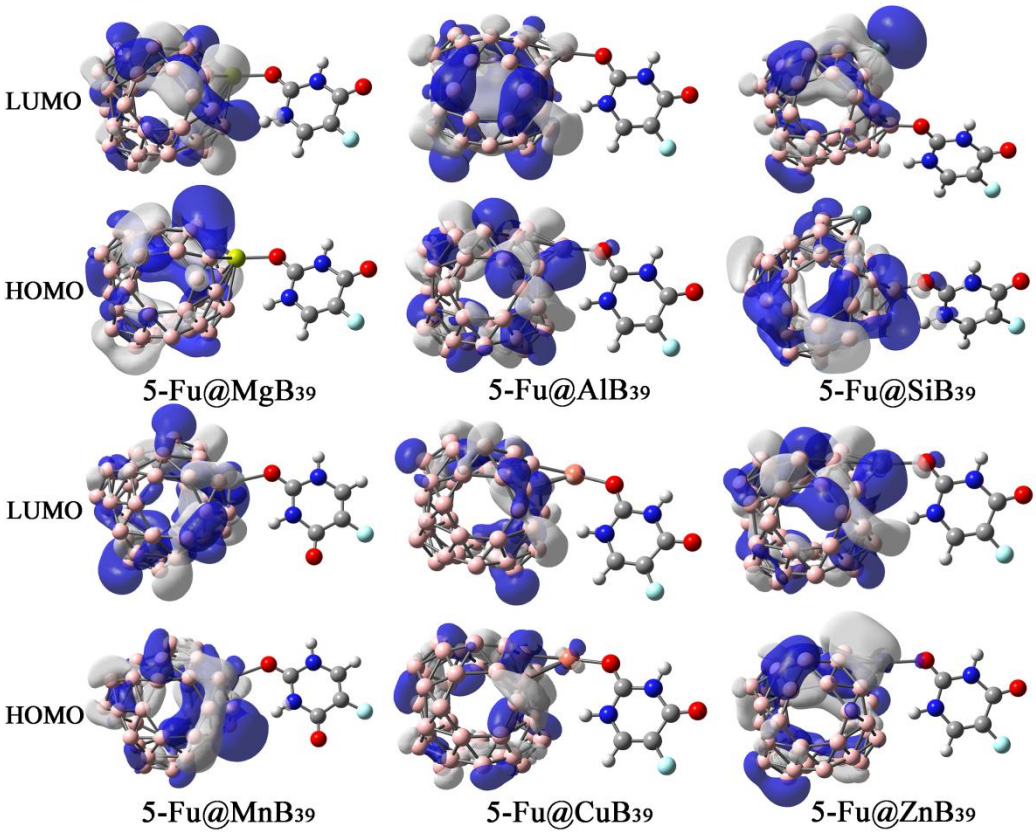


Figure. S8 The HOMO and LUMO orbitals of 5-Fu@B_{39}M (M = Mg, Al, Si, Mn, Cu, and Zn) complexes with isovalue of 0.02 a.u.



3. Cartesian Coordinates

(1) 5-Fu@B_{40} complex at the B3LYP-D3/6-31G(d) level

5-Fu@B_{40}

B	3.24255500	2.13496100	1.48704000
B	1.83074500	2.47428900	2.19251700
B	2.55441900	1.08342800	2.66398800
B	3.18811600	-0.39956100	2.92650000
B	4.04640500	0.50706800	1.89100900
B	4.58435100	1.45801100	0.71165800
B	3.77060800	2.60281200	-0.02406700
B	4.27038300	1.25360300	-0.91839100
B	2.93006400	2.43399000	-1.37582700
B	3.34989200	0.98526600	-2.34854200
B	2.06868700	1.96024000	-2.67162600
B	-0.69332600	1.02052600	1.57911200
B	-0.17269400	-0.02461000	2.69186100
B	0.79112600	1.29125000	2.56372300
B	0.48281100	2.42008700	1.30101000
B	0.24711100	2.99243200	-0.25296200
B	-0.88514500	2.07699100	0.37857500
B	1.18359400	2.64802000	-1.50663400
B	-0.43698700	1.75369700	-1.19997900
B	0.58851100	1.27032500	-2.49155200
B	-0.00046700	-2.28344900	0.86881900
B	1.31066300	-2.77150600	1.74319200
B	0.52161200	-1.44132700	2.26116600
B	-0.79168700	-0.74347800	1.35858200
B	-1.44962000	-1.54087500	0.05892400
B	-0.31784500	-2.46930300	-0.73178100
B	-0.69997300	-1.01794900	-1.43227000
B	0.71528700	-2.06056800	-1.85332600
B	-0.77917400	0.46561700	-2.10846600
B	0.43262700	-0.48077300	-2.64138500
B	1.73038400	-1.40835500	-2.96959000
B	3.86237400	-1.23483700	1.70809600
B	2.28886700	-1.69314900	2.44825600
B	2.75983400	-2.56997800	1.05159500
B	3.21482400	-2.83829800	-0.53187000
B	4.23876100	-2.05116800	0.38557000
B	2.46502900	-2.28486800	-1.83513900
B	4.02389600	-1.49033300	-1.17080700
B	3.15217200	-0.77936800	-2.48721100
B	4.46408400	-0.07674100	-1.81714300

C	-3.84149000	-0.96772000	0.01024100
N	-5.15025000	-1.31523300	-0.05406400
C	-6.26888200	-0.43314100	-0.05102200
C	-5.84928000	0.96711400	0.03682300
C	-4.54897100	1.31320200	0.10290500
N	-3.55967500	0.34496800	0.08308000
H	-4.20773100	2.33836100	0.17233600
O	-2.96056500	-1.88905800	-0.00934200
H	-5.36318500	-2.30675000	-0.11562000
H	-2.57796800	0.64270700	0.16993700
O	-7.40149500	-0.85380700	-0.11426200
F	-6.81642100	1.88034900	0.05025200

(2) 5-Fu@[M@B_{40}] (M = Mg, Al, Si, Mn, Cu, and Zn) complexes at the B3LYP-D3/6-31G(d)&SDD level

5-Fu@[Mg@B_{40}]

B	-0.88710600	2.61590400	-1.14512500
B	-1.79277300	1.77495100	-2.19030200
B	-2.41241000	1.83000800	-0.68230100
B	-2.73728300	1.67503600	0.90752200
B	-1.34948700	2.52203600	0.61389500
B	-0.00051600	3.23710300	0.13165100
B	0.75996700	2.95814300	-1.23044900
B	1.56958900	2.66530000	0.22126900
B	1.97708200	1.95245200	-1.44340000
B	2.75027900	1.39532200	0.08157400
B	3.02962700	0.71452100	-1.38416900
B	-1.73182400	-1.17333100	-2.05880800
B	-3.00560400	-1.02920000	-0.99517300
B	-2.47179900	0.38079500	-1.65926100
B	-1.10751000	0.42784600	-2.74957100
B	0.48536000	0.15850600	-3.27791200
B	-0.43286900	-1.10230000	-3.01318700
B	1.80080900	0.53018200	-2.44993400
B	1.16182600	-1.19921300	-2.53953900
B	2.52574600	-0.83511400	-1.51320000
B	-1.46210500	-2.40727700	1.09339300
B	-2.17775800	-1.34068800	2.10062500
B	-2.82519700	-1.28243600	0.59970500
B	-1.80151800	-2.12538400	-0.65737400
B	-0.61056000	-3.05654800	-0.19653000
B	0.16540800	-2.99342000	1.20664900
B	1.07452400	-2.92547300	-0.20528900
B	1.57840600	-2.27708500	1.42765600

B	1.79056300	-2.30611300	-1.52804200
B	2.43896200	-1.84511900	-0.09095100
B	2.86173200	-1.23126600	1.36405400
B	-1.40970200	1.46691300	1.93582600
B	-2.53004400	0.17476000	1.54757800
B	-1.23671400	-0.11220200	2.68647900
B	0.38361500	-0.20029200	3.15093900
B	-0.27067700	1.34214900	3.16988000
B	1.62682500	-0.81136700	2.40623800
B	1.34080400	0.98361200	2.51090700
B	2.68022500	0.37700400	1.50080300
B	2.20924900	1.94911200	1.52795400
Mg	-0.00130300	-0.48167600	0.54907800
C	0.35297000	5.50692900	3.19469900
N	0.15620300	4.12117500	3.29244900
C	-0.18345800	3.43426600	4.42237100
C	-0.34285700	4.19600800	5.61479700
C	-0.15405900	5.54254800	5.58993900
N	0.18387500	6.16395300	4.41174200
H	-0.26035700	6.15618400	6.47502500
O	0.64201700	6.06737400	2.16230100
H	0.23663800	3.61795900	2.40274600
H	0.32476800	7.16551900	4.37721500
O	-0.33615500	2.16040600	4.42681700
F	-0.67077900	3.55794300	6.74107400

5-Fu@[Al@B_{40}]

B	-0.85608900	2.37840700	-1.64653700
B	-1.52616800	1.25909100	-2.60948400
B	-2.34063300	1.58258400	-1.22761400
B	-2.96861300	1.78114000	0.27792800
B	-1.65243100	2.69521900	-0.00035200
B	-0.24338600	3.35022100	-0.40293000
B	0.75339500	2.82106100	-1.51338600
B	1.24992800	2.79593900	0.10568000
B	1.99159100	1.81632900	-1.29462800
B	2.50381700	1.64277700	0.41135400
B	3.06191700	0.69232200	-0.80824800
B	-1.45256000	-1.64108800	-1.88936100
B	-2.83047900	-1.31952800	-1.06885400
B	-2.24130600	-0.04237300	-1.92216700
B	-0.72839200	-0.13469100	-2.78297400
B	0.92448300	-0.41340400	-2.95393900
B	0.00271800	-1.65646400	-2.58691900
B	2.06462100	0.21158100	-2.00852300

B	1.47816000	-1.53782100	-1.78838500
B	2.65259700	-0.89791200	-0.69665600
B	-1.66859900	-2.09915500	1.48352600
B	-2.53594400	-0.88168900	2.12977900
B	-2.87539100	-1.18162700	0.55896800
B	-1.74924000	-2.32210300	-0.29423700
B	-0.63868300	-3.02645700	0.58678300
B	-0.15579800	-2.82557000	2.20006000
B	0.98677300	-2.73625800	0.77986500
B	1.08342200	-1.68199100	2.21064400
B	1.99325000	-2.37415100	-0.48641400
B	2.29458000	-1.61636300	0.94230600
B	2.40717100	-0.66151500	2.26528200
B	-2.01768300	2.00775600	1.57854400
B	-2.86732100	0.46161900	1.25076800
B	-1.80209400	0.48285200	2.62496200
B	-0.32680000	0.64063600	3.42661100
B	-0.94955200	1.94256800	2.77118200
B	1.02291600	-0.09972100	2.95228600
B	0.69785900	1.68048800	2.58076100
B	2.17540200	0.94193300	2.01843400
B	1.74124600	2.45300600	1.60829300
Al	-0.04261200	-0.49162800	0.16637300
C	-0.88358900	-1.96473500	6.25612400
N	-0.70409400	-2.34270100	4.92383800
C	-0.46826800	-3.62804500	4.47409500
C	-0.40570400	-4.64330700	5.44393700
C	-0.58322800	-4.34860200	6.76997300
N	-0.81201200	-3.03249400	7.14142400
H	-0.55354900	-5.10037900	7.54574400
O	-1.08400300	-0.81688400	6.59963900
H	-0.71669500	-1.57211800	4.25742200
H	-0.94556000	-2.78692300	8.11279600
O	-0.32592900	-3.87980000	3.19928700
F	-0.17997600	-5.90383000	5.04813000

5-Fu@[Si@B_{40}]

B	-2.70557300	3.65202600	-3.44266300
B	-2.95304000	3.10136500	-4.94943300
B	-3.90176200	2.41000400	-3.75926600
B	-4.68907200	1.66579500	-2.53146300
B	-3.64983900	2.80649800	-2.04936300
B	-2.34055100	3.72148500	-1.80045000
B	-1.19935900	4.08335500	-2.84207500
B	-0.78892400	3.24513800	-1.43308700

B	0.20846400	3.34396700	-3.04823000
B	0.68317900	2.34288200	-1.62881800
B	1.49814100	2.35460700	-3.04784300
B	-2.20785700	0.41612500	-5.96487800
B	-3.81734000	0.02071500	-5.38071600
B	-3.58012600	1.61428400	-5.33397100
B	-1.86316300	2.16516300	-5.73981100
B	-0.13601800	2.39885400	-5.81787000
B	-0.77510200	1.03325500	-6.34867900
B	0.75442000	2.51392900	-4.50156600
B	0.65678500	0.97504300	-5.46968700
B	1.45954500	0.97234100	-3.91462000
B	-2.59906800	-1.95276000	-3.49435700
B	-3.74280800	-1.49224500	-2.43444200
B	-3.81709100	-0.75407000	-3.93144800
B	-2.51371800	-1.07867600	-5.17603100
B	-1.36912300	-2.09559300	-4.67371900
B	-0.98555000	-2.46817100	-3.17659700
B	0.09479100	-1.52363400	-4.06212000
B	0.01515800	-1.65068300	-2.23324500
B	1.08651800	-0.40941600	-4.71941300
B	1.20909700	-0.57015200	-3.11324400
B	0.99590300	-0.59179400	-1.48786600
B	-3.77408400	1.22420500	-1.22326300
B	-4.34403900	0.05177500	-2.46116700
B	-3.34006400	-0.53816100	-1.16263100
B	-1.98574600	-0.80909400	-0.08677900
B	-2.81465600	0.63846200	-0.11673000
B	-0.50851100	-0.71221200	-0.85007600
B	-1.18292700	0.81284900	-0.14860200
B	0.39366700	0.78509500	-0.84539600
B	-0.29057700	2.17733300	-0.33918400
Si	-2.11248400	0.72018600	-3.85986000
C	-2.14142600	-3.08296900	0.83683100
N	-2.40830200	-3.93730500	1.85472300
C	-2.37061300	-5.36133700	1.80699800
C	-1.98883000	-5.84372900	0.47830800
C	-1.71940700	-4.99403000	-0.53185500
N	-1.80509600	-3.62509300	-0.34546500
H	-1.42801400	-5.31682400	-1.52361300
O	-2.23171100	-1.82836200	1.05410700
H	-2.67121500	-3.52737100	2.74635800
H	-1.54874600	-3.01159800	-1.13570000
O	-2.63254200	-6.02929600	2.78102900

F	-1.91772000	-7.16276900	0.32002500

5-Fu@[Mn@B_{40}]

B	-2.70740300	0.82905700	-1.17708200
B	-2.51401100	-0.41387800	-2.21571300
B	-2.88371200	-0.83337800	-0.67882900
B	-3.08017500	-1.15860400	0.91183600
B	-2.97025200	0.44460800	0.57362900
B	-2.75859300	1.92372100	0.06595100
B	-2.16886300	2.47873200	-1.39045500
B	-1.34313600	2.73464600	0.20300200
B	-0.50725800	2.53429200	-1.37354600
B	0.35853200	2.90120900	0.09715400
B	1.12319400	2.69803800	-1.33242100
B	-0.13078600	-2.22687300	-2.07869700
B	-0.99488300	-3.04902300	-0.97509100
B	-1.79864600	-1.78312400	-1.66181900
B	-1.03813700	-0.69228800	-2.77813200
B	0.15687900	0.36742200	-3.33346500
B	0.58685700	-1.13514600	-3.01471200
B	0.59080100	1.65045800	-2.45099400
B	1.55888000	0.06869200	-2.36507600
B	2.07796600	1.36200300	-1.39683500
B	0.91041600	-2.57619900	1.17111900
B	-0.38509600	-2.48741100	2.16114100
B	-0.73384900	-2.94512400	0.63506900
B	0.61695000	-2.80097500	-0.58208200
B	2.09118300	-2.50049000	-0.04004000
B	2.38353300	-1.76821800	1.38369000
B	2.96486300	-1.03418800	-0.07461400
B	2.59520500	-0.20651100	1.61219300
B	2.87609000	-0.06188700	-1.39286900
B	2.92595500	0.72943300	0.06428800
B	2.49248600	1.42890600	1.45949600
B	-2.37839100	-0.28159600	2.07023100
B	-1.79998900	-1.89308400	1.59750900
B	-0.84323100	-1.06576800	2.78042100
B	0.15091800	0.17284700	3.31026000
B	-1.36674500	0.52529800	3.01214100
B	1.40493800	0.74616100	2.49853900
B	-0.20754900	1.64039200	2.53047600
B	1.08910900	2.28186000	1.61250200
B	-0.39734100	2.91487400	1.54581100
Mn	0.93434500	-0.47163100	-0.11580200
C	-2.91750900	3.27830900	-3.58974400

N	-3.72495500	4.05057100	-4.35669700
C	-3.77680500	4.08003000	-5.78137600
C	-2.81506900	3.14762600	-6.37322100
C	-2.00962000	2.38367600	-5.60925900
N	-2.07119200	2.45364100	-4.22786500
H	-1.28566200	1.68621800	-6.01219500
O	-3.01214300	3.37363900	-2.31936000
H	-4.37155600	4.66789900	-3.87393300
H	-1.41404900	1.87079600	-3.68593200
O	-4.54499400	4.80957800	-6.36571100
F	-2.77639800	3.09351000	-7.70154300

5-Fu@[Cu@B_{40}]

B	-1.25817000	2.71988500	-0.49041400
B	-1.73519700	2.11552900	-1.91041600
B	-2.49824700	1.52748900	-0.59123900
B	-3.06055700	0.80846300	0.77460500
B	-1.98332900	2.00120300	1.04643700
B	-0.75361500	3.03644500	1.09077700
B	0.23328700	3.36186900	-0.10356600
B	0.86149800	2.64098400	1.29318500
B	1.64646100	2.65913300	-0.37971100
B	2.35083700	1.80305900	1.02274000
B	2.96936300	1.72165600	-0.49413600
B	-1.02945600	-0.62936900	-2.80969400
B	-2.37199700	-1.06463900	-2.00251600
B	-2.15108200	0.55383800	-2.04031800
B	-0.70254100	1.18538100	-2.74129700
B	0.93462900	1.41462700	-2.94729100
B	0.33188800	0.01001800	-3.36604200
B	2.01072200	1.70055400	-1.80102600
B	1.80671200	0.01394900	-2.55923400
B	2.89000300	0.25533300	-1.23023900
B	-0.97220100	-2.84944400	-0.15124500
B	-2.00560500	-2.26279900	1.03321700
B	-2.23505700	-1.73198100	-0.52195600
B	-1.07816800	-2.07723500	-1.78967100
B	0.18212700	-3.17388200	-1.58720400
B	0.67758300	-3.07632700	0.04539200
B	1.66377600	-2.26012600	-1.00253300
B	1.76867500	-2.17395200	0.77753500
B	2.57871200	-1.22211300	-1.85390600
B	2.89255900	-1.21124500	-0.25040200
B	2.87254400	-1.06810100	1.38469100
B	-2.07106100	0.56727200	2.04706200

B	-2.68160300	-0.77567200	0.98108500
B	-1.49650900	-1.19250400	2.17439900
B	0.02297200	-1.14298700	2.89971000
B	-0.90283400	0.15201900	3.06482300
B	1.50066800	-1.24002200	2.25190200
B	0.75479500	0.39082700	2.85787600
B	2.27979600	0.33241100	2.00696000
B	1.54705900	1.73002000	2.44231800
Cu	-0.07871400	-0.99320000	0.41085500
C	0.67972800	-3.10539600	-5.76513300
N	0.58774100	-3.21300600	-4.37756200
C	0.44234500	-4.39633100	-3.66743400
C	0.38525900	-5.58328600	-4.40649700
C	0.47549400	-5.55732800	-5.77733100
N	0.61513600	-4.32917100	-6.41591300
H	0.44428100	-6.44948500	-6.38553400
O	0.80513000	-2.04061300	-6.34025800
H	0.61645600	-2.32667200	-3.87960800
H	0.68092300	-4.27699800	-7.42280800
O	0.38553900	-4.38291600	-2.35123000
F	0.24540000	-6.74898200	-3.75696900

5-Fu@[Zn@B_{40}]

B	-0.75334100	-1.78827200	2.12382400
B	-1.09290300	-0.46813600	3.01170700
B	-2.17391500	-0.84346200	1.86347000
B	-3.06523100	-1.08409100	0.48970200
B	-1.85538500	-2.16657200	0.68245600
B	-0.52291500	-3.02301800	0.96124900
B	0.72355800	-2.54055500	1.81173500
B	0.92795600	-2.82813100	0.14566100
B	2.04269200	-1.80042500	1.26129200
B	2.24720300	-1.90776100	-0.51147500
B	3.13298800	-0.92411600	0.44810500
B	-0.61000800	2.16252000	1.79234300
B	-2.19235600	2.11089800	1.31311800
B	-1.67446500	0.85912200	2.25173600
B	-0.03960300	0.79670800	2.81513700
B	1.61833200	0.80850100	2.70961700
B	0.91882900	2.29725700	2.45055200
B	2.41351700	-0.11253700	1.69344900
B	2.14552700	1.64802900	1.37573100
B	2.94575300	0.67721700	0.16646900
B	-1.41020500	2.28436300	-1.47845600
B	-2.58915100	1.21222100	-1.79184400

B	-2.52450300	1.74373200	-0.25845400
B	-1.18989300	2.84812800	0.26810300
B	-0.17296900	3.29269100	-0.91715500
B	0.03773900	2.55231100	-2.30365900
B	1.32041700	2.55006100	-1.16871800
B	1.10765300	1.39841700	-2.64718600
B	2.51478700	2.22768800	-0.11707300
B	2.43783500	1.25899700	-1.43793800
B	2.15849300	0.16167000	-2.64229100
B	-2.42638700	-1.63437600	-0.90211000
B	-2.95498300	0.05768800	-0.68254200
B	-2.14981000	-0.30101200	-2.17626200
B	-0.88204100	-0.79274100	-3.16052900
B	-1.56709600	-1.89242500	-2.24577500
B	0.63298500	-0.26674900	-3.04082300
B	0.11498300	-1.90340000	-2.34591700
B	1.74826000	-1.36083500	-2.14747800
B	1.19106900	-2.73280200	-1.45332900
Zn	0.02459400	0.08715600	-0.07142900
C	1.33293400	4.69784300	2.79108900
N	1.71276000	5.74001100	3.56971800
C	1.78213700	7.11097300	3.18550800
C	1.37727100	7.29983100	1.79030700
C	0.99881900	6.26304700	1.01726800
N	0.98790800	4.97353400	1.52207500
H	0.69007100	6.37063800	-0.01488000
O	1.33061900	3.52553900	3.29483600
H	1.98135100	5.52985300	4.52678000
H	0.65620100	4.21060000	0.91489600
O	2.13887500	7.96416800	3.96546200
F	1.39967800	8.54582100	1.32609100

(3) 5-Fu@B_{39}M (M = Mg, Al, Si, Mn, Cu, and Zn) complexes at the B3LYP-D3/6-31G(d)&SDD level

5-Fu@B_{39}Mg

B	-2.85352200	2.15534600	-1.45042400
B	-1.34696300	2.47076400	-1.94496200
B	-2.05020100	1.12709400	-2.57350300
B	-2.65699200	-0.31070900	-3.01760200
B	-3.62507600	0.55875000	-2.05646400
B	-4.30117600	1.46403300	-0.91226300
B	-3.57382800	2.52476700	0.01064000
B	-4.21474800	1.12910700	0.72210400
B	-2.93193500	2.25448200	1.45524400

B	-3.49363300	0.75566600	2.24788200
B	-2.25906000	1.69014200	2.81423800
B	1.06898300	0.85458700	-1.16760900
B	0.63793000	0.06318900	-2.57037500
B	-0.28909200	1.37024200	-2.42013300
B	-0.11639600	2.21870800	-0.90161500
B	-0.11513700	2.70973900	0.69871700
B	1.08459800	1.79043200	0.18235400
B	-1.21895900	2.37227200	1.79265800
B	0.43673200	1.44285800	1.72588700
B	-0.75050800	1.02236800	2.90524800
B	0.43953900	-2.21994600	-0.73678400
B	-0.91369500	-2.71171300	-1.67166500
B	-0.05951500	-1.46125200	-2.20265600
B	1.19347800	-0.80356500	-1.33531400
B	0.44340800	-2.34819600	0.90760400
B	0.63209800	-1.41589300	2.17700500
B	-0.83739200	-2.18250200	1.93353300
B	0.59960900	0.17428500	2.71886300
B	-0.69307700	-0.80924100	3.04775500
B	-2.05216200	-1.67504300	3.00902900
B	-3.47352400	-1.22218500	-1.95434200
B	-1.80686100	-1.61133300	-2.48725200
B	-2.45389100	-2.58956400	-1.23668000
B	-3.10100700	-2.92852500	0.27281200
B	-4.00957300	-2.12984300	-0.75331700
B	-2.51655700	-2.51412200	1.71830700
B	-4.01748600	-1.60007500	0.81692700
B	-3.33567100	-0.98874200	2.28838000
B	-4.54789900	-0.24485700	1.50683400
C	4.72410500	0.79962000	0.51815700
N	6.06987900	0.70066900	0.70813400
C	7.06684600	1.64003600	0.32507500
C	6.48370500	2.80941700	-0.33811800
C	5.15568700	2.92315600	-0.53287800
N	4.29603800	1.92383100	-0.10970800
H	4.70525000	3.77916000	-1.01932200
O	3.94713300	-0.10430500	0.90770200
H	6.40426800	-0.13732900	1.17477700
H	3.27759500	2.01242400	-0.23796500
O	8.23997400	1.44185900	0.54781000
F	7.33131400	3.75505700	-0.73825200
Mg	2.00703300	-0.48043600	0.76877400

5-Fu@$B_{39}Al$

B	-3.06064200	2.07510100	-1.50230400
B	-1.64807000	2.45458900	-2.18712400
B	-2.31720500	1.04892200	-2.67008600
B	-2.88295700	-0.45319100	-2.94355400
B	-3.79349100	0.41870800	-1.92023300
B	-4.39006200	1.34656700	-0.75054900
B	-3.63250700	2.52061600	0.00068800
B	-4.09778700	1.15098600	0.88233900
B	-2.81692800	2.38913400	1.37344100
B	-3.19082100	0.91937100	2.32956500
B	-1.96070700	1.95221400	2.68280800
B	0.95702300	1.10190600	-1.55093400
B	0.48111100	0.09673700	-2.73639200
B	-0.54934800	1.34506600	-2.59642700
B	-0.31415900	2.42757300	-1.27378500
B	-0.15145000	3.02100600	0.27185700
B	1.04391400	2.16159200	-0.32540700
B	-1.07999200	2.64860900	1.51950600
B	0.57641800	1.83641700	1.25729500
B	-0.43853800	1.33896800	2.56573600
B	0.38699200	-2.17047500	-0.82392200
B	-0.88644400	-2.69558600	-1.70928800
B	-0.11081100	-1.37378400	-2.25802000
B	1.26282000	-0.63640700	-1.50754700
B	0.71044400	-2.34081400	0.79970100
B	0.97947900	-0.92202800	1.63425900
B	-0.38362500	-2.01593700	1.93667000
B	0.97008500	0.59217900	2.21243300
B	-0.20715900	-0.42038900	2.74825600
B	-1.48696200	-1.39145400	2.99909800
B	-3.52481600	-1.31665700	-1.72831200
B	-1.89396400	-1.65475500	-2.42645800
B	-2.35389000	-2.57104400	-1.03662900
B	-2.83708400	-2.89097600	0.52977300
B	-3.87721000	-2.15502800	-0.41627600
B	-2.12614300	-2.31307200	1.84531500
B	-3.72633200	-1.57433300	1.13495400
B	-2.91809900	-0.82914700	2.46387700
B	-4.24878200	-0.18912100	1.77473100
Al	2.32993600	-1.34777100	0.06093900
C	4.64435200	0.25215700	0.43270600
N	5.95096500	0.38321100	0.76864500
C	6.72296400	1.58300200	0.77256500
C	5.92358300	2.73565800	0.35393900

C	4.62564800	2.60956400	0.01669700
N	4.00215500	1.37283700	0.05135700
H	4.00302600	3.44166600	-0.28837200
O	4.09734900	-0.89595400	0.49152400
H	6.43911100	-0.45884700	1.06035100
H	2.99827100	1.34683500	-0.20833800
O	7.88833800	1.57752400	1.09552500
F	6.54166900	3.91273600	0.32665900

5-Fu@B_{39}Si

B	-1.68627700	-2.22928500	2.16734300
B	-0.50324400	-1.33491000	2.81061700
B	-2.00774900	-0.76188500	2.99230300
B	-3.49027400	-0.06551200	2.87745200
B	-3.40994000	-1.54117300	2.20218400
B	-3.06095700	-2.88378400	1.40413300
B	-1.62181700	-3.30702500	0.89030700
B	-2.83590400	-2.96298900	-0.24576700
B	-0.98991500	-3.01920500	-0.55603100
B	-2.18355200	-2.50729200	-1.78106300
B	-0.56281500	-2.43776500	-1.99795100
B	0.38391700	1.17452000	1.46670600
B	-0.76484700	1.87360300	2.39144600
B	-0.57167700	0.28414600	2.65945400
B	0.52977500	-0.62934500	1.74546600
B	1.23027700	-1.24150000	0.39244100
B	1.58134200	0.38800100	0.62399100
B	0.36566200	-1.91973600	-0.74386500
B	0.95442000	-0.21583000	-0.89875000
B	0.03948600	-0.93464600	-2.20491800
B	-2.17686600	2.82958300	0.05415900
B	-3.57012100	2.49606700	0.86389400
B	-2.17793200	2.30768900	1.66517600
B	-0.62267200	2.50382100	0.90457300
B	-1.94675500	2.76217000	-1.58904000
B	-0.61721500	1.79690700	-1.97631500
B	-2.35324400	1.49803700	-2.47199100
B	0.47849200	0.63470200	-2.19167900
B	-1.01621600	0.35145400	-2.79875500
B	-2.56743300	0.04453800	-3.20139400
B	-4.45410600	-0.25588700	1.58606900
B	-3.62497400	1.27306800	1.94950600
B	-4.47717100	1.22389700	0.46253400
B	-4.85583100	0.68893100	-1.06866100
B	-5.15384800	-0.29669400	0.13910000

B	-3.79185500	0.47042700	-2.24048000
B	-4.45376800	-0.95406000	-1.22779100
B	-3.22857000	-1.22341200	-2.41196800
B	-3.77691800	-2.40695800	-1.43241700
C	4.09253200	0.34043800	0.39436500
N	5.26275700	1.01908300	0.48468500
C	6.56098800	0.52112100	0.17400900
C	6.51030800	-0.87312500	-0.27715700
C	5.34752800	-1.54838200	-0.36473600
N	4.15177200	-0.93250700	-0.03404800
H	5.28774500	-2.57789800	-0.69437000
O	3.01582600	0.94321000	0.72425500
H	5.21497600	1.98308600	0.80363300
H	3.23962400	-1.43246800	-0.05769500
O	7.54572000	1.21313100	0.28968800
F	7.67095400	-1.43744800	-0.59682600
Si	-0.23483500	3.50742200	-0.82536600

5-Fu@B_{39}Mn

B	-3.69358100	1.03891600	-2.11381200
B	-2.43910200	1.45077000	-3.04441000
B	-2.71727900	-0.15534200	-2.87319600
B	-2.85754400	-1.74160100	-2.51873000
B	-3.95760700	-0.79746500	-1.80612300
B	-4.76786600	0.33657400	-1.00664900
B	-4.34654100	1.84895700	-0.80662300
B	-4.43926900	0.84105400	0.55119600
B	-3.53446600	2.45522900	0.43386400
B	-3.50875100	1.42276500	1.88349700
B	-2.58916000	2.78235600	1.70705000
B	0.40021800	1.01784500	-2.25532900
B	0.14222300	-0.42597600	-3.01717600
B	-1.13170000	0.54834600	-3.22884800
B	-1.08919900	2.06179000	-2.32388600
B	-1.11194100	3.17711300	-1.08982800
B	0.26113400	2.43176700	-1.40318200
B	-1.92950100	3.12945700	0.28224600
B	-0.08545600	2.77324000	0.21539700
B	-0.94599700	2.62094700	1.70396200
B	0.82933000	-1.56569600	-0.40536300
B	-0.31092900	-2.75436400	-0.76400400
B	0.05656800	-1.72123100	-1.94792700
B	1.02137000	-0.38121100	-1.65621400
B	1.10109300	-0.81504300	1.03601500
B	1.08915500	0.56947400	1.79179800

B	-0.10105800	-0.52370800	2.18680200
B	0.59963400	2.15831100	1.56793000
B	-0.26921900	1.19504300	2.59827400
B	-1.28352700	0.09799600	3.22498800
B	-3.21605000	-2.20041300	-1.00554300
B	-1.59046500	-2.40643700	-1.71266200
B	-1.75170000	-2.80024400	-0.04845700
B	-2.08863000	-2.50789800	1.56519500
B	-3.30843300	-2.53540200	0.55452700
B	-1.55671700	-1.33630800	2.53266900
B	-3.34184300	-1.37766300	1.74095600
B	-2.78677800	0.01317700	2.62541300
B	-4.23243400	-0.04094800	1.89434000
C	4.63589300	0.87056300	0.27293900
N	4.48065900	-0.09596000	1.22186600
C	5.50232600	-0.75446100	1.95220800
C	6.84209700	-0.28372400	1.57759200
C	7.02164900	0.66871300	0.64395700
N	5.92784000	1.23308000	0.00488200
H	8.00140300	1.02830000	0.35680100
O	3.69121100	1.41514900	-0.33562000
H	3.51406700	-0.37443900	1.43470500
H	6.04953100	1.94859000	-0.69970200
O	5.25193700	-1.60075100	2.78108900
F	7.87500600	-0.84222500	2.20724100
Mn	1.60227300	1.07147300	-0.23846200

5-Fu@B_{39}Cu

B	-2.85265200	2.11527600	-1.52553400
B	-1.36632900	2.51626700	-2.02331500
B	-1.97746000	1.12081700	-2.63645800
B	-2.56465500	-0.34648100	-3.08828600
B	-3.56513300	0.48504000	-2.11647200
B	-4.27851900	1.38123700	-0.99033800
B	-3.61231900	2.51201700	-0.09726900
B	-4.20863000	1.12197900	0.65470800
B	-2.99198500	2.33988400	1.37110600
B	-3.48487000	0.82548500	2.19625400
B	-2.34094600	1.85867700	2.78030100
B	0.97868000	0.93113200	-0.98209300
B	0.66899400	0.00231100	-2.26877900
B	-0.28479000	1.33302600	-2.22276000
B	-0.19836700	2.45172800	-0.90856000
B	-0.20277200	2.97625500	0.65566300
B	0.98059300	2.01531700	0.21439200

B	-1.29656100	2.57592000	1.76353400
B	0.38306200	1.83653700	1.76622800
B	-0.80077900	1.30338700	2.89215600
B	0.23665800	-2.39786900	-0.76094200
B	-0.86587300	-2.82618600	-1.84732100
B	0.02226400	-1.48155900	-2.17965300
B	0.72638900	-0.76434800	-0.76750100
B	0.67115100	-1.78649200	0.65890600
B	0.77610100	-0.84783500	2.00878200
B	-0.64674800	-1.71734100	1.76707600
B	0.65678100	0.58660300	2.76164000
B	-0.53911300	-0.50288900	3.03197600
B	-1.84153600	-1.44495800	2.91663300
B	-3.35665000	-1.25373500	-1.99065300
B	-1.74549400	-1.67865500	-2.59544800
B	-2.39210600	-2.64428600	-1.31724700
B	-2.90819200	-2.85242500	0.25905000
B	-3.89072800	-2.11618400	-0.74572100
B	-2.25935000	-2.31938200	1.62599900
B	-3.90852100	-1.59956900	0.81345900
B	-3.23079000	-0.90628000	2.24684000
B	-4.49067100	-0.24754300	1.47396000
C	4.91562500	0.28808300	0.55669500
N	6.26426600	0.50376300	0.52360500
C	6.94318700	1.68473300	0.12013600
C	6.00838800	2.73516600	-0.28956900
C	4.67587000	2.54038700	-0.26538900
N	4.14561300	1.33312700	0.15493000
H	3.95993300	3.29698400	-0.56230600
O	4.45793600	-0.81529700	0.93828400
H	6.85372100	-0.26690400	0.82301300
H	3.12460500	1.22054300	0.13219900
O	8.15283800	1.75400600	0.13593200
F	6.54000100	3.89068200	-0.68681000
Cu	2.58954800	-1.27546400	1.15821600

5-Fu@B_{39}Zn

B	-2.99724000	2.09789400	-1.53123900
B	-1.56102000	2.44693400	-2.18196900
B	-2.25423500	1.05243800	-2.67779700
B	-2.83856300	-0.43719000	-2.97042000
B	-3.75472600	0.45051600	-1.97079600
B	-4.36340200	1.39259100	-0.82336300
B	-3.60272900	2.53595500	-0.03451700
B	-4.12056400	1.16508400	0.81410100

B	-2.83787600	2.39178400	1.37037000
B	-3.28161700	0.92562000	2.30485100
B	-2.05423800	1.94391500	2.71779800
B	0.95572700	0.99482200	-1.46745500
B	0.49334200	0.05240700	-2.73411800
B	-0.48329900	1.33174600	-2.61435600
B	-0.24448500	2.35027800	-1.22947400
B	-0.15013900	2.91067100	0.34425400
B	1.02752100	1.99286900	-0.20016100
B	-1.11719600	2.59483100	1.57221600
B	0.51555900	1.73375700	1.38689300
B	-0.52808800	1.31382000	2.69620100
B	0.42570700	-2.13862700	-0.80350300
B	-0.91333500	-2.71846100	-1.67410600
B	-0.13641200	-1.44028500	-2.25608400
B	1.18986200	-0.70390900	-1.49292700
B	0.58552500	-2.27141600	0.83241700
B	0.88677000	-0.97227300	1.79520800
B	-0.51355000	-1.98702500	1.96803300
B	0.86507000	0.53970100	2.41138300
B	-0.34243100	-0.46862700	2.88282100
B	-1.65115500	-1.41109400	3.04677800
B	-3.52927300	-1.30192200	-1.78493900
B	-1.89642000	-1.66765000	-2.43437200
B	-2.39887300	-2.58720700	-1.07376300
B	-2.90276000	-2.86215000	0.49818800
B	-3.92242200	-2.14482200	-0.48224100
B	-2.22561100	-2.32075200	1.85717400
B	-3.80894100	-1.53395300	1.05925000
B	-3.03524100	-0.81415800	2.42777200
B	-4.34055600	-0.15964700	1.71319400
C	4.78779800	0.27617700	0.37839400
N	6.11805800	0.45191000	0.62484400
C	6.84727300	1.67277700	0.60948800
C	5.98814900	2.81274400	0.28178200
C	4.67430800	2.65504300	0.03092100
N	4.09215200	1.39966900	0.07439200
H	4.01255800	3.47805200	-0.20933300
O	4.27843800	-0.87123800	0.43812400
H	6.65172800	-0.38058100	0.85602900
H	3.08580700	1.32856600	-0.12735200
O	8.03407200	1.70120100	0.84947600
F	6.56854600	4.01093500	0.24589800
Zn	2.35208600	-1.36704300	0.21928200