Supporting Information

Comparison of pnicogen and tetrel bonds in the complexes containing carbenes CX_2 (X =F, Cl, Br, OH, OMe, NH_2, and NMe_2)

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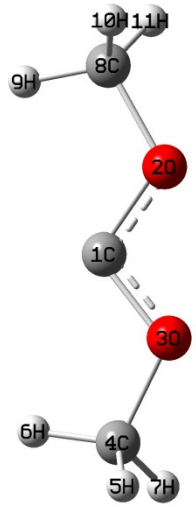
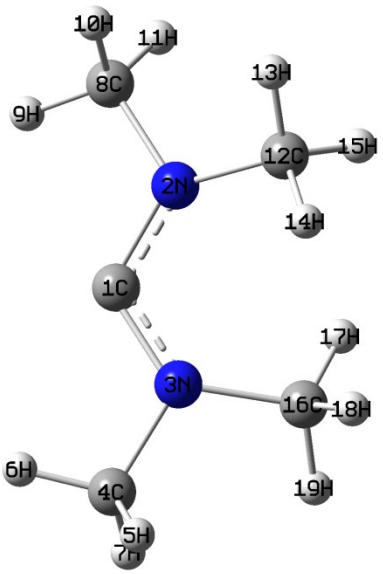
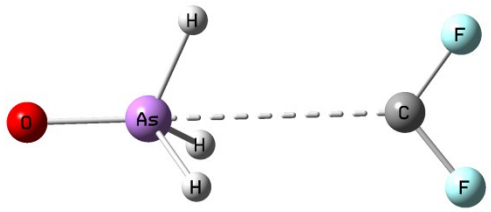
Table S1 Second-order stabilization energies ($E^{(2)}$, kcal/mol) associated in $C(OMe)_2$ and

Table S2: Equilibrium geometries(Å) and total energies (a.u.) for complexes $C(NMe_2)_2$.





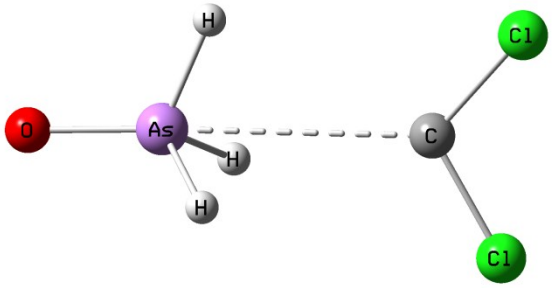
Donor NBO(i)	Acceptor NBO(j)	$E^{(2)}$	Donor NBO(i)	Acceptor NBO(j)	$E^{(2)}$
BD(1)C4-H5	BD*(1)C1-O3	1.67	BD(1)C8-H10	BD*(1)C1-N2	2.03
BD(1)C4-H7	BD*(1)C1-O3	1.67	BD(1)C8-H10	BD*(2)C1-N2	1.03
BD(1)C8-H10	BD*(1)C1-O2	1.67	BD(1)C8-H11	BD*(1)C1-N2	2.92
BD(1)C8-H11	BD*(1)C1-O2	1.67	BD(1)C8-H11	BD*(2)C1-N2	1.16
			BD(1)C12-H13	BD*(1)C1-N2	4.23
			BD(1)C12-H13	BD*(2)C1-N2	1.16
			BD(1)C12-H15	BD*(1)C1-N2	2.15
			BD(1)C12-H15	BD*(2)C1-N2	1.01
			BD(1)C4-H5	BD*(1)C1-N3	2.89
			BD(1)C4-H7	BD*(1)C1-N3	2.05
			BD(1)C16-H18	BD*(1)C1-N3	2.13
			BD(1)C16-H19	BD*(1)C1-N3	4.87



$H_3AsO\cdots CF_2$

MP2= -2548.688623

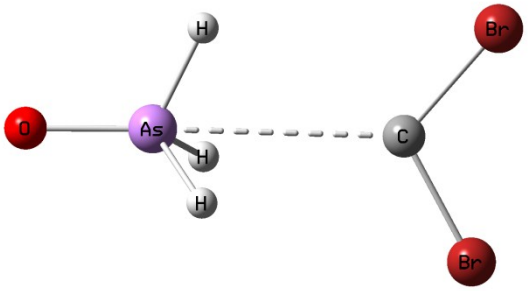
As	1.26386900	0.00167200	-0.00134900
H	0.61491200	-0.83610500	-1.05271700
H	0.62231900	1.33382500	-0.20788000
H	0.60697400	-0.48278400	1.24856500
O	2.89824300	-0.00639600	0.00533000
C	-2.19101100	-0.00074300	-0.00147700
F	-2.97746700	-1.03239700	0.00125300
F	-2.97717400	1.03078600	0.00127900



$H_3AsO\cdots CCl_2$

MP2= -3268.622155

As	-1.82573500	-0.04713200	0.00049900
H	-1.22593200	-1.41336200	0.00363700
H	-1.15868300	0.60741400	1.16458500
H	-1.15515600	0.60372600	-1.16364700
O	-3.46042600	0.00831300	-0.00222700
C	1.46290400	-0.05138400	0.00235600
Cl	2.58822900	-1.32730000	-0.00057400
Cl	2.27618400	1.44491100	-0.00044800



$H_3AsO\cdots CBr_2$

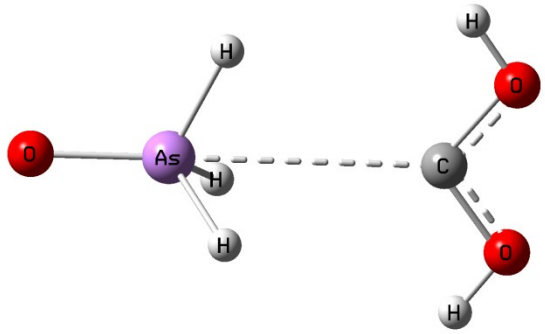
MP2= -7494.586437

As	-2.56704700	-0.08184600	-0.00226600
H	-1.91857100	0.69903800	-1.09687600
H	-1.94233400	-1.42958100	-0.14374100
H	-1.90329200	0.46158700	1.21967200
O	-4.20284400	-0.05852400	0.01081200
C	0.66966900	-0.04854200	-0.01471500
Br	1.56851400	1.57585600	0.00127800
Br	1.86238600	-1.46930500	0.00150800

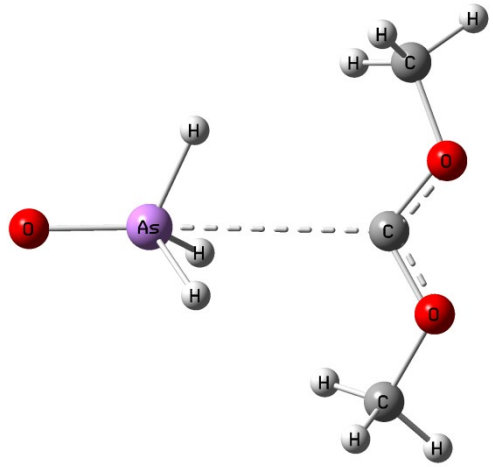
$H_3AsO\cdots C(OH)_2$

MP2= -2500.67299

As	1.18388900	0.00286100	0.00020200
H	0.53496700	-0.66216400	-1.16694600
H	0.55145400	1.35438500	0.00137400
H	0.53650700	-0.66351900	1.16741500



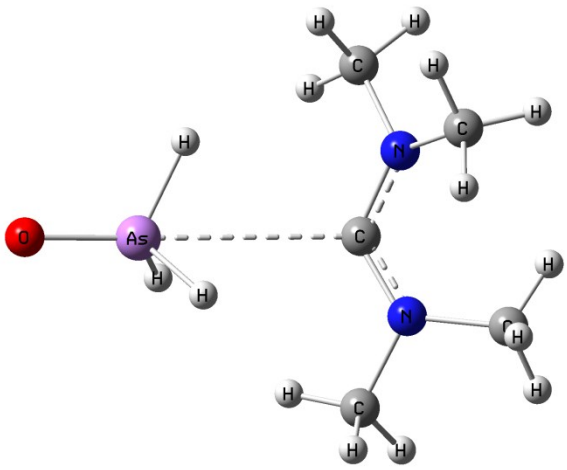
O	2.81940300	-0.00433100	-0.00091400
C	-2.07899300	0.00393100	0.00117500
O	-2.86968500	-1.05581900	-0.00060800
H	-2.29180000	-1.82867300	0.00077300
O	-2.89783800	1.04170100	-0.00060600
H	-2.34054600	1.82956300	0.00070400



$H_3AsO\cdots C(OMe)_2$

MP2= -2579.03143

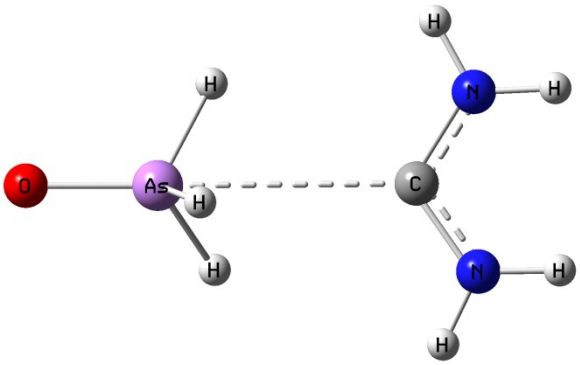
As	-1.57919500	-0.06845600	0.02223800
H	-0.85431100	0.80653900	-0.94598900
H	-0.90891500	-1.38639600	-0.16717700
H	-1.04943200	0.38453500	1.34096200
O	-3.20883400	-0.07704100	-0.12514600
C	1.68645000	0.04269000	0.12479500
O	2.31737100	1.16174600	-0.16788900
O	2.53286900	-0.92283900	-0.16757500
C	2.04276800	-2.25105700	0.08637800
H	2.85782700	-2.80471300	0.54113700
H	1.18813200	-2.20911200	0.75486800
H	1.76712300	-2.70531000	-0.86166300
C	1.56815000	2.36096400	0.09330000
H	0.69393000	2.12722000	0.69359300
H	2.22704300	3.03864200	0.62684600
H	1.27659200	2.79714700	-0.85839600



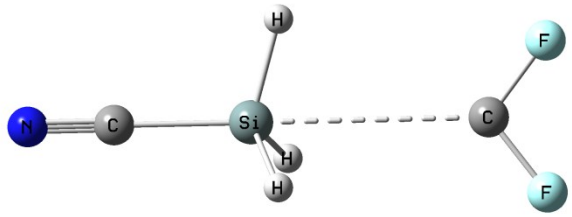
$H_3AsO\cdots C(NMe_2)_2$

MP2= -2617.67295

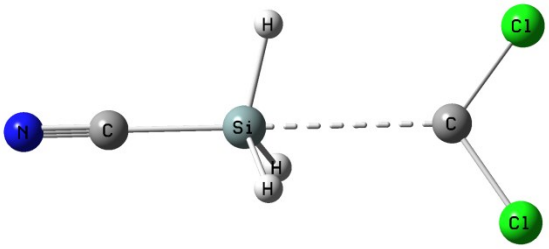
As	-2.02249800	-0.04135000	0.02293000
H	-1.36875100	1.29556700	-0.01238200
H	-1.74724200	-0.59552200	-1.33242700
H	-1.11947100	-0.83356000	0.90789700
O	-3.59796100	-0.03098200	0.47853400
C	1.06831000	-0.01834800	-0.51433900
N	1.61255000	1.17025100	-0.18165000
N	1.71020800	-1.12759300	-0.10531500
C	1.05470900	-2.40020500	-0.36562700

	H	0.96124900	-2.98040600	0.55465000
	H	0.06871900	-2.20115600	-0.77086000
	H	1.63149200	-2.98497200	-1.08641000
	C	1.03793700	2.35471700	-0.79982000
	H	0.35832900	2.03645800	-1.58357800
	H	0.50277700	2.96008300	-0.06218300
	H	1.82675100	2.96837400	-1.23906500
	C	2.49018900	1.48139300	0.94631000
	H	2.08357200	2.35696900	1.45507700
	H	2.50048300	0.65719700	1.65208900
	H	3.51242200	1.71347000	0.64128300
	C	3.11638400	-1.27025900	0.27403700
	H	3.68023500	-0.40281500	-0.05377800
	H	3.25573600	-1.41253900	1.34705800
	H	3.51534600	-2.14713000	-0.23695300
	$H_3AsO\cdots C(NH_2)_2$ MP2= -2460.932106			
	As	-1.18300900	-0.00526400	-0.00067600
	H	-0.54177300	-0.29105900	1.31314700
	H	-0.54528400	1.27571000	-0.41857400
	H	-0.55765400	-1.00429700	-0.91228600
	O	-2.82209000	0.00574300	0.00543200
	C	2.03529800	-0.00677600	-0.00912100
	N	2.75045000	1.12237300	0.00194500
	H	3.76500300	1.16043900	0.01670500
	H	2.27137300	2.00264400	-0.00570700
	N	2.79830100	-1.10415100	0.00219800
	H	2.35779300	-2.00427200	-0.00594100
	H	3.81352800	-1.09829100	0.01722400

	$H_3SiCN\cdots CF_2$ MP2= -620.880042			
	Si	1.12129600	0.00095000	-0.00150400
	H	0.70655000	1.38886900	-0.25592600
	H	0.70511600	-0.47327900	1.32722100



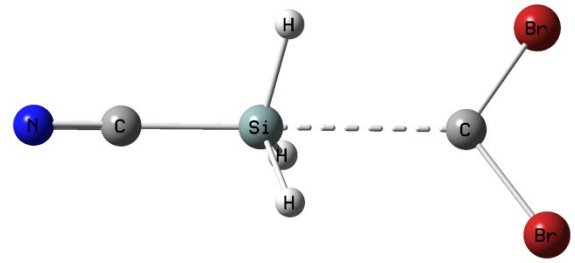
H	0.70747800	-0.91432100	-1.07595900
C	2.98720900	0.00104300	0.00034400
N	4.16191300	0.00036500	0.00214900
C	-2.11358700	0.00298600	-0.00296400
F	-2.89274800	-1.03382000	0.00147000
F	-2.90641000	1.02923200	0.00146400



$H_3SiCN\cdots CCl_2$

MP2= -1340.813931

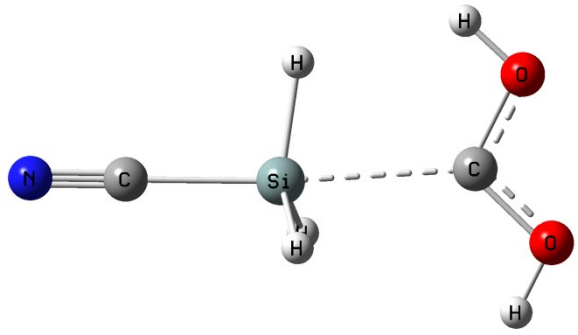
Si	-1.65809100	-0.01059200	-0.01851100
H	-1.29548200	1.08269000	-0.93305100
H	-1.29440200	-1.34900300	-0.50736300
H	-1.26477200	0.23678800	1.37762000
C	-3.53563900	-0.00734600	0.00759200
N	-4.71059100	-0.00497300	0.02462000
C	1.21224200	-0.00881400	-0.03347300
Cl	2.20163800	-1.38712800	0.00910500
Cl	2.15027000	1.40533900	0.00883000



$H_3SiCN\cdots CBr_2$

MP2= -5566.778394

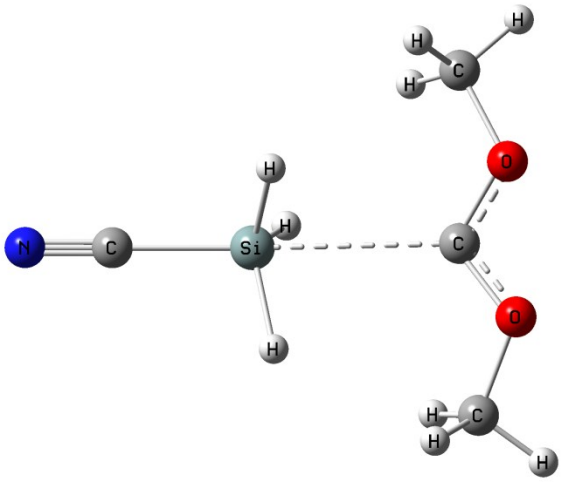
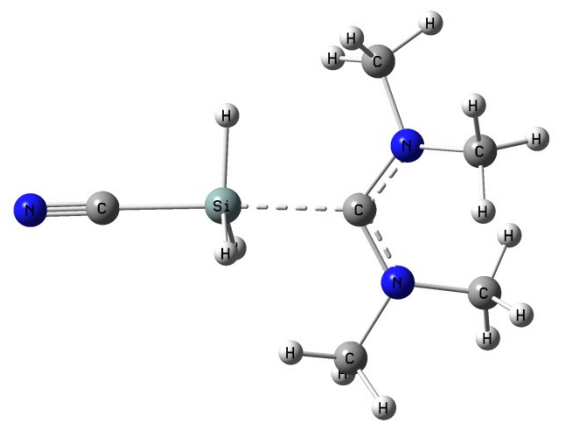
Si	2.36379500	-0.03451700	-0.04024300
H	2.03465200	1.06943700	-0.95541300
H	1.96396000	0.20885300	1.35590000
H	2.02168800	-1.37512800	-0.54011900
C	4.24489700	-0.03593700	0.01702100
N	5.41956800	-0.03669600	0.05348600
C	-0.40071500	-0.01676800	-0.07012300
Br	-1.47921100	-1.51525600	0.00946900
Br	-1.38123200	1.54820500	0.00902300

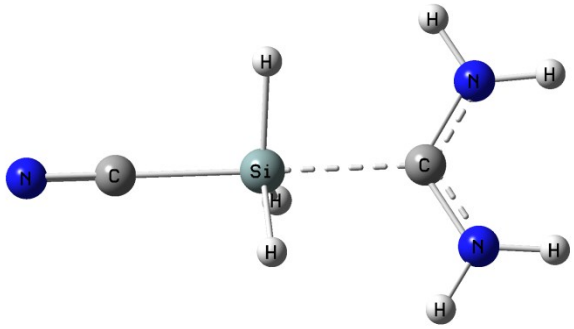


$H_3SiCN\cdots C(OH)_2$

MP2= -572.865849

Si	-0.70395200	-0.08928800	0.00010400
H	-0.48886900	-0.83440700	-1.25367200
H	-0.48889100	-0.83148300	1.25559900
H	-0.44052400	1.37034600	-0.00149400
C	-2.61514500	-0.00817700	-0.00001400
N	-3.79009000	0.04364100	-0.00013800

	C 1.70104100 -0.01642100 0.00010300 O 2.61187500 -0.96070400 -0.00010300 H 2.14655000 -1.80864000 -0.00004900 O 2.32604000 1.13296600 -0.00006600 H 1.63900100 1.81821600 -0.00006500
	$H_3SiCN\cdots C(OMe_2)_2$ MP2= -651.223396 Si 1.34675700 -0.05107200 0.08843400 H 0.96076300 0.97673200 -0.89021200 H 1.10703600 0.30617100 1.49321100 H 0.98508200 -1.42518800 -0.28430400 C 3.23016600 -0.06566900 -0.04194000 N 4.40277700 -0.07330200 -0.12273700 C -1.46466100 0.02116100 0.08873300 O -2.28319800 -0.97270100 -0.17547200 O -2.14320200 1.11632300 -0.17239700 C -1.43993000 2.34742800 0.08261000 H -2.18091000 3.04935600 0.45011500 H -0.66402100 2.18871100 0.82482800 H -1.01186100 2.70715600 -0.84898300 C -1.75006200 -2.28719900 0.07868700 H -1.01315500 -2.24439100 0.87401800 H -2.59447400 -2.90184400 0.37137200 H -1.30437000 -2.67187800 -0.83455500
	$H_3SiCN\cdots C(NMe_2)_2$ MP2= -689.8683456 Si 1.62950700 -0.10140800 -0.04038600 H 1.57540600 0.84516100 -1.17949900 H 1.45768800 0.39942700 1.34711700 H 1.55516800 -1.55686300 -0.26290000 C 3.59076100 -0.08556700 0.05609400 N 4.76671900 -0.06508100 0.11677700 C -0.59860000 -0.02464900 -0.07652100 N -1.40810100 -1.09938500 -0.03203700 N -1.20592300 1.17086700 0.00034200 C -0.42404400 2.39308200 0.16643300 H -1.00974700 3.09470200 0.76013000

	H 0.50050800 2.18847600 0.69145000 H -0.20366200 2.84621600 -0.80134900 C -0.92297800 -2.41919300 -0.42310400 H -0.11461100 -2.32676000 -1.13632800 H -0.58299600 -2.98930100 0.44364000 H -1.74736300 -2.95515400 -0.89401200 C -2.67000600 -1.15984300 0.70355300 H -2.64154000 -2.05354600 1.32833200 H -2.76315500 -0.29366200 1.35131100 H -3.54139600 -1.22625600 0.05055700 C -2.57698000 1.43736400 -0.43282200 H -2.94627800 0.60281200 -1.02109800 H -3.25554200 1.62970900 0.39900300 H -2.55335800 2.32278900 -1.06832000
	$H_3SiCN\cdots C(NH_2)_2$ MP2= -533.132590 Si 0.59059400 -0.00000200 0.01190100 H 0.47245900 1.30948700 -0.68805000 H 0.45172000 -0.00035500 1.48955900 H 0.47259700 -1.30907600 -0.68882800 C 2.54264400 0.00006400 -0.00051900 N 3.71977100 -0.00007000 -0.01208000 C -1.57370800 -0.00002000 -0.02537800 N -2.25266700 1.13616000 -0.00197000 H -3.25984000 1.20844100 0.03932300 H -1.72953200 1.99497600 -0.04529100 N -2.25277000 -1.13614300 -0.00194200 H -1.72973600 -1.99501800 -0.04523300 H -3.25995400 -1.20833000 0.03923000

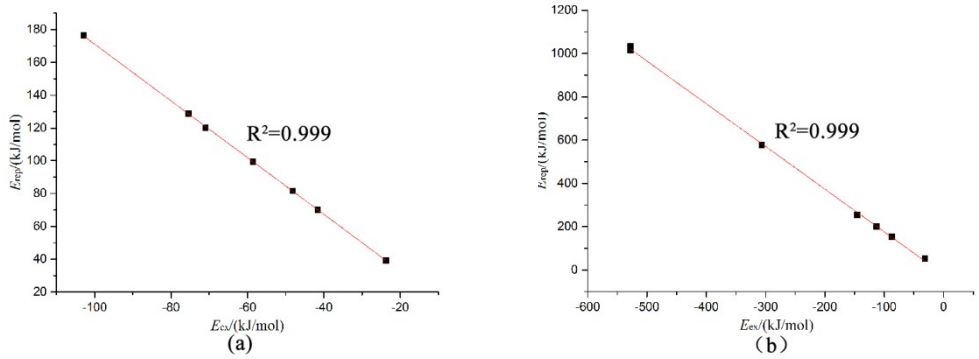


Figure S1: Linear relationship between the exchange energy（E_{ex}）and polarization energy (E_{rep}) for complexes (a): $H_3AsO\cdots CX_2$; (b): $H_3SiCN\cdots CX_2$. (X= F, Cl, Br, OH, NH_2, OMe, $(NMe_2)_2$,)

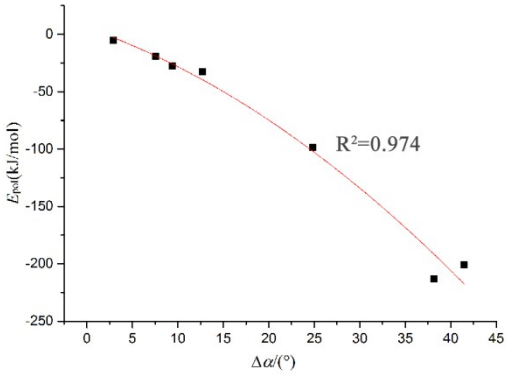


Figure S2: Polynomial correlation between the polarization energy (E_{pol}) and the change of dihedral angle of SiH_3 fragment ($\Delta\alpha$) for $H_3SiCN\cdots CX_2$. (X= F, Cl, Br, OH, NH_2, OMe, $(NMe_2)_2$,)

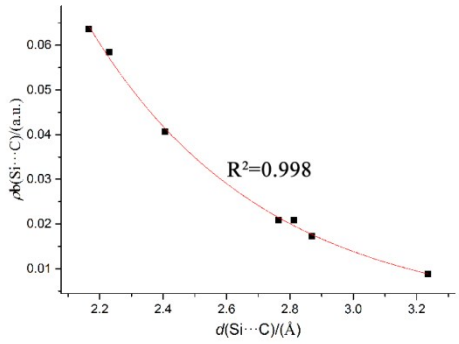


Figure S3: Exponential correlation between the electron density at the BCPs (ρ_b (Si···C)) and the binding distances (d(Si··· C)) of $H_3SiCN\cdots CX_2$. (X= F, Cl, Br, OH, NH_2, OMe, $(NMe_2)_2$,)