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Supplementary Information

Rational Design of Chemical Sensor Array Using Carbonitrile Neutral Receptors. *Sensors* 2013, *13*, 13835-13860

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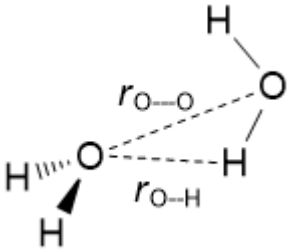
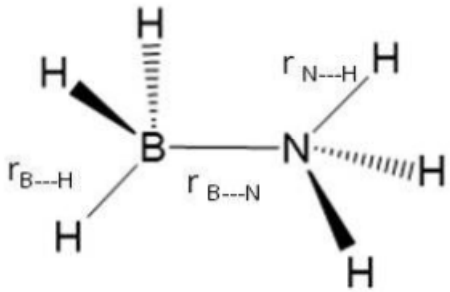
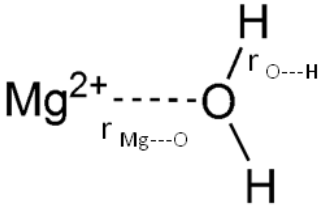
1. Benchmark Structures



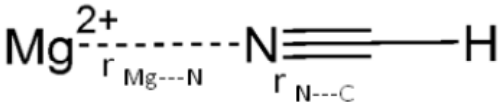
i. water dimer



ii. ammonia-borane



iii. Mg(II)-H2O



iv. Mg(II)-HCN

HCN

Symbol	*X*	*Y*	*Z*
C	*0*	*0*	*−0.5117*
N	*0*	*0*	*0.664423*
H	*0*	*0*	*−1.58079*

Mg(II)-H_2O

Symbol	*X*	*Y*	*Z*
O	*0*	*0*	*−1.00818*
H	*0*	*0.786319*	*−1.60806*
H	*0*	*−0.78632*	*−1.60806*
Mg	*0*	*0*	*0.940131*

Mg(II)-HCN

Symbol	*X*	*Y*	*Z*
Mg	*0*	*0*	*1.441744*
N	*0*	*0*	*−0.57422*
C	*0*	*0*	*−1.74209*
H	*0*	*0*	*−2.82887*

NH_3—BH_3

Symbol	*X*	*Y*	*Z*
N	−0.71562	0.000025	0.000009
B	0.910729	−1.2E-05	−9E-06
H	−1.09918	−0.27609	−0.90494
H	−1.09925	0.921743	0.213351
H	−1.09923	−0.6456	0.691599
H	1.25129	0.341064	1.114228
H	1.250837	−1.13564	−0.26173
H	1.251215	0.794417	−0.85252

2. Geometrical Structures

CH_3CN

Symbol	*X*	*Y*	*Z*
C	0.273053	0.000036	0.000074
N	1.450787	−1.4E-05	−3.1E-05
C	−1.18659	−5E-06	−8E-06
H	−1.55806	0.578153	−0.84747
H	−1.55804	−1.023	−0.07707
H	−1.55821	0.44476	0.92436

Sum of electronic and thermal Enthalpies
= −131.883190 hartrees

Mg—CH_3CN

Symbol	*X*	*Y*	*Z*
C	−0.98716	−0.04353	0.00006
N	0.1805	−0.11206	−1.8E-05
C	−2.43712	0.051242	−8E-06
Mg	2.306119	0.042253	−3E-06
H	−2.72551	1.103334	−0.01879
H	−2.83394	−0.45229	−0.88248
H	−2.83178	−0.41993	0.901111

Sum of electronic and thermal Enthalpies
= −331.340853 hartrees

Be—CH_3CN

Symbol	*X*	*Y*	*Z*
C	0.202038	−0.02106	0.00021
N	−0.96325	−0.04274	0.000144
C	1.645698	0.018501	−9.6E-05
H	2.012613	−0.395	0.941093
H	2.017835	−0.57094	−0.83993
H	1.965726	1.057331	−0.10184
Be	−2.58497	0.055774	−0.00025

Sum of electronic and thermal Enthalpies
= −146.253335 hartrees

Malono nitrile

Symbol	*X*	*Y*	*Z*
C	−1.20945	0.035464	0.000048
C	0	0.86391	0.000049
C	1.209446	0.035465	−4.3E-05
H	−3.2E-05	1.510394	−0.88341
H	0.000034	1.510297	0.883583
N	2.190386	−0.61641	−0.00012
N	−2.19039	−0.61641	0.000047

Sum of electronic and thermal Enthalpies
= −223.604231 hartees

Be—Malono nitrile

Symbol	*X*	*Y*	*Z*
C	1.072616	−0.38718	0
C	0	−1.4118	0.000003
C	−1.07262	−0.38718	0.000001
H	−1E-06	−2.02876	−0.90343
Be	0	1.735182	−2E-06
N	−1.44656	0.730978	−1E-06
N	1.446562	0.730977	−2E-06
H	0	−2.02876	0.903441

Sum of electronic and thermal Enthalpies
= −237.904143 hartees

n-Pentane carbonitrile

Symbol	*X*	*Y*	*Z*
C	−1.51004	0.698612	0.000025
C	−0.34329	−0.31358	−2E-06
C	1.018701	0.390409	−3E-06
C	2.198832	−0.59019	0.000031
C	3.562087	0.11097	−3.3E-05
C	−2.82349	0.051256	−0.00001
N	−3.85925	−0.47726	−2.4E-05
H	−1.45642	1.348367	0.881268
H	−1.45639	1.348435	−0.88117
H	−0.4295	-0.95983	0.881359
H	−0.42952	-0.95981	−0.88137
H	1.089979	1.044742	0.880264
H	1.090016	1.044713	−0.88029
H	2.124338	−1.24476	0.879088
H	2.124294	−1.24496	−0.87887
H	3.680138	0.746221	0.885851
H	3.679016	0.748205	−0.88465
H	4.381984	−0.61541	−0.00137

Sum of electronic and thermal Enthalpies

= −289.875391 hartrees

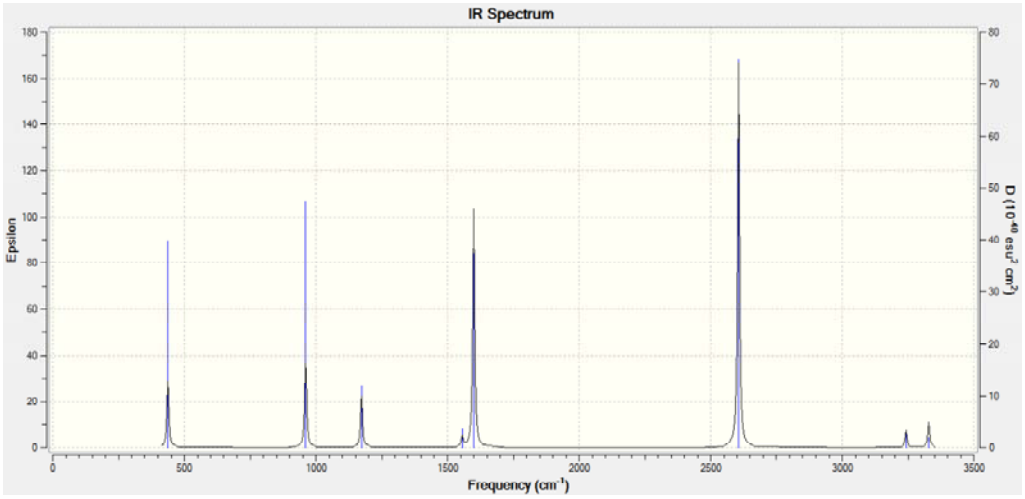
Mg--n-Pentane carbonitrile

Symbol	*X*	*Y*	*Z*
C	−0.35078	1.051676	−0.00016
C	0.661714	−0.12041	0.000039
C	2.106823	0.391662	0.000031
C	3.133631	−0.74925	−0.00014
C	4.582535	−0.2488	0.000091
C	−1.7287	0.585066	0.000074
N	−2.81294	0.181437	0.000177
H	−0.22021	1.687538	0.883119
H	−0.22029	1.687097	−0.88376
H	0.48477	−0.7446	0.882675
H	0.484807	−0.74484	−0.88244
H	2.268574	1.02775	0.881041
H	2.268527	1.027944	−0.88085
H	2.965515	−1.38574	0.878959
H	2.965642	−1.38533	−0.87955
H	4.788885	0.363893	0.885586
H	4.789054	0.36424	−0.88512
H	5.290031	−1.08485	−9E-06
Mg	−4.71717	−0.62857	−4.3E-05

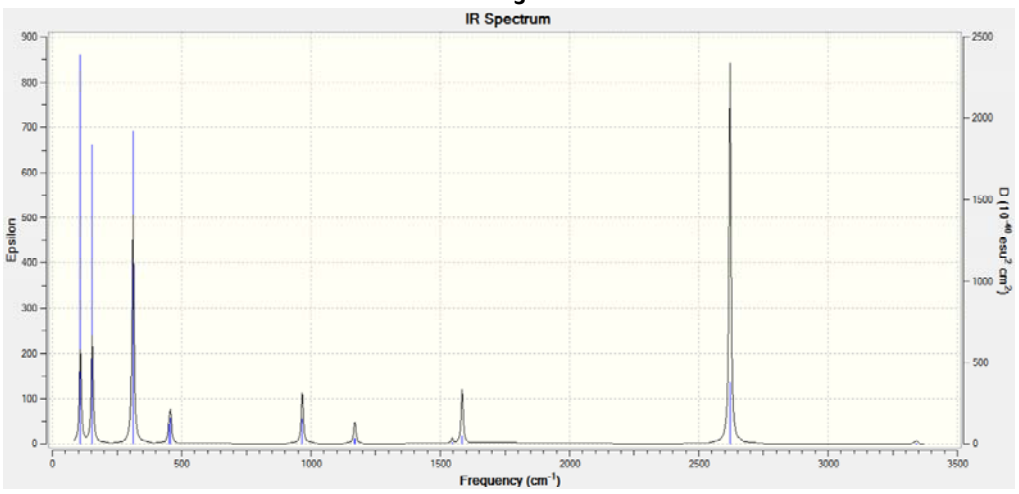
Sum of electronic and thermal Enthalpies

= −489.750237 hartrees

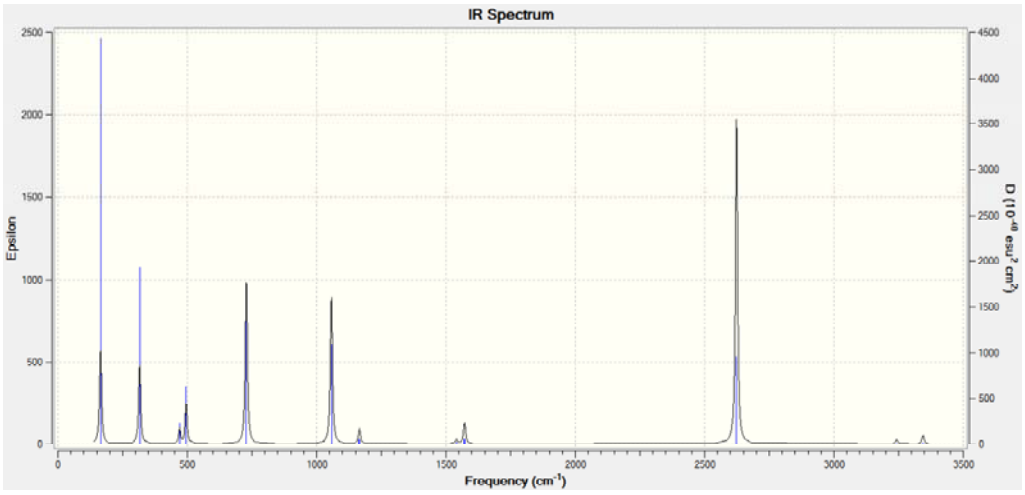
3. IR spectra



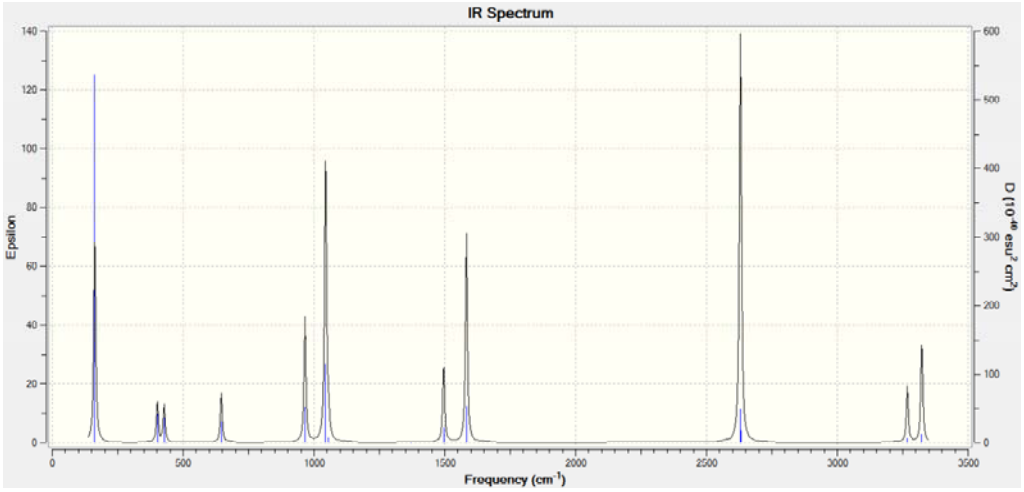
CH_3CN



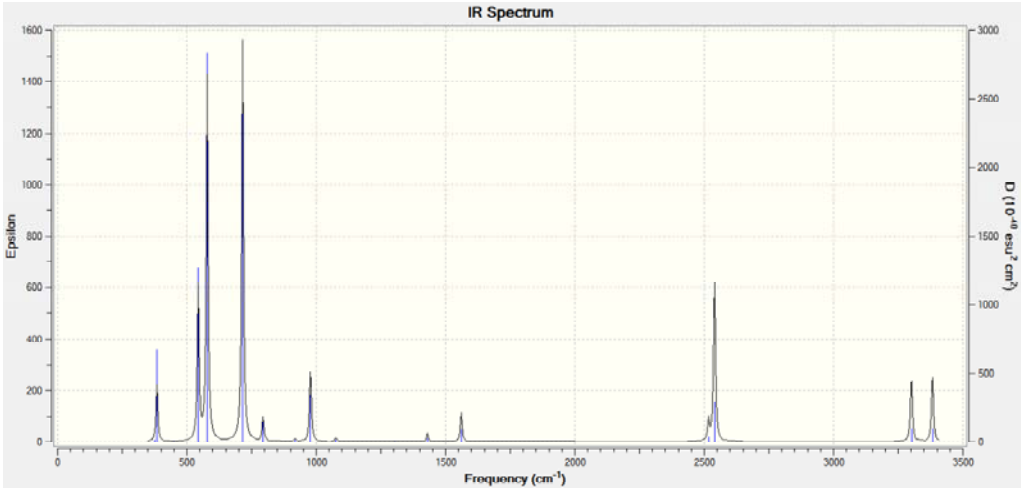
$Mg—CH_3CN$



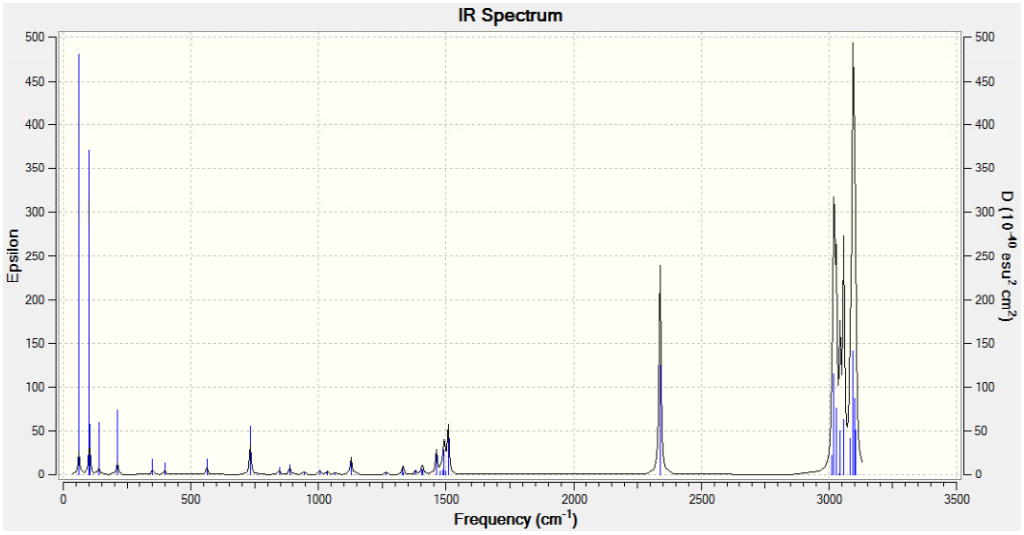
$Be—CH_3CN$



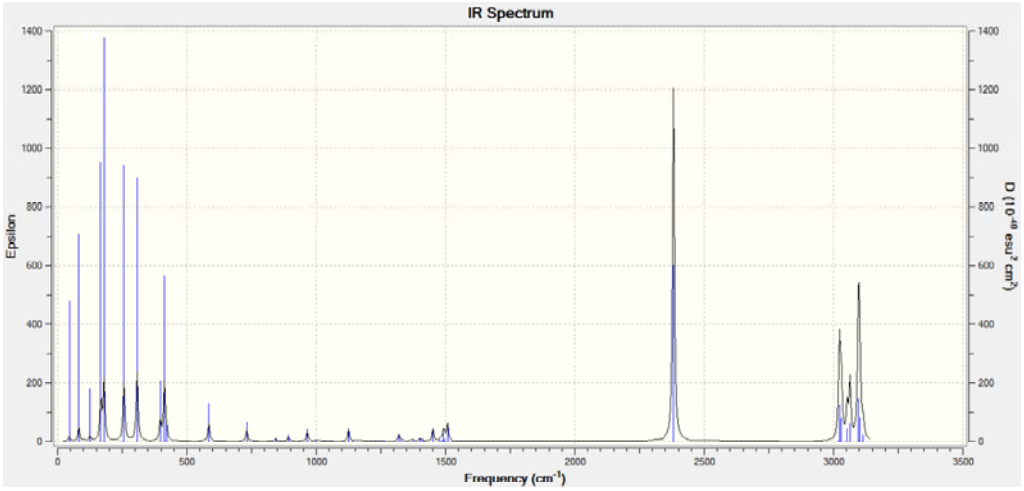
Malono Nitrile



Be—Malono Nitrile



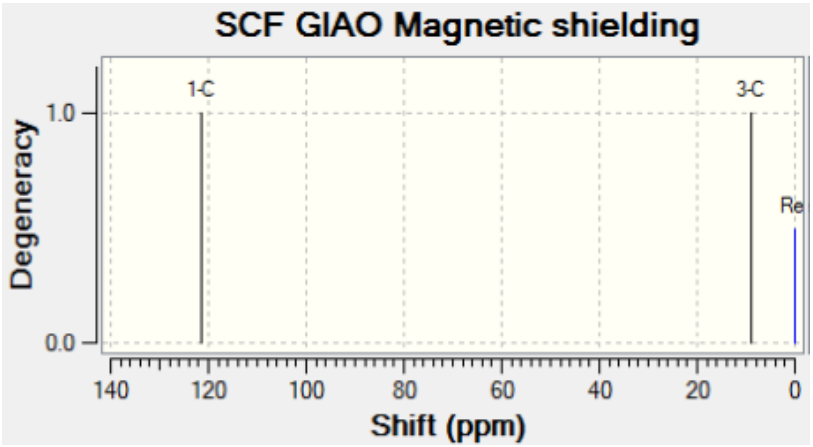
n-Pentane Carbonitrile



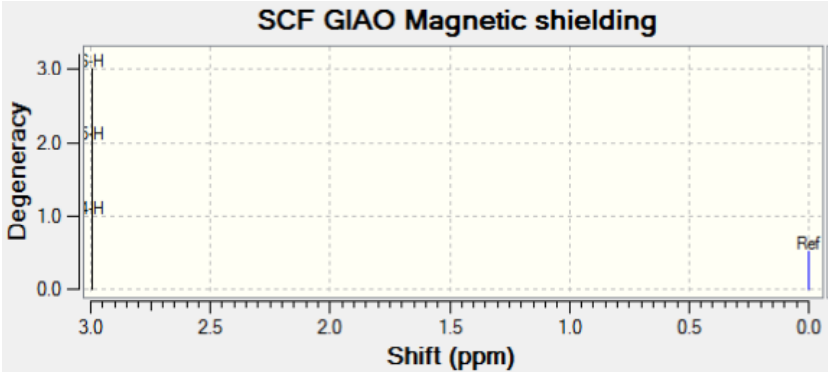
Mg--*n*-Pentane Carbonitrile

4. NMR GIAO Spectra

CH3CN

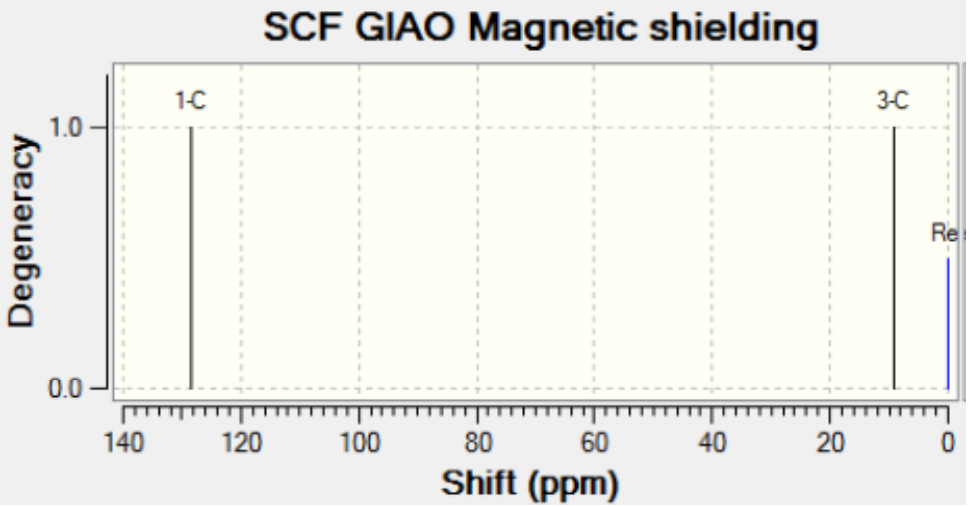


^{13}C NMR GIAO against reference TMS HF/6-31G(d) GIAO

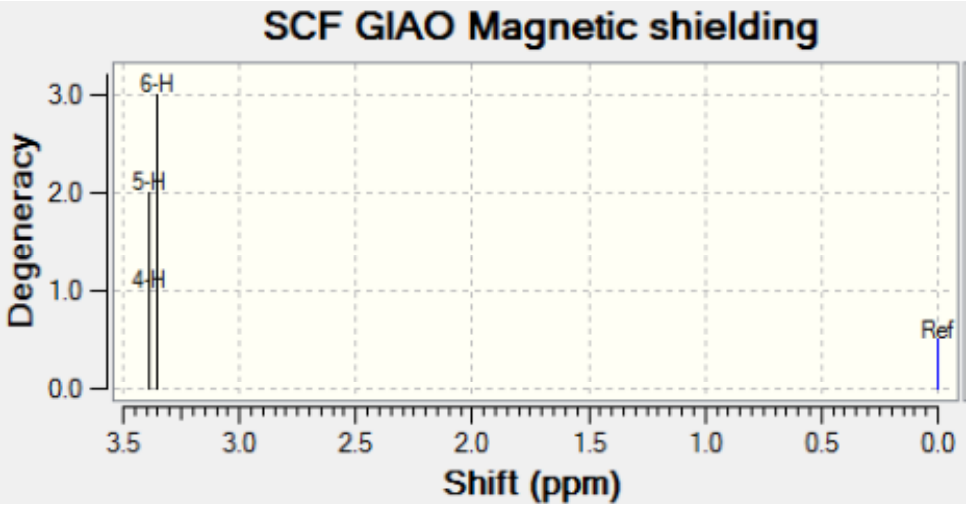


^{1}H NMR GIAO against reference TMS HF/6-31G(d) GIAO

Mg—CH3CN

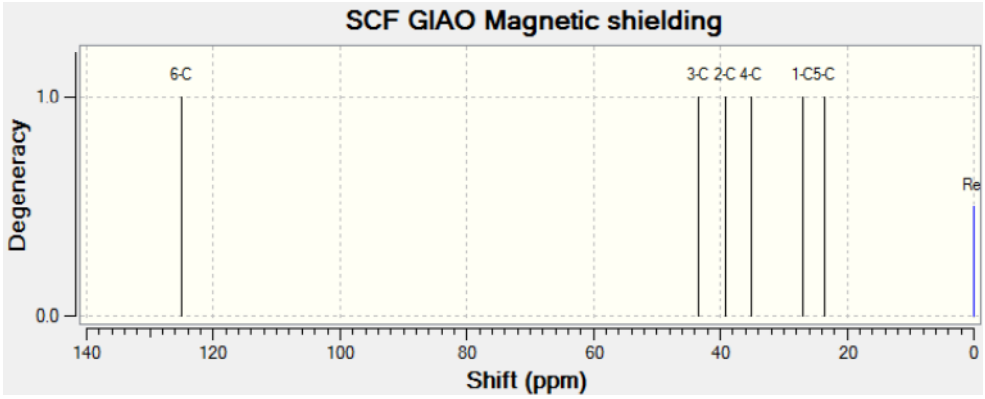


^{13}C NMR GIAO against reference TMS HF/6-31G(d) GIAO

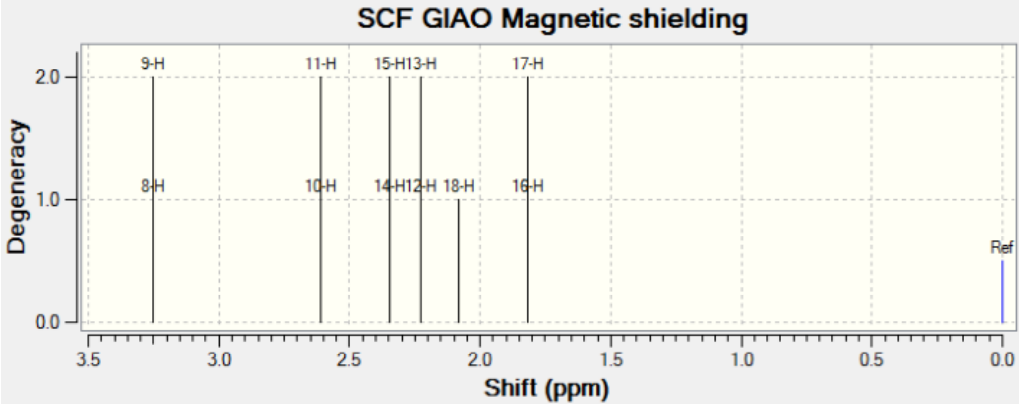


^{1}H NMR GIAO against reference TMS HF/6-31G(d) GIAO

n-Pentane Carbonitrile

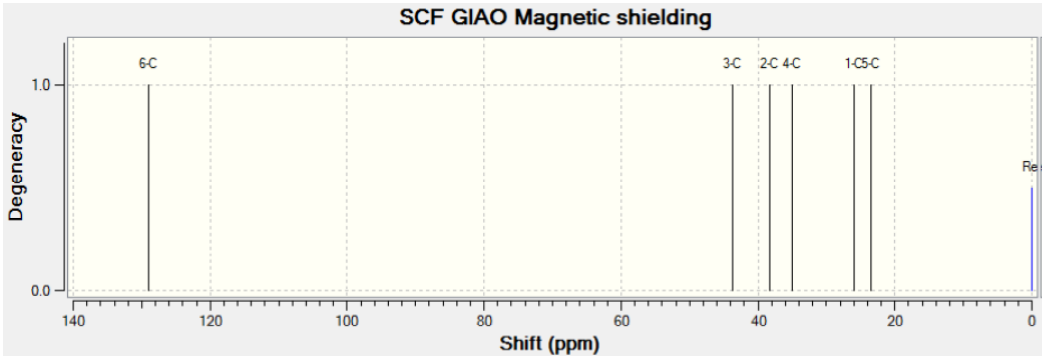


^{13}C NMR GIAO against reference TMS HF/6-31G(d) GIAO

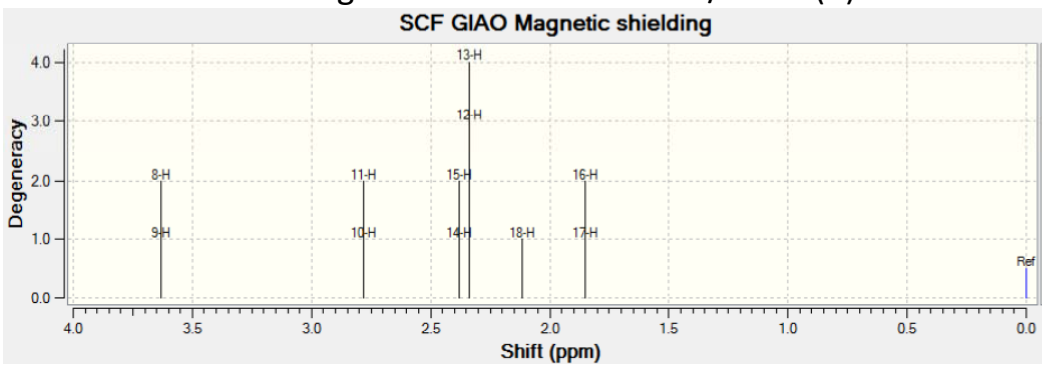


^{1}H NMR GIAO against reference TMS HF/6-31G(d) GIAO

Mg--*n*-Pentane Carbonitrile

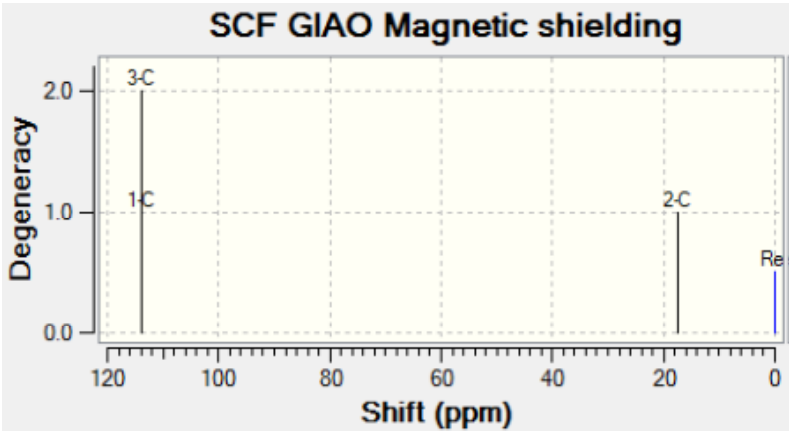


^{13}C NMR GIAO against reference TMS HF/6-31G(d) GIAO

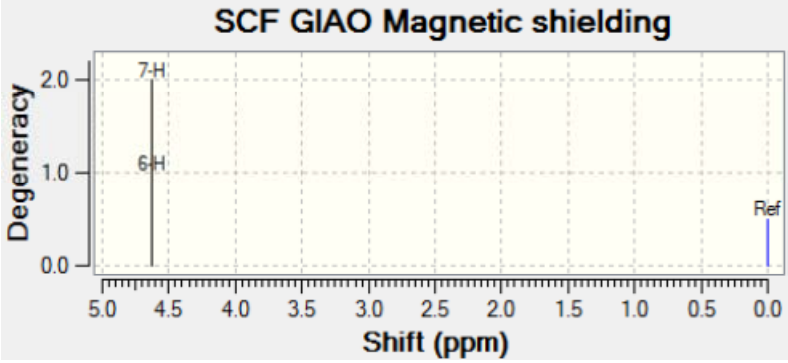


^{1}H NMR GIAO against reference TMS HF/6-31G(d) GIAO

Malono Nitrile

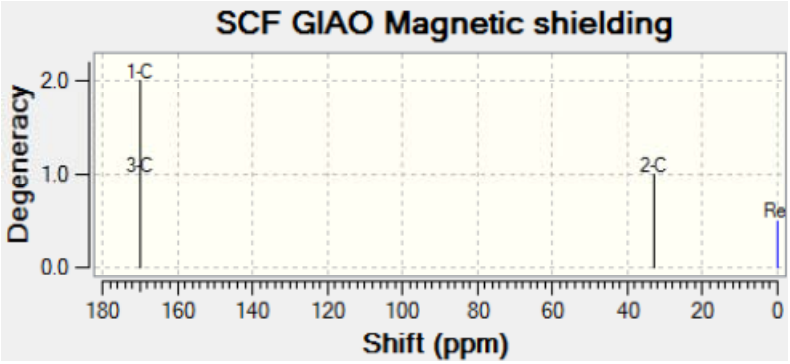


^{13}C NMR GIAO against reference TMS HF/6-31G(d) GIAO

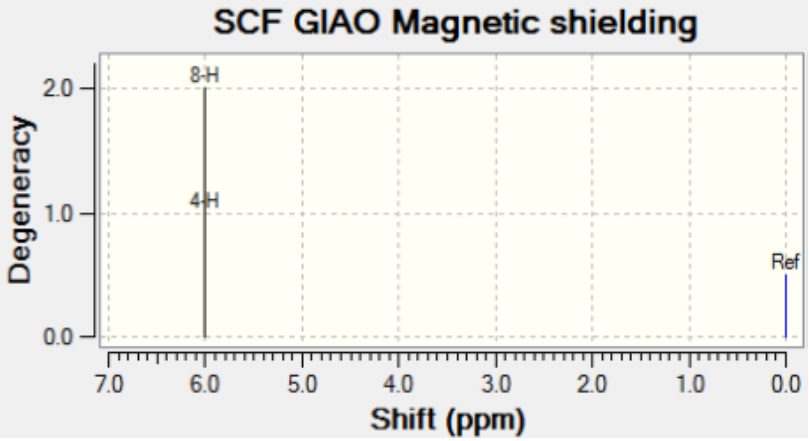


^{1}H NMR GIAO against reference TMS HF/6-31G(d) GIAO

Be—Malono Nitrile

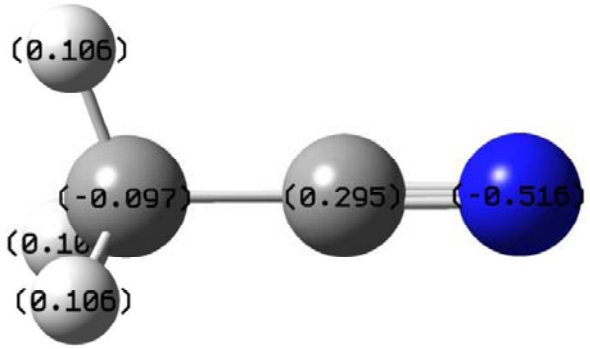


^{13}C NMR GIAO against reference TMS HF/6-31G(d) GIAO

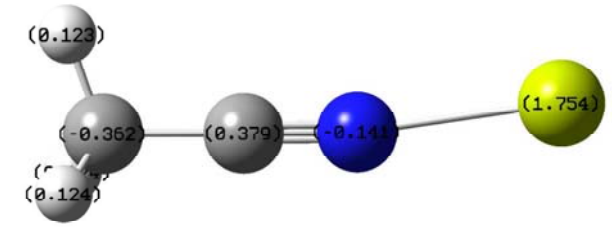


^{1}H NMR GIAO against reference TMS HF/6-31G(d) GIAO

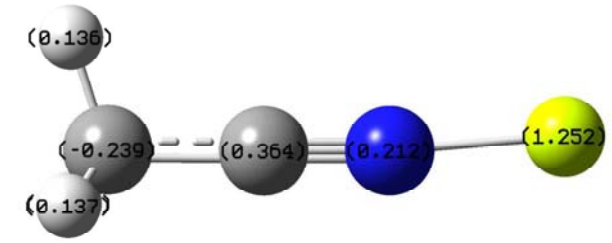
5. Mulliken Charges



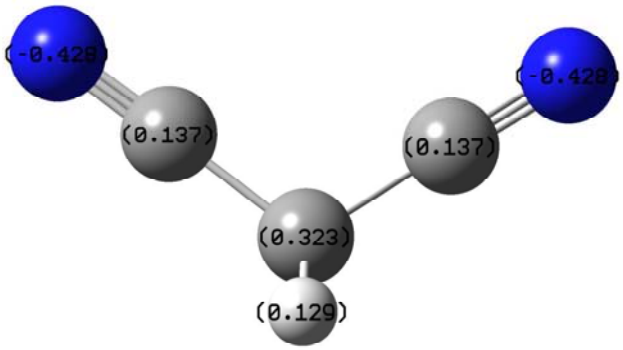
CH3CN



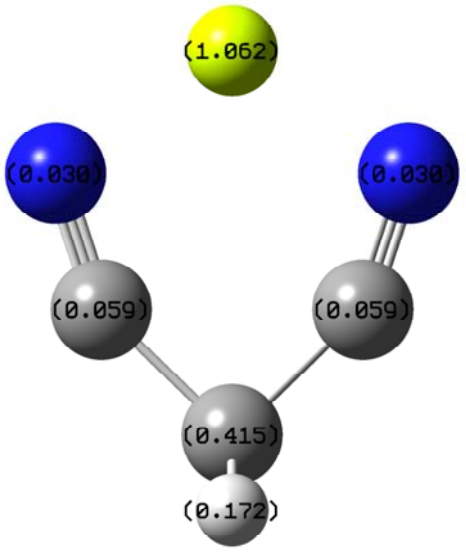
Mg-CH3CN



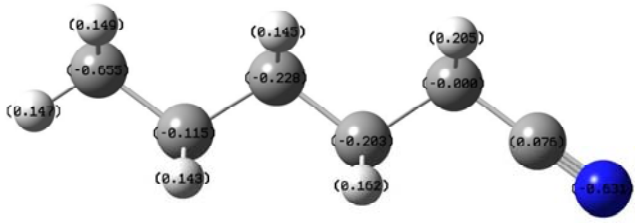
Be-CH3CN



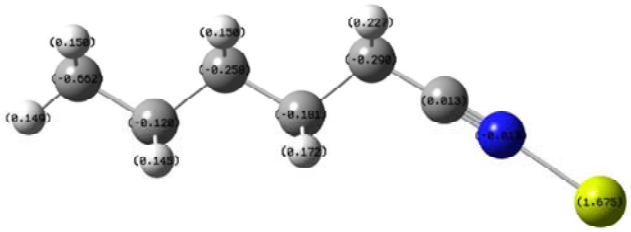
Malono nitrile



Be-Malono Nitrile

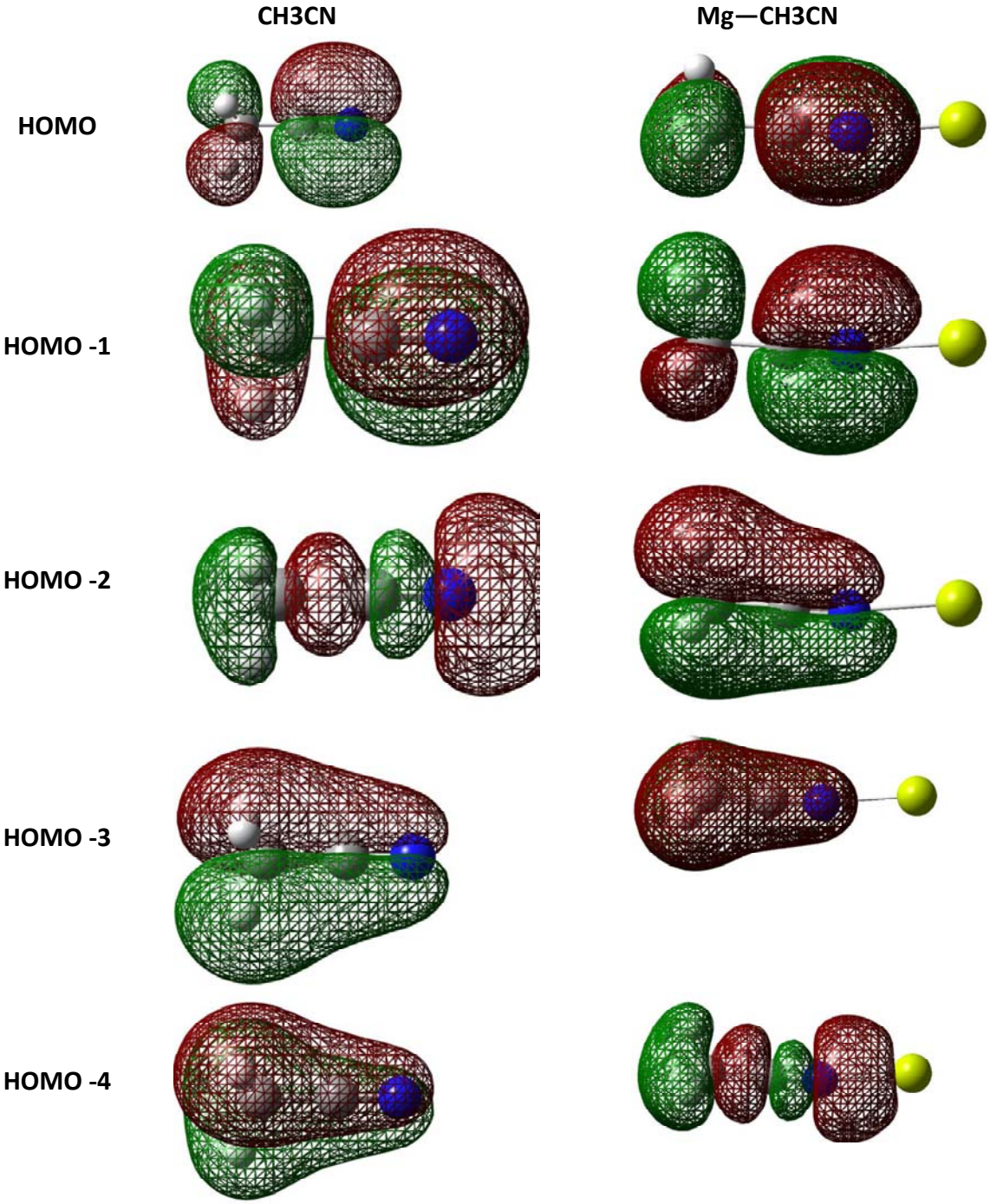


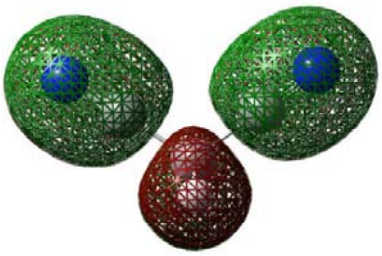
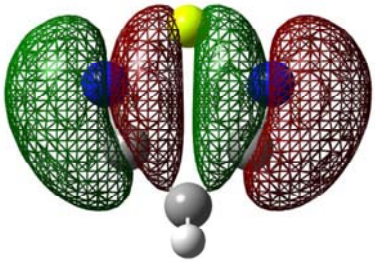
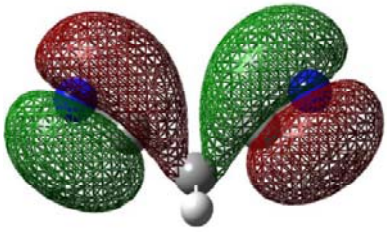
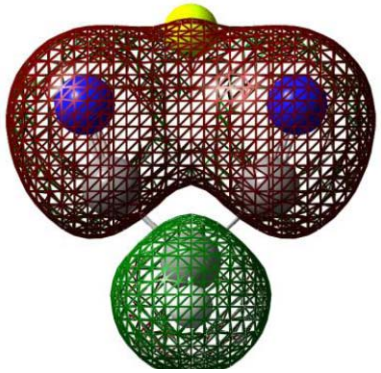
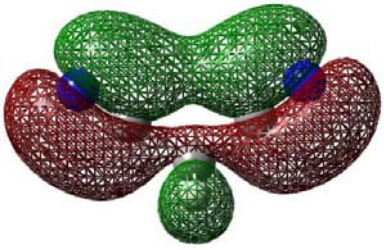
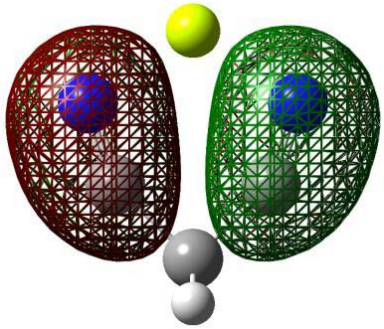
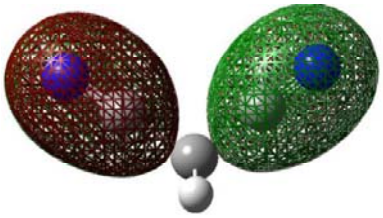
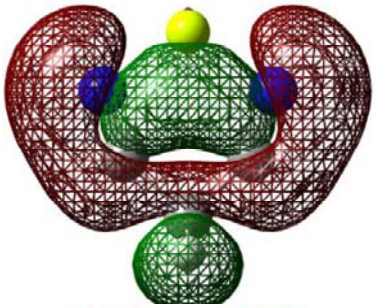
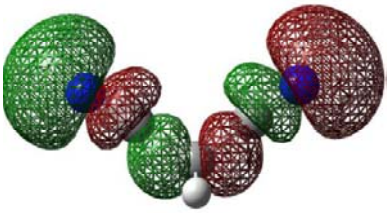
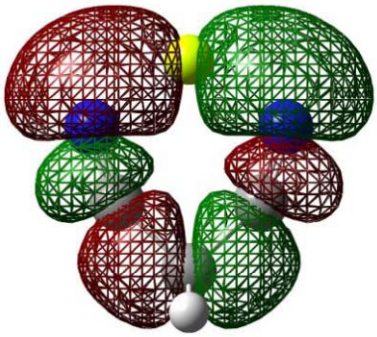
n-Pentane carbonitrile



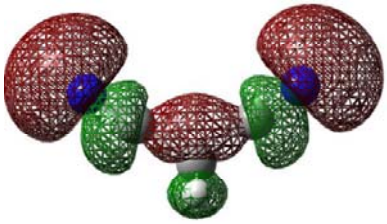
Mg--*n*-Pentane carbonitrile

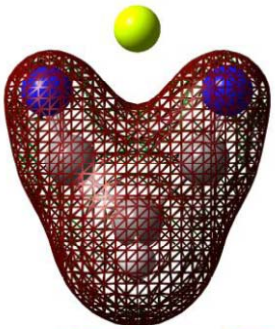
7. Molecular Orbitals



	Malono Nitrile	Be--Malono Nitrile
HOMO		
HOMO -1		
HOMO -2		
HOMO -3		
HOMO -4		

HOMO -5





HOMO -6