

- Electronic Supplementary Information -

Computational Study of 1,2,3-Triazol-5-ylidenes with *p*-Block

Element Substituents

Shiqing Huang, Yedong Wang, Chubin Hu and Xiaoyu Yan*

Department of Chemistry, Renmin University of China, Beijing 100872, People's
Republic of China

Corresponding author's contact: yanxy@ruc.edu.cn

Table of contents

Figure S1. Frontier molecular orbital energies trend of HOMO and LUMO calculated at different functional (B3LYP, PBE0, BP86, M06-2X) with basis set of def2TZVP.

Figure S2. The frontier molecular energies trend of **MIC-Icosagen** with methyl and H attached to group 13 elements, respectively.

Figure S3. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+1 of **MIC-H** with corresponding energy in the brackets. Isovalue=0.05.

Figure S4. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Al** with corresponding energy in the brackets. Isovalue=0.05.

Figure S5. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Si** with corresponding energy in the brackets. Isovalue=0.05.

Figure S6. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-P** with corresponding energy in the brackets. Isovalue=0.05.

Figure S7. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-S** with corresponding energy in the brackets. Isovalue=0.05.

Figure S8. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Cl** with corresponding energy in the brackets. Isovalue=0.05.

Figure S9. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Ga** with corresponding energy in the brackets. Isovalue=0.05.

Figure S10. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Ge** with

corresponding energy in the brackets. Isovalue=0.05.

Figure S11. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-As** with corresponding energy in the brackets. Isovalue=0.05.

Figure S12. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Se** with corresponding energy in the brackets. Isovalue=0.05.

Figure S13. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Br** with corresponding energy in the brackets. Isovalue=0.05.

Figure S14. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-In** with corresponding energy in the brackets. Isovalue=0.05.

Figure S15. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Sn** with corresponding energy in the brackets. Isovalue=0.05.

Figure S16. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Sb** with corresponding energy in the brackets. Isovalue=0.05.

Figure S17. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Te** with corresponding energy in the brackets. Isovalue=0.05.

Figure S18. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-I** with corresponding energy in the brackets. Isovalue=0.05.

Figure S19. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Tl** with corresponding energy in the brackets. Isovalue=0.05.

Figure S20. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Pb** with corresponding energy in the brackets. Isovalue=0.05.

Figure S21. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Bi** with corresponding energy in the brackets. Isovalue=0.05.

Table 1. Calculated bond lengths and N₁-C₄-C₅ bond angles of singlet and triplet states along with the singlet-triplet gaps of the investigated systems.

Table 2. Calculated atom contribution for HOMO-1 of **MIC-Pnictogen** using Hirshfeld method.

Table 3. Calculated atom contribution for HOMO-1 of **MIC-Chalcogen** using Hirshfeld method.

Cartesian Coordinate

Figure S1. Frontier molecular orbital energies trend of HOMO and LUMO calculated at different functional (B3LYP, PBE0, BP86, M06-2X) with basis set of def2TZVP.

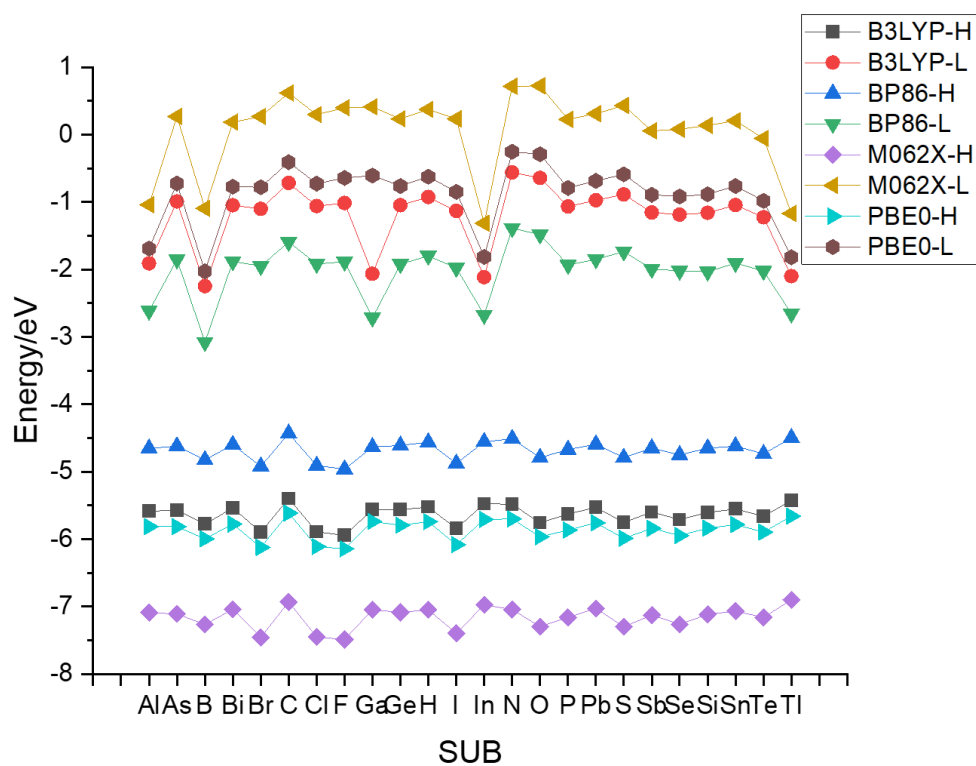


Figure S2. The frontier molecular energies trend of **MIC-Icosagen** with methyl and H attached to group 13 elements, respectively.

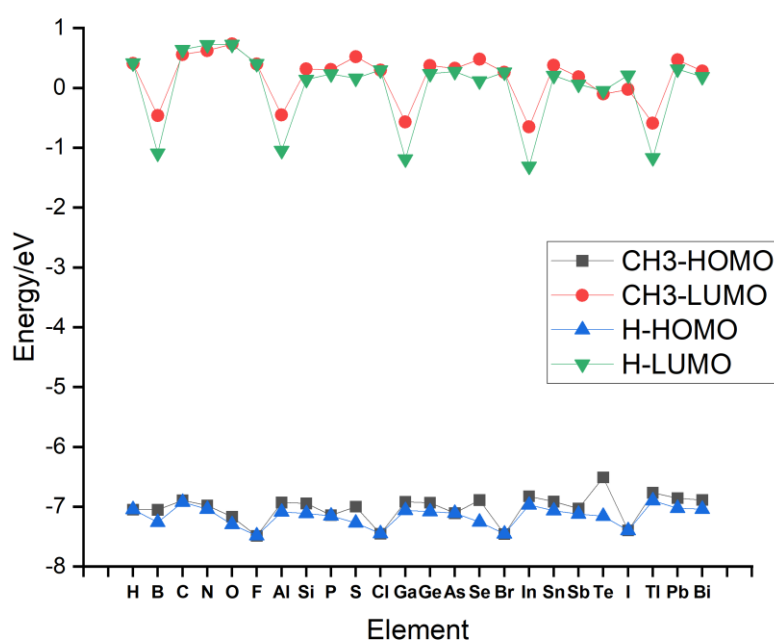


Figure S3. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+1 of **MIC-H** with corresponding energy in the brackets. Isovalue=0.05.

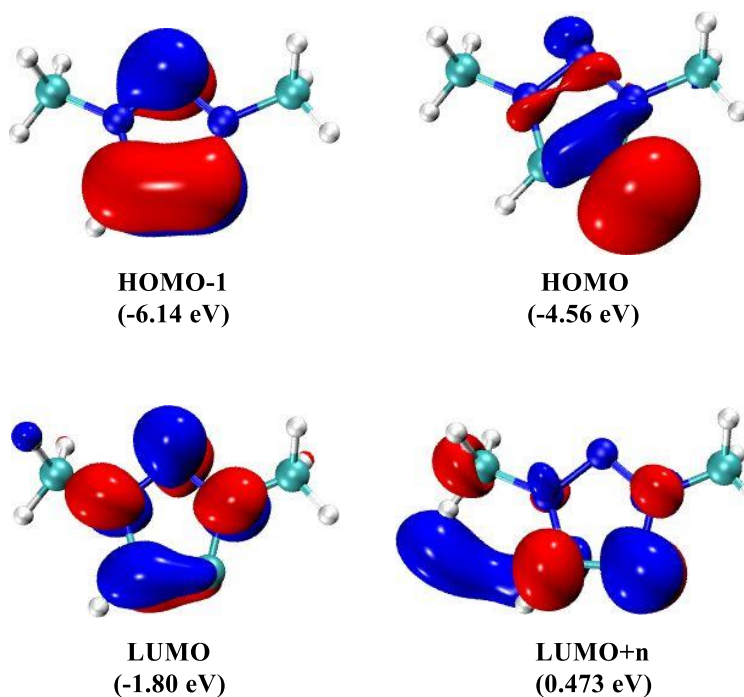


Figure S4. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Al** with corresponding energy in the brackets. Isovalue=0.05.

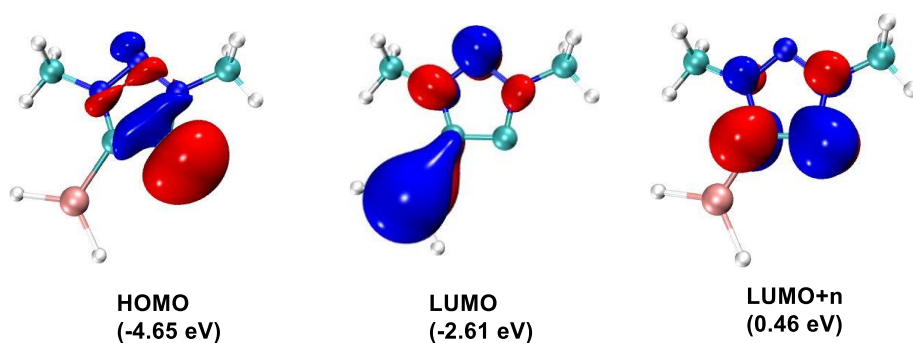


Figure S5. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Si** with corresponding energy in the brackets. Isovalue=0.05.

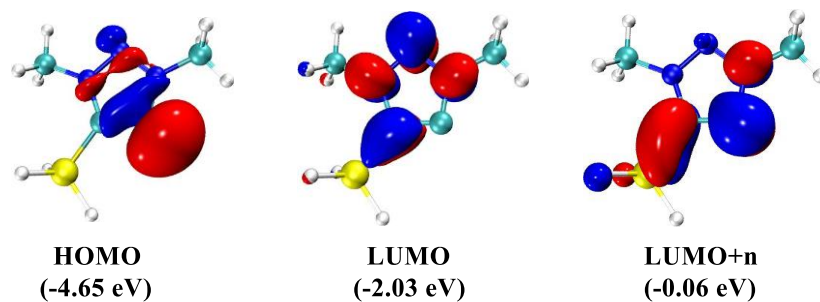


Figure S6. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-P** with corresponding energy in the brackets. Isovalue=0.05.

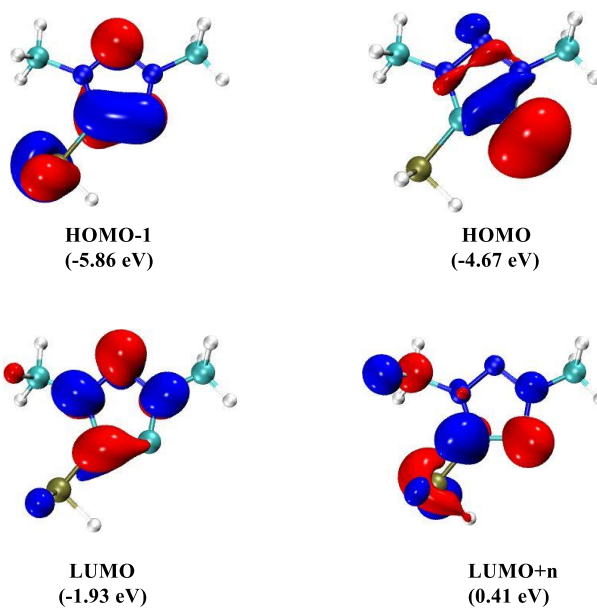


Figure S7. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-S** with corresponding energy in the brackets. Isovalue=0.05.

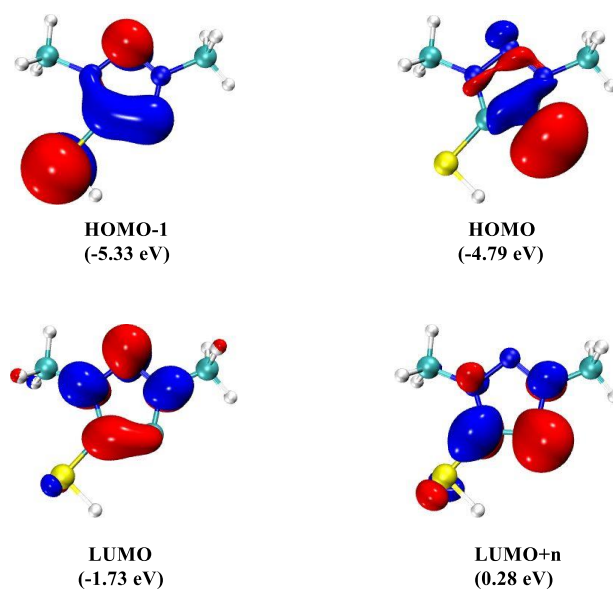


Figure S8. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Cl** with corresponding energy in the brackets. Isovalue=0.05.

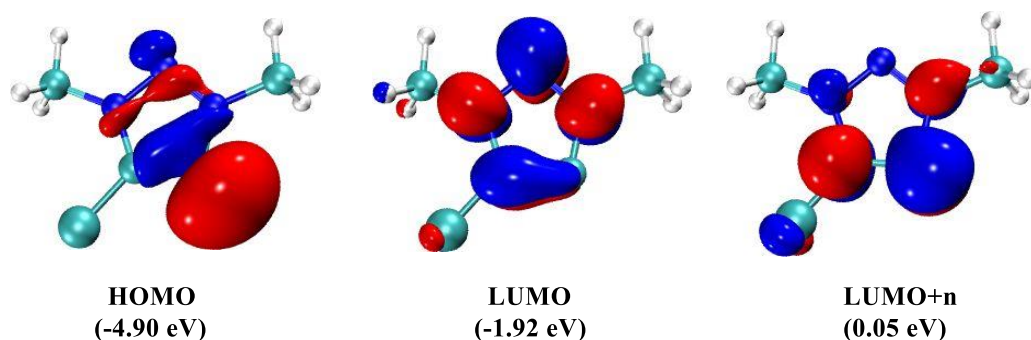


Figure S9. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Ga** with corresponding energy in the brackets. Isovalue=0.05.

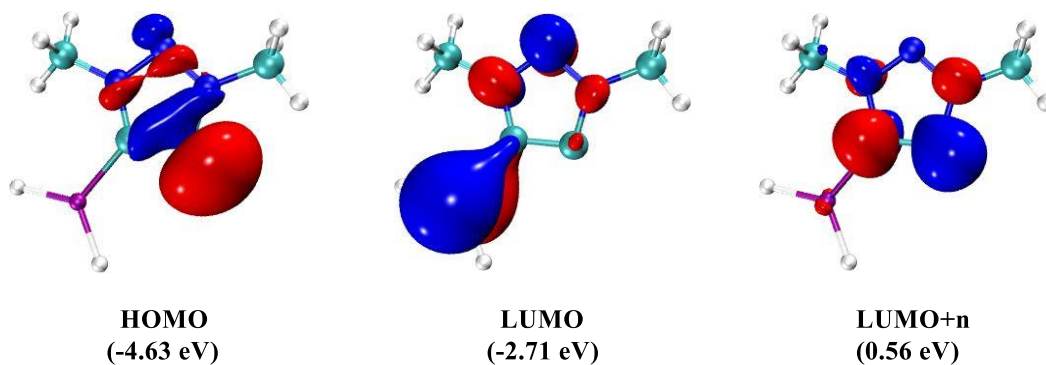


Figure S10. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Ge** with corresponding energy in the brackets. Isovalue=0.05.

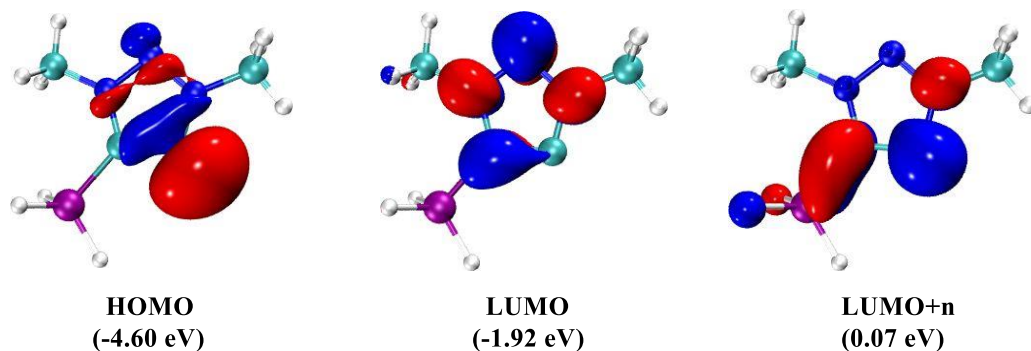


Figure S11. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-As** with corresponding energy in the brackets. Isovalue=0.05.

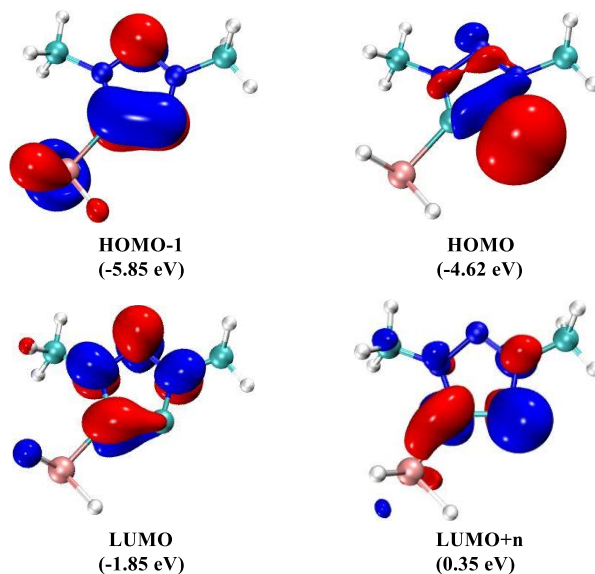


Figure S12. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Se** with corresponding energy in the brackets. Isovalue=0.05.

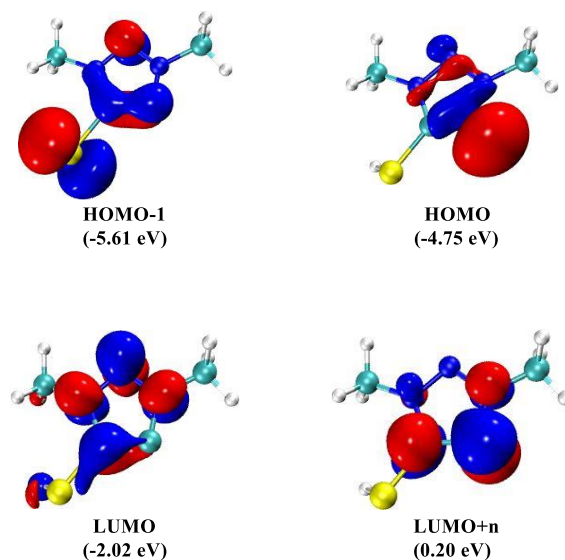


Figure S13. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Br** with corresponding energy in the brackets. Isovalue=0.05.

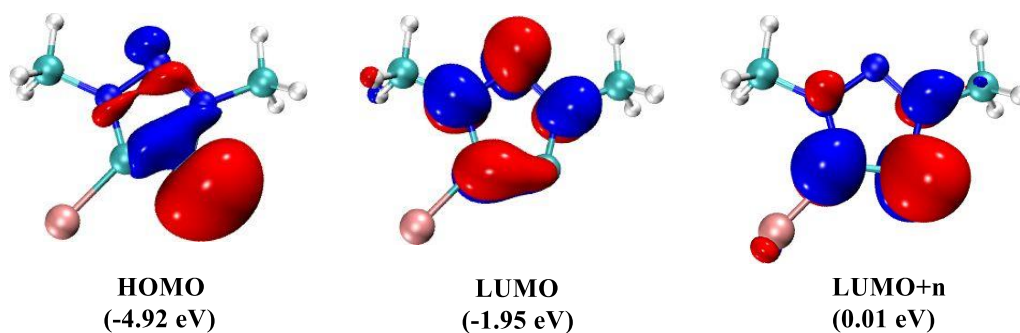


Figure S14. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-In** with corresponding energy in the brackets. Isovalue=0.05.

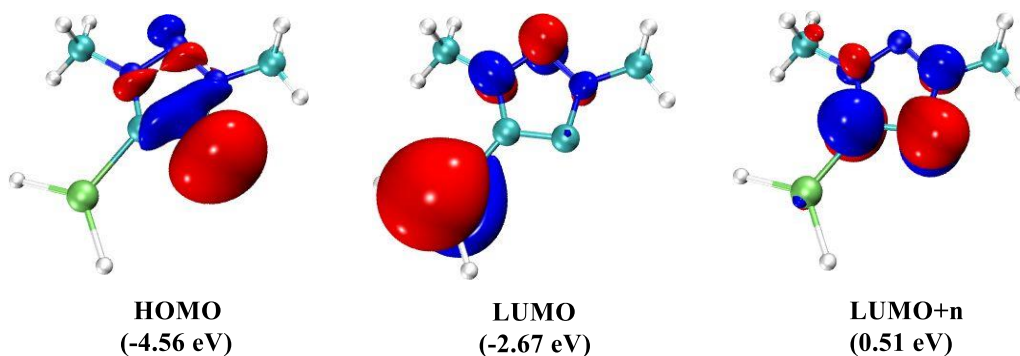


Figure S15. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Sn** with corresponding energy in the brackets. Isovalue=0.05.

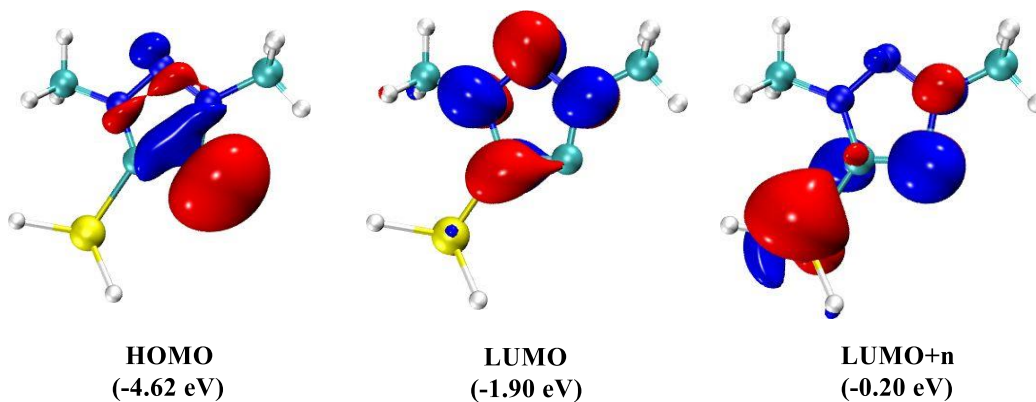


Figure S16. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Sb** with corresponding energy in the brackets. Isovalue=0.05.

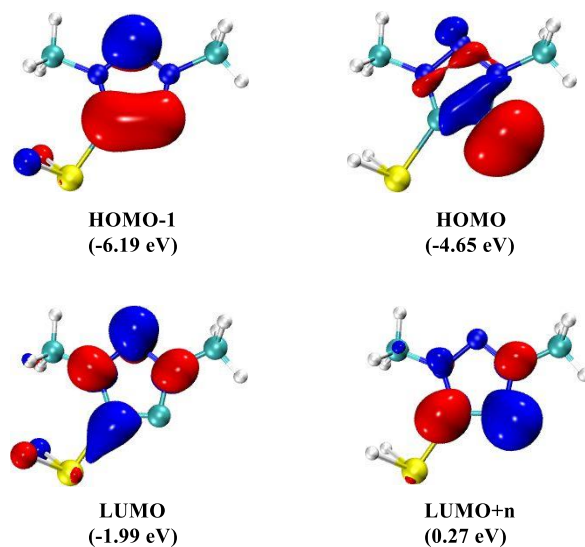


Figure S17. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Te** with corresponding energy in the brackets. Isovalue=0.05.

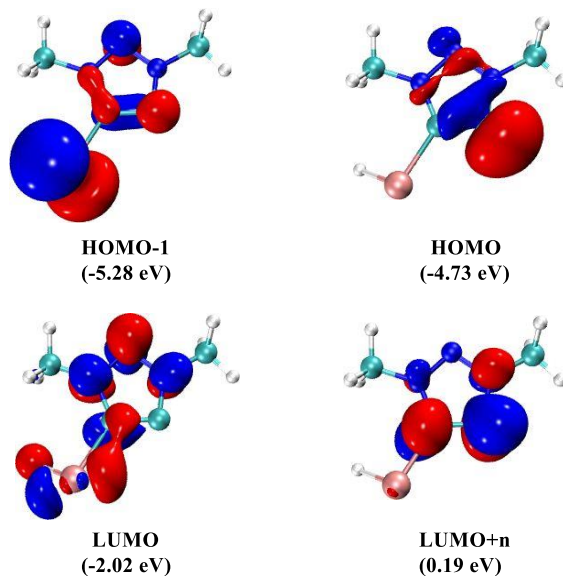


Figure S18. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-I** with corresponding energy in the brackets. Isovalue=0.05.

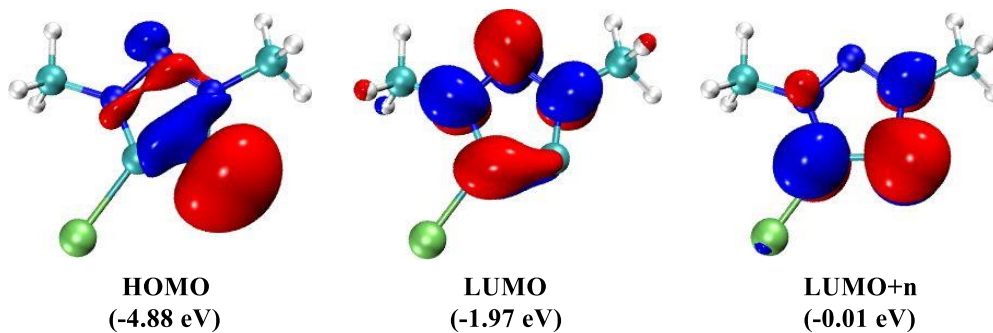


Figure S19. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Tl** with corresponding energy in the brackets. Isovalue=0.05.

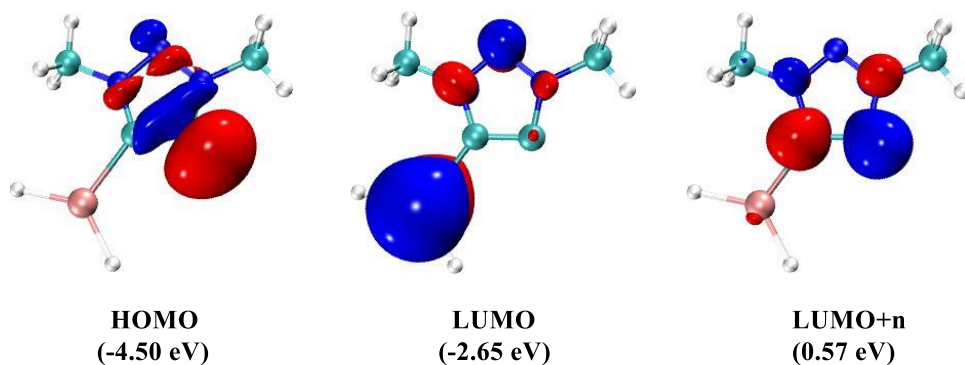


Figure S20. Frontier orbitals of calculated HOMO, LUMO and LUMO+n of **MIC-Pb** with corresponding energy in the brackets. Isovalue=0.05.

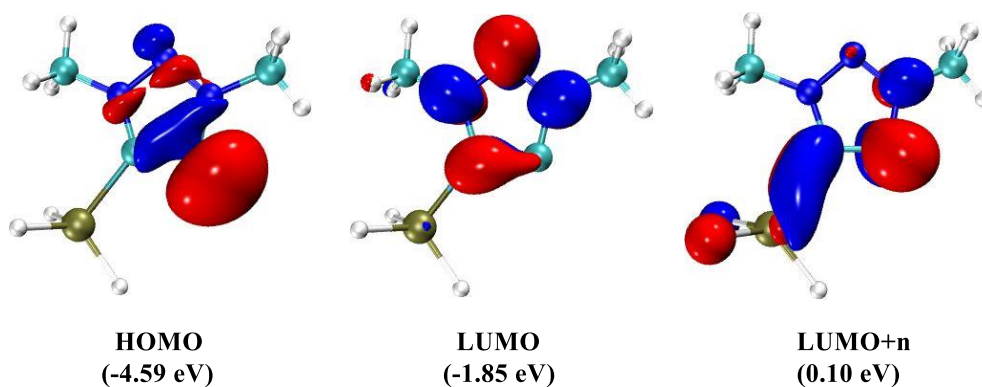


Figure S21. Frontier orbitals of calculated HOMO-1, HOMO, LUMO and LUMO+n of **MIC-Te** with corresponding energy in the brackets. Isovalue=0.05.

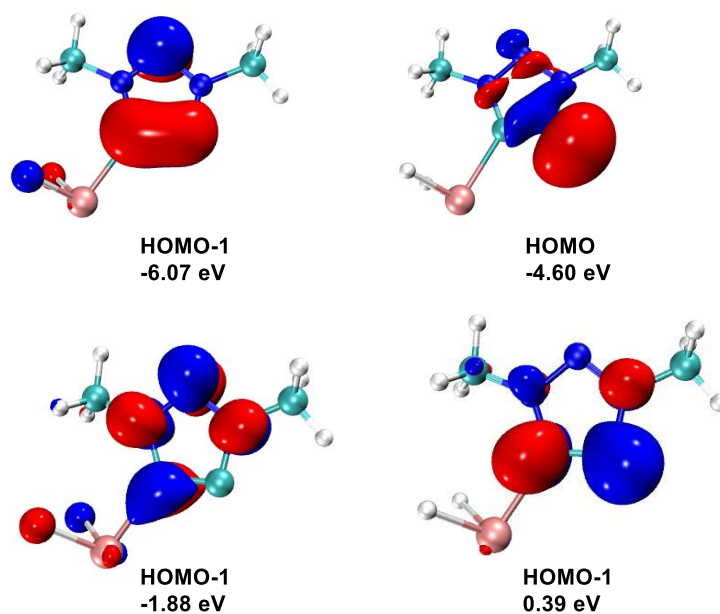


Table 1. Calculated bond lengths and N₁–C₄–C₅ bond angles of singlet and triplet states along with the singlet-triplet gaps of the investigated systems.

Compounds	singlet			triplet			Gap (S-T) kcal/mol
	C ₅ –N ₁	C ₄ –C ₅	N ₁ –C ₄ –C ₅	C ₅ –N ₁	C ₄ –C ₅	N ₁ –C ₄ –C ₅	
	(Å)	(Å)	(°)	(Å)	(Å)	(°)	
MIC-H	1.38	1.41	98.7	1.38	1.37	110.0	60.0
MIC-B	1.38	1.43	100.2	1.34	1.41	111.6	45.1
MIC-Al	1.38	1.43	100.3	1.34	1.39	112.0	50.2
MIC-Ga	1.38	1.43	100.0	1.34	1.39	111.8	56.4
MIC-In	1.38	1.42	100.0	1.35	1.38	111.5	54.3
MIC-Tl	1.38	1.42	99.8	1.36	1.37	109.9	47.8
MIC-C	1.38	1.41	99.3	1.38	1.37	110.2	58.3
MIC-Si	1.38	1.42	99.5	1.36	1.38	111.4	58.5
MIC-Ge	1.39	1.42	99.4	1.37	1.37	111.2	59.6
MIC-Sn	1.39	1.41	99.6	1.37	1.37	111.3	58.9
MIC-Pb	1.39	1.41	99.3	1.36	1.37	110.1	59.1
MIC-N	1.38	1.41	98.9	1.39	1.39	104.3	54.1
MIC-P	1.38	1.42	99.2	1.37	1.37	110.7	60.2
MIC-As	1.38	1.41	99.1	1.37	1.37	110.8	59.2
MIC-Sb	1.39	1.41	99.3	1.36	1.37	111.1	59.0
MIC-Bi	1.39	1.41	99.3	1.37	1.37	111.0	48.0
MIC-O	1.38	1.40	98.3	1.40	1.39	104.5	61.4
MIC-S	1.38	1.41	98.5	1.39	1.38	106.8	61.3
MIC-Se	1.38	1.41	98.9	1.36	1.37	109.3	59.3
MIC-Te	1.38	1.41	98.9	1.37	1.39	104.8	54.6
MIC-F	1.38	1.39	97.5	1.39	1.37	106.8	65.5
MIC-Cl	1.38	1.40	98.1	1.38	1.37	108.2	61.5
MIC-Br	1.38	1.40	98.1	1.38	1.37	108.6	60.7
MIC-I	1.38	1.40	98.4	1.37	1.38	105.2	53.7

Table 2. Calculated atom contribution for HOMO-1 of **MIC-Pnictogen** using Hirshfeld method.

HOMO-1	C2	C3	Hetero
MIC-N	17	20	25
MIC-P	21	18	25
MIC-As	28	20	18
MIC-Sb	30	24	5
MIC-Bi	30	24	5

Table 3. Calculated atom contribution for HOMO-1 of **MIC-Chalcogen** using Hirshfeld method.

HOMO-1	C2	C3	Hetero
MIC-O	19	23	20
MIC-S	14	16	41
MIC-Se	9	8	65
MIC-Te	6	7	71

Cartesian Coordinate

ligands MIC

MIC-H

E (SCF) = -320.925573367 a.u.

7	0.024477000	-0.864731000	0.004338000
7	-1.021034000	-0.052317000	0.013923000
6	-0.643052000	1.268165000	0.005290000
6	0.755368000	1.357357000	-0.008320000
7	1.055635000	0.012605000	-0.009584000
6	-2.361799000	-0.624924000	-0.007408000
6	2.398135000	-0.559571000	0.001430000
1	-1.401566000	2.045950000	0.010902000
1	-2.443448000	-1.403102000	0.761226000
1	-3.079550000	0.177057000	0.200632000
1	-2.572291000	-1.060515000	-0.993523000
1	3.095621000	0.269313000	-0.150830000
1	2.596693000	-1.043600000	0.967995000
1	2.499089000	-1.300162000	-0.803093000

MIC-B

E (SCF) = -346.372259148 a.u.

7	0.698348000	-0.553880000	-0.000067000
6	0.749096000	0.848324000	0.000169000
6	-0.600416000	1.312759000	0.000198000
7	-1.274677000	0.120650000	-0.000026000
7	-0.524466000	-1.016236000	-0.000189000
6	-2.724143000	-0.056247000	-0.000111000
6	1.803635000	-1.510729000	-0.000186000
5	2.046990000	1.635740000	0.000350000
1	-3.160763000	0.946801000	0.000066000
1	-3.039017000	-0.607476000	-0.896578000
1	-3.039080000	-0.607822000	0.896120000
1	2.420968000	-1.354738000	0.892945000
1	1.383260000	-2.521427000	-0.000377000
1	2.421043000	-1.354431000	-0.893210000
1	2.003609000	2.832268000	0.000549000
1	3.111564000	1.069743000	0.000294000

MIC-Al

E (SCF) = -563.977417863 a.u.

7	0.075711000	0.926740000	0.000095000
6	0.609814000	-0.359064000	-0.000084000
6	-0.484991000	-1.264786000	-0.000113000
7	-1.541135000	-0.384572000	0.000052000
7	-1.241884000	0.936158000	0.000179000
6	-2.958050000	-0.736088000	0.000113000
6	0.771228000	2.212354000	0.000166000
13	2.459084000	-0.942243000	-0.000239000
1	-3.008911000	-1.828987000	-0.000045000
1	-3.449283000	-0.333035000	0.896282000
1	-3.449426000	-0.332767000	-0.895856000
1	1.849271000	2.015533000	0.000228000
1	0.498112000	2.784828000	-0.895728000
1	0.497993000	2.784788000	0.896047000
1	2.817183000	-2.484432000	-0.000479000
1	3.600116000	0.180452000	-0.000115000

MIC-Ga

E (SCF) = -2246.63460884 a.u.

7	-0.604204000	1.027453000	0.014621000
6	0.093002000	-0.175914000	-0.015690000
6	-0.866278000	-1.221782000	-0.026844000
7	-2.030084000	-0.489336000	-0.005233000
7	-1.912140000	0.859322000	0.017468000
6	-3.386506000	-1.028695000	0.010743000
6	-0.089147000	2.394458000	-0.022554000
31	2.025308000	-0.427268000	0.004977000
1	-3.291592000	-2.115760000	-0.068499000
1	-3.891010000	-0.761194000	0.949482000
1	-3.962031000	-0.632548000	-0.836790000
1	-0.757557000	3.045797000	0.551614000
1	0.915416000	2.401845000	0.414985000
1	-0.034977000	2.747431000	-1.061834000
1	2.954985000	0.845135000	0.135658000
1	2.600796000	-1.875888000	-0.100800000

MIC-In

E (SCF) = -511.754262041 a.u.

7	1.132713000	1.055451000	-0.009080000
6	0.352500000	-0.092212000	0.025556000
6	1.231671000	-1.204573000	0.031843000
7	2.446921000	-0.558555000	0.003537000
7	2.428566000	0.793842000	-0.018320000

6	3.759465000	-1.196572000	-0.018890000
6	0.718302000	2.455392000	0.027901000
49	-1.781727000	-0.255878000	-0.004463000
1	3.584735000	-2.274196000	0.054186000
1	4.280915000	-0.961281000	-0.957052000
1	4.364579000	-0.849559000	0.829690000
1	1.401307000	3.051250000	-0.588306000
1	-0.302662000	2.527866000	-0.364358000
1	0.738068000	2.827859000	1.061676000
1	-2.500505000	-1.807579000	0.163572000
1	-2.690859000	1.216292000	-0.212128000

MIC-TI

E (SCF) = -494.137784598 a.u.

N	1.63166900	1.07018800	-0.00580400
C	0.81814500	-0.05885200	0.01981700
C	1.66095600	-1.20281600	0.02403300
N	2.89865400	-0.58421600	0.00247400
N	2.91908100	0.76564700	-0.01352500
C	4.19223500	-1.26091800	-0.01505800
C	1.26046400	2.48143600	0.02101800
H	3.98481500	-2.34328500	0.04648200
H	4.73781100	-1.03312400	-0.95296000
H	4.80910500	-0.94024200	0.84808800
H	0.18898700	2.56717400	-0.23679000
H	1.42959300	2.90807400	1.03040100
H	1.86980300	3.04007900	-0.71431800
H	-2.08867200	-1.74400000	0.12724100
H	-2.28142200	1.36870200	-0.16025300
TI	-1.38748900	-0.15231900	-0.00208300

MIC-C

E (SCF) = -360.260884125 a.u.

7	-0.601473185	0.629676444	0.000000879
6	-0.706948213	-0.742900795	0.000000136
6	0.587377756	-1.294417685	-0.000002062
7	1.328913798	-0.134286666	-0.000002404
7	0.663005239	1.040045939	-0.000000476
6	2.786061102	-0.058170099	0.000001543
6	-1.667770862	1.621455443	-0.000000041
6	-2.035609540	-1.422069721	0.000000973
1	3.154584684	-1.088176144	-0.000102309
1	3.138533563	0.471256729	-0.895929436
1	3.138539225	0.471071879	0.896039722
1	-2.293393532	1.496616683	-0.894724336
1	-2.293400020	1.496611116	0.894718864

1	-1.213989993	2.617687654	0.000004618
1	-2.636102319	-1.165314852	0.888857316
1	-2.636104901	-1.165312200	-0.888852897
1	-1.870449092	-2.505873761	-0.000000825

MIC-Si

E (SCF) = -611.660448223 a.u.

7	0.037485000	0.911788000	0.000014000
6	0.523574000	-0.384238000	0.000014000
6	-0.580008000	-1.266820000	-0.000037000
7	-1.612125000	-0.353210000	-0.000061000
7	-1.283872000	0.956763000	-0.000031000
6	-3.036464000	-0.673623000	-0.000114000
6	0.784543000	2.165421000	0.000057000
14	2.330275000	-0.850360000	0.000068000
1	-3.111113000	-1.765038000	-0.000137000
1	-3.518536000	-0.259965000	0.896155000
1	-3.518476000	-0.259931000	-0.896399000
1	1.418074000	2.216561000	-0.896063000
1	0.071204000	2.995839000	0.000049000
1	1.418022000	2.216531000	0.896215000
1	3.019448000	-0.279492000	1.201589000
1	2.437708000	-2.331772000	0.000081000
1	3.019518000	-0.279509000	-1.201420000

MIC-Ge

E (SCF) = -2399.39674105 a.u.

7	-0.626791000	1.016870000	0.000109000
6	0.028766000	-0.198570000	-0.000019000
6	-0.936693000	-1.225814000	-0.000091000
7	-2.085821000	-0.463993000	0.000008000
7	-1.944245000	0.878799000	0.000128000
6	-3.451516000	-0.979649000	-0.000003000
6	-0.061746000	2.362096000	0.000220000
32	1.963081000	-0.410964000	-0.000086000
1	-3.373740000	-2.070858000	-0.000139000
1	-3.986504000	-0.637139000	0.896306000
1	-3.986572000	-0.636919000	-0.896188000
1	0.558027000	2.502451000	-0.896018000
1	-0.884671000	3.084047000	0.000298000
1	0.558055000	2.502291000	0.896463000
1	2.574026000	0.275404000	1.248497000
1	2.273927000	-1.914210000	-0.000249000
1	2.573967000	0.275662000	-1.248557000

MIC-Sn

E (SCF) = -536.526343906 a.u.

7	1.150623000	1.054926000	0.009289000
6	0.392889000	-0.099471000	0.006733000
6	1.267532000	-1.204998000	-0.001843000
7	2.478887000	-0.546753000	-0.004231000
7	2.452430000	0.802770000	0.003304000
6	3.795245000	-1.177673000	-0.003414000
6	0.713365000	2.447592000	-0.003454000
50	-1.737155000	-0.250207000	-0.000260000
1	3.624994000	-2.257094000	-0.056295000
1	4.377778000	-0.840425000	-0.871445000
1	4.336940000	-0.925311000	0.918601000
1	0.017281000	2.621667000	0.827432000
1	1.594760000	3.087618000	0.106387000
1	0.208469000	2.671709000	-0.953339000
1	-2.314366000	-0.280841000	-1.618350000
1	-2.176939000	-1.674081000	0.832036000
1	-2.398934000	1.137788000	0.781294000

MIC-Pb

E (SCF) = -515.090918000 a.u.

7	1.628034000	1.060823000	0.000003000
6	0.853916000	-0.079263000	0.000001000
6	1.702755000	-1.200980000	0.000002000
7	2.926401000	-0.564316000	0.000004000
7	2.926961000	0.785638000	0.000005000
6	4.230492000	-1.220332000	0.000006000
6	1.210917000	2.458920000	0.000004000
1	4.039006000	-2.297474000	0.000004000
1	4.798519000	-0.935706000	-0.896268000
1	4.798516000	-0.935708000	0.896282000
1	0.610978000	2.666455000	-0.896658000
1	0.610975000	2.666454000	0.896664000
1	2.107339000	3.087360000	0.000006000
1	-1.964990000	0.697970000	1.439166000
1	-1.964985000	0.697970000	-1.439173000
1	-1.816118000	-1.848099000	-0.000003000
82	-1.360701000	-0.152735000	-0.000002000

MIC-N

E (SCF) = -376.313368281 a.u.

7	0.644483000	0.611567000	-0.009373000
6	0.696216000	-0.761040000	0.003590000
6	-0.609536000	-1.280455000	0.012210000
7	-1.309620000	-0.100769000	0.019333000

7	-0.616725000	1.059423000	0.022625000
6	-2.763802000	0.012853000	-0.007964000
6	1.750587000	1.553262000	-0.019907000
7	1.925627000	-1.424542000	-0.083961000
1	-3.181231000	-0.788018000	0.611628000
1	-3.056708000	0.996315000	0.379130000
1	-3.127093000	-0.103303000	-1.038793000
1	2.530935000	1.163896000	-0.688147000
1	1.386487000	2.518752000	-0.387356000
1	2.167337000	1.681575000	0.990758000
1	1.758694000	-2.430669000	-0.109227000
1	2.574419000	-1.206012000	0.674074000

MIC-P

E (SCF) = -662.924273298 a.u.

7	-0.086021000	0.900338000	-0.013488000
6	-0.535259000	-0.406207000	0.022054000
6	0.584407000	-1.266430000	0.028480000
7	1.591166000	-0.328744000	0.011151000
7	1.237129000	0.975003000	-0.005936000
6	3.022011000	-0.618250000	-0.003893000
6	-0.858620000	2.137638000	0.000842000
15	-2.313641000	-0.811557000	-0.095375000
1	3.124960000	-1.701828000	0.105500000
1	3.464552000	-0.291805000	-0.955210000
1	3.520742000	-0.100226000	0.826167000
1	-1.713878000	2.030883000	-0.679815000
1	-1.226844000	2.343504000	1.015818000
1	-0.211676000	2.956380000	-0.331184000
1	-2.090490000	-2.218201000	-0.079863000
1	-2.633909000	-0.752030000	1.302219000

MIC-As

E (SCF) = -2557.67033564 a.u.

7	0.601825000	1.011253000	-0.001459000
6	-0.031851000	-0.211207000	0.045528000
6	0.942061000	-1.229230000	0.042075000
7	2.078959000	-0.452036000	0.005803000
7	1.924518000	0.889027000	-0.014696000
6	3.450050000	-0.953055000	-0.013202000
6	0.019698000	2.348095000	0.004779000
33	-1.978766000	-0.393429000	-0.065157000
1	3.385933000	-2.044227000	0.030774000
1	3.954994000	-0.639704000	-0.937260000
1	4.005634000	-0.569094000	0.853156000
1	-0.709361000	2.434682000	-0.812868000

1	-0.485787000	2.531706000	0.963248000
1	0.824522000	3.076686000	-0.136226000
1	-1.923825000	-1.834414000	0.441758000
1	-2.269680000	0.162205000	1.344973000

MIC-Sb

E (SCF) = -561.897256582 a.u.

7	-1.133512000	1.057045000	0.000003000
6	-0.386870000	-0.105098000	-0.000002000
6	-1.266479000	-1.205623000	-0.000010000
7	-2.472459000	-0.537892000	-0.000009000
7	-2.436010000	0.811755000	-0.000002000
6	-3.793780000	-1.158311000	-0.000016000
6	-0.681054000	2.443570000	0.000011000
51	1.747866000	-0.301903000	0.000003000
1	-3.631613000	-2.240253000	-0.000023000
1	-4.353829000	-0.858438000	0.896258000
1	-4.353825000	-0.858427000	-0.896289000
1	-0.070803000	2.630532000	0.893628000
1	-0.070799000	2.630543000	-0.893601000
1	-1.561850000	3.093662000	0.000013000
1	1.982264000	0.917926000	1.213613000
1	1.982271000	0.917943000	-1.213588000

MIC-Bi

E (SCF) = -536.304495193 a.u.

7	-1.653104000	1.074913000	0.000004000
6	-0.854994000	-0.048652000	0.000002000
6	-1.679449000	-1.189607000	0.000002000
7	-2.916736000	-0.580406000	0.000005000
7	-2.944805000	0.769443000	0.000006000
6	-4.207073000	-1.262572000	0.000006000
6	-1.262849000	2.480087000	0.000004000
1	-3.994233000	-2.335751000	0.000011000
1	-4.780965000	-0.989642000	0.896209000
1	-4.780961000	-0.989651000	-0.896202000
1	-0.660989000	2.693101000	0.893519000
1	-0.660992000	2.693103000	-0.893512000
1	-2.171201000	3.091153000	0.000006000
1	1.558907000	1.114829000	-1.265989000
1	1.558912000	1.114820000	1.265992000
83	1.380244000	-0.182110000	-0.000003000

MIC-O

E (SCF) = -396.191300753 a.u.

7	-0.678330000	0.590981000	-0.013044000
6	-0.679703000	-0.774782000	-0.000988000
6	0.625072000	-1.272701000	0.008496000
7	1.296115000	-0.075719000	0.007442000
7	0.575271000	1.067239000	-0.004118000
6	2.747646000	0.072347000	-0.001399000
6	-1.813422000	1.500657000	0.006569000
8	-1.875308000	-1.418716000	-0.001077000
1	3.150352000	-0.342150000	-0.934686000
1	2.995280000	1.137299000	0.077836000
1	3.168110000	-0.482806000	0.845948000
1	-2.228741000	1.570922000	1.021932000
1	-1.472151000	2.487075000	-0.324908000
1	-2.586522000	1.118808000	-0.671786000
1	-1.652812000	-2.370041000	-0.013749000

MIC-S

E (SCF) = -719.177931039 a.u.

7	-0.133736000	0.892815000	0.002413000
6	-0.533150000	-0.419670000	-0.000020000
6	0.596880000	-1.260287000	-0.007749000
7	1.575461000	-0.295865000	-0.009823000
7	1.197567000	1.000251000	-0.003403000
6	3.012367000	-0.554844000	0.007449000
6	-0.954365000	2.094946000	0.000628000
16	-2.241144000	-0.842401000	0.002189000
1	3.145457000	-1.624914000	-0.176455000
1	3.508148000	0.035390000	-0.774261000
1	3.432214000	-0.288350000	0.987425000
1	-1.585594000	2.111465000	-0.899302000
1	-1.596288000	2.105590000	0.892980000
1	-0.290527000	2.965240000	0.007488000
1	-1.960549000	-2.167285000	0.000943000

MIC-Se

E (SCF) = -2722.75436093 a.u.

7	-0.567336000	1.014796000	-0.011238000
6	0.045001000	-0.222176000	0.042705000
6	-0.933362000	-1.230347000	0.050804000
7	-2.057893000	-0.439402000	0.014749000
7	-1.889000000	0.901872000	-0.006768000
6	-3.435331000	-0.923309000	-0.009568000
6	0.033423000	2.341586000	-0.026311000
34	1.936721000	-0.454250000	-0.037542000
1	-3.392982000	-2.004737000	0.149273000

1	-4.017784000	-0.440423000	0.786200000
1	-3.895749000	-0.704052000	-0.982986000
1	0.882551000	2.333274000	-0.722354000
1	-0.725399000	3.061088000	-0.350713000
1	0.394124000	2.607639000	0.977416000
1	2.247942000	0.456325000	1.096624000

MIC-Te

E (SCF) = -589.077736500 a.u.

7	-1.603447000	1.059048000	-0.000001000
6	-0.815532000	-0.078979000	-0.000001000
6	-1.676961000	-1.202220000	0.000000000
7	-2.900717000	-0.567532000	0.000000000
7	-2.899059000	0.784139000	0.000000000
6	-4.205728000	-1.221196000	0.000001000
6	-1.194589000	2.460718000	0.000000000
1	-4.015237000	-2.298640000	0.000003000
1	-4.773957000	-0.936325000	0.896171000
1	-4.773956000	-0.936329000	-0.896172000
1	-0.592761000	2.670342000	0.893933000
1	-0.592761000	2.670343000	-0.893933000
1	-2.094772000	3.083829000	0.000000000
1	2.089750000	-1.733266000	-0.000005000
1	2.195508000	1.399301000	0.000007000
81	1.379477000	-0.155540000	0.000000000

MIC-F

E (SCF) = -420.204808849 a.u.

7	0.692141000	0.562760000	0.013550000
6	0.648134000	-0.807005000	0.000730000
6	-0.655098000	-1.283054000	-0.008395000
7	-1.293389000	-0.065846000	-0.005474000
7	-0.543761000	1.062182000	0.007354000
6	-2.741500000	0.117319000	-0.000557000
6	1.847957000	1.448869000	-0.008872000
9	1.810746000	-1.470364000	0.002944000
1	-3.158018000	-0.320474000	0.915419000
1	-2.962039000	1.190309000	-0.044582000
1	-3.169121000	-0.398399000	-0.868971000
1	2.720318000	0.879217000	0.330450000
1	2.024495000	1.817757000	-1.028570000
1	1.665751000	2.294423000	0.664307000

MIC-Cl

E (SCF) = -780.584981676 a.u.

7	0.169586000	0.866315000	-0.000033000
6	0.510631000	-0.467426000	0.000033000
6	-0.632158000	-1.269854000	0.000034000
7	-1.575240000	-0.270253000	-0.000035000
7	-1.150393000	1.014396000	-0.000076000
6	-3.019998000	-0.481713000	-0.000031000
6	1.034736000	2.038295000	-0.000073000
17	2.171108000	-0.914849000	0.000092000
1	-3.298894000	-1.054197000	0.893197000
1	-3.520762000	0.493504000	-0.000347000
1	-3.298798000	-1.054739000	-0.892938000
1	1.672018000	2.024927000	-0.894057000
1	0.398649000	2.928927000	-0.000105000
1	1.672013000	2.024988000	0.893915000

MIC-Br

E (SCF) = -2894.75614577 a.u.

7	0.527624000	1.005598000	-0.000125000
6	-0.038268000	-0.249139000	0.000028000
6	0.947954000	-1.236571000	0.000092000
7	2.050653000	-0.415969000	-0.000036000
7	1.853290000	0.922403000	-0.000168000
6	3.437280000	-0.873901000	-0.000042000
6	-0.114330000	2.313764000	-0.000238000
35	-1.912138000	-0.435448000	0.000120000
1	3.612835000	-1.486240000	-0.893096000
1	4.099051000	0.000109000	-0.000157000
1	3.612903000	-1.486057000	0.893123000
1	-0.743998000	2.413822000	-0.894077000
1	-0.743931000	2.414008000	0.893628000
1	0.671189000	3.075889000	-0.000346000

MIC-I

E (SCF) = -618.168574344 a.u.

7	1.038687000	1.036823000	0.003719000
6	0.376623000	-0.171423000	-0.001572000
6	1.292710000	-1.228558000	-0.015299000
7	2.454205000	-0.492865000	-0.017771000
7	2.354445000	0.855681000	-0.004952000
6	3.804202000	-1.048959000	0.014299000
6	0.506192000	2.393791000	0.000967000
53	-1.704346000	-0.265555000	0.001360000
1	3.797294000	-1.980048000	-0.561420000
1	4.504505000	-0.326156000	-0.421502000
1	4.093092000	-1.266709000	1.051953000

1	-0.103606000	2.548612000	-0.899070000
1	-0.122312000	2.543282000	0.888800000
1	1.351648000	3.088852000	0.011827000

ligand-CuCl

MIC-H-CuCl

E (SCF) = -2422.11429577 a.u.

7	-2.541377000	0.825050000	0.006409000
7	-2.666398000	-0.494728000	-0.017692000
6	-1.458729000	-1.129231000	-0.023119000
7	-1.215523000	1.001349000	0.016663000
6	-4.000706000	-1.085001000	0.019607000
6	-0.696364000	2.365942000	-0.007819000
1	-1.386415000	-2.210726000	-0.038650000
1	-4.725789000	-0.311284000	-0.252873000
1	-4.046337000	-1.912176000	-0.699121000
1	-4.215539000	-1.458655000	1.029786000
1	0.290656000	2.348662000	0.469026000
1	-0.588663000	2.703652000	-1.047402000
1	-1.385042000	3.024509000	0.533405000
6	-0.454946000	-0.157084000	-0.003147000
29	1.411956000	-0.237620000	-0.003425000
17	3.513998000	-0.269555000	0.009079000

MIC-B-CuCl

E (SCF) = -2447.56193769 a.u.

7	2.604862000	-0.187232000	0.000475000
6	1.425773000	-0.926756000	0.005192000
7	1.067146000	1.226605000	-0.010993000
7	2.403256000	1.107532000	-0.007923000
6	0.494778000	2.570978000	0.013265000
6	3.979852000	-0.682496000	-0.007691000
5	1.346608000	-2.446281000	0.012896000
1	-0.550769000	2.480812000	-0.303377000
1	0.535873000	2.975343000	1.033427000
1	1.054779000	3.219668000	-0.670382000
1	4.143756000	-1.285598000	-0.908989000
1	4.651053000	0.181958000	0.001097000
1	4.145749000	-1.305873000	0.879110000
1	0.264825000	-2.956083000	0.015597000
1	2.349032000	-3.110231000	0.016567000
6	0.375691000	0.031933000	-0.001254000
29	-1.475790000	-0.148496000	0.001390000
17	-3.571344000	-0.273676000	-0.005637000

MIC-C-CuCl

E (SCF) = -2461.45308699 a.u.

7	-2.568362000	-0.153843000	-0.001050000
6	-1.382793000	-0.837626000	-0.007248000
7	-1.073949000	1.297344000	0.013664000
7	-2.404110000	1.166461000	0.010471000
6	-0.509864000	2.643162000	-0.016997000
6	-3.917991000	-0.702596000	0.010847000
6	-1.293287000	-2.322680000	-0.015298000
1	0.496796000	2.584075000	0.412765000
1	-0.440750000	2.994827000	-1.055332000
1	-1.147397000	3.317557000	0.566133000
1	-4.067464000	-1.335021000	-0.874322000
1	-4.065873000	-1.305132000	0.917136000
1	-4.625095000	0.132722000	-0.002329000
1	-1.768060000	-2.769469000	0.872777000
1	-1.768389000	-2.759645000	-0.908073000
1	-0.231683000	-2.601134000	-0.017034000
6	-0.355580000	0.117650000	0.001279000
29	1.504120000	-0.080687000	-0.000560000
17	3.592969000	-0.322120000	0.006320000

MIC-N-CuCl

E (SCF) = -2477.50590547 a.u.

7	2.560770000	-0.232995000	0.002061000
6	1.341753000	-0.848287000	-0.005908000
7	1.130271000	1.288741000	0.012936000
7	2.454226000	1.105341000	0.032331000
6	0.624998000	2.657164000	-0.019232000
6	3.872133000	-0.859486000	0.009773000
7	1.194873000	-2.220319000	-0.107473000
1	-0.371623000	2.650460000	0.436781000
1	1.308338000	3.307392000	0.538696000
1	0.545801000	2.999022000	-1.060147000
1	3.873695000	-1.680466000	-0.720212000
1	4.614537000	-0.105129000	-0.270403000
1	4.108502000	-1.253737000	1.009092000
1	0.204978000	-2.473130000	-0.100164000
1	1.721665000	-2.774037000	0.567201000
6	0.355258000	0.152467000	-0.005290000
29	-1.504536000	-0.034637000	-0.006692000
17	-3.583541000	-0.344848000	0.019893000

MIC-O-CuCl

E (SCF) = -2497.38071196 a.u.

7	-2.555533000	-0.269972000	-0.004880000
6	-1.324071000	-0.844683000	-0.009871000

7	-1.152384000	1.281838000	0.015549000
7	-2.472920000	1.070106000	0.011010000
6	-0.673735000	2.659816000	-0.017508000
6	-3.851743000	-0.933423000	0.013989000
8	-1.207438000	-2.183708000	-0.018769000
1	-0.501210000	2.966992000	-1.057855000
1	-1.422717000	3.309583000	0.448547000
1	0.274424000	2.695478000	0.531117000
1	-3.976814000	-1.478569000	0.959019000
1	-4.623972000	-0.163920000	-0.083892000
1	-3.910072000	-1.640670000	-0.823101000
1	-0.244418000	-2.374411000	-0.024797000
6	-0.352776000	0.161334000	0.001375000
29	1.506306000	-0.024588000	0.000776000
17	3.580071000	-0.350814000	0.005820000

MIC-F-CuCl

E (SCF) = -2521.38836688 a.u.

7	-2.594585000	-0.128326000	0.006331000
6	-1.427720000	-0.829319000	0.010747000
7	-1.021566000	1.246576000	-0.010635000
7	-2.359103000	1.184870000	-0.007203000
6	-0.389171000	2.562277000	0.015017000
6	-3.958671000	-0.642713000	-0.022766000
9	-1.468290000	-2.154696000	0.020206000
1	0.457010000	2.545689000	-0.682238000
1	-1.130216000	3.314414000	-0.276891000
1	-0.011785000	2.765226000	1.025886000
1	-4.066380000	-1.419827000	0.743659000
1	-4.635031000	0.192292000	0.185397000
1	-4.176377000	-1.068318000	-1.011297000
6	-0.342057000	0.041090000	0.002020000
29	1.514674000	-0.167818000	0.002191000
17	3.610844000	-0.292961000	-0.010557000

MIC-Al-CuCl

E (SCF) = -2665.16915671 a.u.

7	-2.521792000	-0.195409000	-0.008934000
6	-1.393143000	0.600603000	0.010500000
7	-0.921214000	-1.532797000	0.005355000
7	-2.257721000	-1.489890000	-0.008789000
6	-0.270466000	-2.839996000	-0.035002000
6	-3.922273000	0.221106000	0.040309000
13	-1.218604000	2.548240000	-0.025406000
1	0.780383000	-2.682636000	0.234470000
1	-0.757529000	-3.516105000	0.677793000

1	-0.332370000	-3.257406000	-1.048881000
1	-4.028974000	1.163618000	-0.508557000
1	-4.537331000	-0.560146000	-0.418794000
1	-4.229861000	0.370109000	1.084341000
1	0.219390000	3.176435000	0.134915000
1	-2.568395000	3.374000000	-0.217201000
6	-0.297805000	-0.297651000	0.016963000
29	1.545945000	0.006011000	0.010707000
17	3.627727000	0.297234000	-0.001668000

MIC-Si-CuCl

E (SCF) = -2712.85207081 a.u.

7	2.485554000	0.243374000	0.000091000
6	1.350886000	-0.530817000	-0.002463000
7	0.894004000	1.590322000	0.006554000
7	2.230001000	1.542991000	0.004811000
6	0.247940000	2.900193000	-0.010492000
6	3.876137000	-0.200860000	0.006818000
14	1.251322000	-2.403174000	-0.005264000
1	-0.820146000	2.729538000	0.166801000
1	0.673857000	3.532959000	0.777655000
1	0.391720000	3.375206000	-0.989895000
1	4.067163000	-0.816649000	-0.882034000
1	4.518969000	0.684958000	-0.005197000
1	4.067524000	-0.792415000	0.912017000
1	1.933689000	-2.938029000	1.212039000
1	-0.193534000	-2.744058000	-0.024116000
1	1.965039000	-2.934507000	-1.206175000
6	0.259218000	0.360724000	0.001057000
29	-1.579724000	0.027225000	0.000045000
17	-3.646047000	-0.356138000	0.003622000

MIC-P-CuCl

E (SCF) = -2764.11650855 a.u.

7	-2.487056000	0.174699000	-0.002098000
6	-1.327085000	-0.558090000	0.013718000
7	-0.934363000	1.568553000	0.004939000
7	-2.269417000	1.484395000	0.004569000
6	-0.325007000	2.895151000	-0.028979000
6	-3.862981000	-0.310582000	0.028722000
15	-1.265165000	-2.382100000	-0.112206000
1	0.737791000	2.763946000	0.204395000
1	-0.433705000	3.330323000	-1.031277000
1	-0.808149000	3.541493000	0.713552000
1	-3.966454000	-1.132992000	-0.691158000
1	-4.111083000	-0.672150000	1.035906000

1	-4.524196000	0.518255000	-0.243705000
1	0.164023000	-2.393435000	-0.136194000
1	-1.342366000	-2.659323000	1.291810000
6	-0.261330000	0.363376000	0.010440000
29	1.581170000	0.053533000	0.007213000
17	3.641292000	-0.355867000	0.007960000

MIC-S-CuCl

E (SCF) = -2820.36977656 a.u.

7	-2.487468000	0.102439000	-0.000209000
6	-1.301062000	-0.572586000	0.003789000
7	-0.983624000	1.553288000	-0.011893000
7	-2.314983000	1.429169000	-0.008949000
6	-0.415756000	2.898075000	0.017776000
6	-3.834091000	-0.451549000	-0.009384000
16	-1.190898000	-2.316858000	0.009387000
1	0.624344000	2.816664000	-0.317482000
1	-0.990653000	3.550978000	-0.649185000
1	-0.442625000	3.291237000	1.042825000
1	-3.973677000	-1.064609000	-0.910577000
1	-3.980437000	-1.074949000	0.883510000
1	-4.543970000	0.381432000	-0.007121000
1	0.172495000	-2.261653000	0.008926000
6	-0.264220000	0.379893000	-0.003001000
29	1.582183000	0.089674000	-0.001309000
17	3.629346000	-0.369835000	-0.004167000

MIC-Cl-CuCl

E (SCF) = -2881.77070396 a.u.

7	2.476661000	0.282950000	-0.002444000
6	1.374443000	-0.528604000	0.004912000
7	0.798833000	1.526550000	-0.011442000
7	2.136238000	1.567832000	-0.010963000
6	0.066278000	2.789723000	0.021415000
6	3.883213000	-0.099731000	-0.016204000
17	1.524909000	-2.225651000	0.011714000
1	-0.224422000	3.018535000	1.055304000
1	0.707988000	3.582360000	-0.378880000
1	-0.839012000	2.666941000	-0.584775000
1	4.093902000	-0.688625000	-0.918216000
1	4.478088000	0.818705000	-0.012096000
1	4.105706000	-0.704406000	0.872258000
6	0.223247000	0.270146000	-0.000266000
29	-1.610749000	-0.084199000	0.001776000
17	-3.688187000	-0.390953000	-0.009966000

MIC-Ga-CuCl

E (SCF) = -4347.82723819 a.u.

7	-2.208640000	0.951987000	-0.000185000
6	-1.230797000	-0.020304000	-0.001342000
7	-0.402769000	1.996796000	0.006645000
7	-1.727069000	2.183324000	0.004043000
6	0.461241000	3.174345000	-0.015060000
6	-3.659187000	0.775002000	0.012054000
31	-1.443421000	-1.973189000	-0.004317000
1	1.477860000	2.827370000	0.203390000
1	0.434301000	3.640094000	-1.009133000
1	0.126190000	3.892532000	0.743034000
1	-4.124117000	1.765078000	-0.029520000
1	-3.961593000	0.177206000	-0.856668000
1	-3.958380000	0.255073000	0.931004000
1	-2.916478000	-2.525452000	-0.012340000
1	-0.134917000	-2.815687000	0.000781000
6	0.001686000	0.673242000	0.002074000
29	1.759571000	0.044365000	0.000723000
17	3.747489000	-0.639553000	0.004848000

MIC-Ge-CuCl

E (SCF) = -4500.58932203 a.u.

7	2.190535000	0.965805000	0.000741000
6	1.194313000	0.024546000	-0.001700000
7	0.403871000	2.041375000	0.007459000
7	1.730060000	2.210552000	0.005416000
6	-0.445831000	3.228773000	-0.013870000
6	3.634057000	0.750360000	0.008756000
32	1.392338000	-1.921176000	-0.003587000
1	-1.465285000	2.894220000	0.210040000
1	-0.098587000	3.944911000	0.740626000
1	-0.417632000	3.691247000	-1.009454000
1	3.923007000	0.174484000	-0.880398000
1	4.126026000	1.728064000	-0.001784000
1	3.917545000	0.196602000	0.913689000
1	2.182377000	-2.343432000	1.256253000
1	-0.039520000	-2.471371000	-0.012001000
1	2.195826000	-2.339204000	-1.256403000
6	-0.024937000	0.726082000	0.001846000
29	-1.781493000	0.085771000	0.000633000
17	-3.743068000	-0.669879000	0.004139000

MIC-As-CuCl

E (SCF) = -4658.86372824 a.u.

7	-2.201565000	0.917693000	0.012752000
6	-1.180184000	0.006508000	0.030583000

7	-0.440830000	2.037422000	-0.004367000
7	-1.771005000	2.175863000	0.000476000
6	0.380312000	3.243743000	-0.052124000
6	-3.638910000	0.668502000	0.051478000
33	-1.401070000	-1.940667000	-0.070872000
1	1.411068000	2.934939000	0.156300000
1	0.322496000	3.696043000	-1.051048000
1	0.030579000	3.958688000	0.702401000
1	-3.903669000	-0.047851000	-0.737364000
1	-3.919412000	0.257221000	1.030564000
1	-4.154262000	1.619654000	-0.115583000
1	0.119906000	-2.114275000	0.042085000
1	-1.606736000	-2.121306000	1.444489000
6	0.022639000	0.736231000	0.012416000
29	1.785355000	0.112688000	0.010519000
17	3.738277000	-0.662107000	0.014455000

MIC-Se-CuCl

E (SCF) = -4823.94373685 a.u.

7	2.165715000	0.981424000	0.001046000
6	1.191472000	0.016740000	0.036960000
7	0.335358000	1.988733000	0.008587000
7	1.654518000	2.209916000	0.003617000
6	-0.559075000	3.141888000	-0.045808000
6	3.611878000	0.810444000	0.001078000
34	1.478640000	-1.859066000	-0.044160000
1	-1.514166000	2.835312000	0.396086000
1	-0.113781000	3.971669000	0.514884000
1	-0.720491000	3.436364000	-1.091536000
1	3.874810000	0.041516000	-0.737316000
1	4.067582000	1.769876000	-0.263475000
1	3.956013000	0.494822000	0.995764000
1	2.609727000	-1.854059000	0.920824000
6	-0.055068000	0.664761000	0.033648000
29	-1.803929000	0.007310000	0.019696000
17	-3.784935000	-0.691927000	-0.003117000

MIC-Br-CuCl

E (SCF) = -4995.94224649 a.u.

7	-2.121598000	1.022752000	-0.003969000
6	-1.181310000	0.028579000	0.002374000
7	-0.249401000	1.950323000	-0.010706000
7	-1.558479000	2.226929000	-0.010361000
6	0.694374000	3.064582000	0.024986000
6	-3.574709000	0.903634000	-0.018373000

35	-1.654612000	-1.777127000	0.006752000
1	1.574473000	2.774660000	-0.561032000
1	0.211402000	3.952867000	-0.397060000
1	1.001268000	3.253219000	1.062328000
1	-3.888442000	0.362353000	-0.920242000
1	-3.903845000	0.349331000	0.869841000
1	-3.991512000	1.915437000	-0.014640000
6	0.093468000	0.611293000	-0.001306000
29	1.835619000	-0.063695000	0.001011000
17	3.822973000	-0.741755000	-0.010333000

MIC-In-CuCl

E (SCF) = -2612.94819881 a.u.

7	-1.695071000	1.701270000	-0.002683000
6	-0.967771000	0.532968000	0.030273000
7	0.300361000	2.308031000	0.004233000
7	-0.944727000	2.794352000	-0.013081000
6	1.411597000	3.254377000	-0.040146000
6	-3.146192000	1.863769000	0.032416000
49	-1.640645000	-1.526741000	-0.007466000
1	2.324491000	2.683418000	0.165459000
1	1.475828000	3.710390000	-1.037024000
1	1.264832000	4.033863000	0.717473000
1	-3.391305000	2.872827000	-0.314963000
1	-3.605399000	1.114232000	-0.622851000
1	-3.512699000	1.724577000	1.058585000
1	-0.449199000	-2.708431000	0.311912000
1	-3.324791000	-1.715713000	-0.363899000
6	0.389837000	0.927212000	0.031236000
29	1.956461000	-0.094609000	0.017201000
17	3.713161000	-1.250396000	-0.017037000

MIC-Sn-CuCl

E (SCF) = -2637.71952976 a.u.

7	-1.682594000	1.708629000	0.000347000
6	-0.936833000	0.558758000	-0.001013000
7	0.305913000	2.337687000	0.004908000
7	-0.943384000	2.812383000	0.003359000
6	1.408787000	3.294675000	-0.009660000
6	-3.136120000	1.842795000	0.006115000
50	-1.595786000	-1.490284000	-0.001615000
1	2.330170000	2.718725000	0.134396000
1	1.440416000	3.814675000	-0.976134000
1	1.279446000	4.022173000	0.801145000
1	-3.544953000	1.374771000	0.911514000
1	-3.381753000	2.909431000	-0.006194000

1	-3.553058000	1.352080000	-0.883332000
1	-2.579569000	-1.721437000	-1.390160000
1	-0.155013000	-2.394565000	-0.022247000
1	-2.546510000	-1.734076000	1.407369000
6	0.413491000	0.957823000	0.001342000
29	1.975919000	-0.073256000	0.000520000
17	3.702529000	-1.272844000	0.002842000

MIC-Sb-CuCl

E (SCF) = -2663.08962937 a.u.

7	-1.658162000	1.714765000	0.001678000
6	-0.926506000	0.553700000	-0.001916000
7	0.343352000	2.308422000	0.009368000
7	-0.898136000	2.803399000	0.007286000
6	1.462557000	3.245800000	-0.019390000
6	-3.108446000	1.873998000	0.011889000
51	-1.606867000	-1.495137000	-0.003283000
1	2.354646000	2.690552000	0.292816000
1	1.605345000	3.626446000	-1.039650000
1	1.261885000	4.077779000	0.665882000
1	-3.534567000	1.386850000	-0.874558000
1	-3.521362000	1.404854000	0.914321000
1	-3.332564000	2.945321000	0.002910000
1	-2.805705000	-1.166892000	-1.214237000
1	-2.799579000	-1.170495000	1.214570000
6	0.429463000	0.928004000	0.002156000
29	1.988407000	-0.107548000	0.000585000
17	3.729797000	-1.283450000	0.006097000

MIC-Te-CuCl

E (SCF) = -2690.26877838 a.u.

7	1.755784000	1.618009000	-0.006084000
6	0.959570000	0.505824000	0.032107000
7	-0.218080000	2.309526000	-0.009197000
7	1.044726000	2.748475000	-0.018729000
6	-1.292660000	3.297955000	0.011168000
6	3.209198000	1.699879000	-0.037184000
52	1.513243000	-1.520443000	-0.008167000
1	-2.197559000	2.799854000	-0.355614000
1	-1.458286000	3.647413000	1.039071000
1	-1.021993000	4.142136000	-0.633503000
1	3.587520000	1.090887000	-0.869293000
1	3.486046000	2.749307000	-0.179106000
1	3.624811000	1.326440000	0.908530000
1	3.086653000	-1.186990000	0.475247000
6	-0.378034000	0.941007000	0.027107000

29	-1.972745000	-0.038211000	0.017163000
17	-3.744217000	-1.164584000	-0.024676000

MIC-I-CuCl

E (SCF) = -2719.35569437 a.u.

7	-1.613690000	1.667897000	-0.004215000
6	-0.895896000	0.500698000	0.001241000
7	0.406597000	2.202173000	-0.010594000
7	-0.820464000	2.734539000	-0.009754000
6	1.553580000	3.105900000	0.026703000
6	-3.059922000	1.854601000	-0.018273000
53	-1.778618000	-1.371080000	0.004494000
1	2.371168000	2.626954000	-0.524831000
1	1.271057000	4.059736000	-0.432667000
1	1.865981000	3.262207000	1.067817000
1	-3.480412000	1.390415000	-0.919820000
1	-3.497709000	1.381675000	0.870271000
1	-3.257011000	2.931089000	-0.014937000
6	0.471809000	0.821602000	-0.002207000
29	2.045305000	-0.188425000	0.000411000
17	3.850313000	-1.261740000	-0.009929000

MIC-Tl-CuCl

E (SCF) = -2595.33386049 a.u.

7	-0.782842000	2.358478000	-0.003049000
6	-0.412909000	1.037061000	0.005056000
7	1.302188000	2.386582000	-0.000732000
7	0.243455000	3.203695000	-0.004890000
6	2.634472000	2.982709000	-0.017324000
6	-2.133012000	2.912064000	0.023280000
1	3.350702000	2.155932000	0.052877000
1	2.787439000	3.534347000	-0.954136000
1	2.750952000	3.661788000	0.836839000
1	-2.734712000	2.433205000	-0.758808000
1	-2.592582000	2.722595000	1.002483000
1	-2.069082000	3.990219000	-0.156343000
1	-0.410433000	-2.090445000	0.073357000
1	-3.305763000	-0.553798000	-0.087168000
81	-1.611915000	-0.874735000	-0.002392000
6	0.999951000	1.036800000	0.005292000
29	2.173826000	-0.422041000	0.003951000
17	3.404529000	-2.130250000	0.001938000

MIC-Pb-CuCl

E (SCF) = -2616.28577461 a.u.

7	0.776599000	2.353850000	0.000339000
6	0.385247000	1.043630000	0.000144000

7	-1.309271000	2.397621000	0.000518000
7	-0.245191000	3.207082000	0.000566000
6	-2.637804000	3.002708000	0.000588000
6	2.133411000	2.891261000	0.000384000
1	-3.359756000	2.178119000	0.001541000
1	-2.767056000	3.620909000	0.898214000
1	-2.767850000	3.619424000	-0.897955000
1	2.664255000	2.546359000	0.897493000
1	2.664251000	2.546492000	-0.896777000
1	2.069681000	3.984069000	0.000467000
1	2.599204000	-0.815666000	-1.449464000
1	2.599406000	-0.816161000	1.448821000
1	0.271161000	-2.017427000	-0.000374000
82	1.582614000	-0.853479000	-0.000257000
6	-1.021504000	1.044962000	0.000253000
29	-2.193352000	-0.417715000	0.000090000
17	-3.403028000	-2.138373000	-0.000098000

MIC-Bi-CuCl

E (SCF) = -2637.49896736 a.u.

7	-0.758926000	2.336590000	0.000509000
6	-0.368741000	1.023961000	-0.001054000
7	1.329024000	2.370342000	0.004649000
7	0.267093000	3.182544000	0.003409000
6	2.658817000	2.972644000	-0.009191000
6	-2.113887000	2.877822000	0.005282000
1	3.378029000	2.156586000	0.125383000
1	2.834470000	3.470986000	-0.971617000
1	2.745952000	3.699332000	0.808022000
1	-2.649962000	2.522868000	-0.884344000
1	-2.640669000	2.532496000	0.904288000
1	-2.044825000	3.970204000	-0.000860000
1	-2.716974000	-0.189350000	1.266991000
1	-2.720278000	-0.187559000	-1.265106000
83	-1.601476000	-0.868672000	-0.000954000
6	1.037436000	1.018655000	0.001183000
29	2.223618000	-0.430067000	0.000550000
17	3.477042000	-2.116982000	0.002540000

ligand-Se

MIC-H-Se

E (SCF) = -2722.81746990 a.u.

7	-1.855920000	0.936367000	-0.000002000
7	-2.071145000	-0.373835000	-0.000002000
6	-0.930553000	-1.107931000	0.000000000

7	-0.514930000	1.025834000	0.000000000
6	-3.446420000	-0.858164000	0.000001000
6	0.125750000	2.327146000	0.000001000
1	-0.931343000	-2.190726000	0.000000000
1	-4.108546000	0.013833000	0.000003000
1	-3.624187000	-1.464379000	-0.897878000
1	-3.624184000	-1.464380000	0.897881000
1	0.767799000	2.411298000	0.888177000
1	0.767796000	2.411301000	-0.888177000
1	-0.656068000	3.094060000	0.000004000
6	0.150272000	-0.206027000	0.000001000
34	1.973777000	-0.437050000	0.000000000

MIC-B-Se

E (SCF) = -2748.27109635 a.u.

7	2.018878000	0.019027000	0.000000000
6	0.967596000	-0.893420000	0.000000000
7	0.312280000	1.231862000	0.000000000
7	1.645828000	1.274339000	0.000000000
6	-0.449079000	2.468835000	-0.000001000
6	3.448090000	-0.275238000	0.000001000
5	1.146050000	-2.393232000	-0.000001000
1	-1.094770000	2.492904000	-0.888571000
1	-1.094769000	2.492904000	0.888570000
1	0.259288000	3.304104000	-0.000002000
1	3.700214000	-0.859432000	-0.893543000
1	3.985431000	0.678710000	0.000005000
1	3.700212000	-0.859440000	0.893540000
1	0.177858000	-3.095418000	-0.000001000
1	2.254229000	-2.862645000	-0.000002000
6	-0.213248000	-0.068295000	0.000000000
34	-1.999323000	-0.423336000	0.000000000

MIC-C-Se

E (SCF) = -2762.15724276 a.u.

7	-1.995351000	0.076425000	0.000000000
6	-0.940102000	-0.782115000	0.000000000
7	-0.304672000	1.309065000	0.000000000
7	-1.647891000	1.363168000	0.000000000
6	0.468014000	2.536370000	0.000001000
6	-3.410157000	-0.265461000	0.000000000
6	-1.055350000	-2.260962000	0.000001000
1	1.114845000	2.554355000	-0.888476000
1	-0.230303000	3.380216000	0.000004000
1	1.114850000	2.554350000	0.888474000
1	-3.650831000	-0.853424000	-0.895925000

1	-3.650831000	-0.853424000	0.895925000
1	-3.981239000	0.668669000	0.000000000
1	-1.584078000	-2.635166000	0.891499000
1	-1.584056000	-2.635169000	-0.891510000
1	-0.035473000	-2.671811000	0.000013000
6	0.222605000	0.020894000	0.000000000
34	2.012131000	-0.418869000	0.000000000

MIC-N-Se

E (SCF) = -2778.21115186 a.u.

7	2.004244000	-0.002270000	-0.005648000
6	0.905389000	-0.797213000	0.009842000
7	0.362747000	1.309410000	0.000491000
7	1.710323000	1.312727000	0.010268000
6	-0.358934000	2.567337000	0.004866000
6	3.393173000	-0.425950000	-0.013772000
7	0.920845000	-2.173838000	-0.081304000
1	-1.028845000	2.594301000	0.875806000
1	0.372982000	3.381093000	0.043973000
1	-0.975746000	2.634126000	-0.902369000
1	3.506038000	-1.250873000	-0.730533000
1	4.006625000	0.427902000	-0.320641000
1	3.703706000	-0.761507000	0.986647000
1	-0.051338000	-2.510212000	-0.065894000
1	1.489948000	-2.653594000	0.615890000
6	-0.219417000	0.056330000	0.003850000
34	-2.009758000	-0.393720000	0.000052000

MIC-O-Se

E (SCF) = -2798.08828240 a.u.

7	-1.999766000	-0.082502000	-0.007576000
6	-0.858859000	-0.801450000	-0.002005000
7	-0.420862000	1.317059000	0.002065000
7	-1.769194000	1.249468000	-0.003195000
6	0.235546000	2.610683000	-0.000692000
6	-3.365997000	-0.582523000	0.007180000
8	-0.815143000	-2.134953000	-0.003277000
1	0.862873000	2.696365000	-0.899006000
1	-0.536995000	3.386674000	0.011923000
1	0.883791000	2.687520000	0.883343000
1	-3.590191000	-1.034376000	0.982893000
1	-4.033305000	0.265737000	-0.177618000
1	-3.483736000	-1.338356000	-0.779620000
1	0.164661000	-2.332508000	-0.007382000
6	0.219658000	0.097070000	0.001671000
34	2.005903000	-0.370067000	0.001050000

MIC-F-Sc

E (SCF) = -2822.09003215 a.u.

7	-2.007714000	0.017822000	0.000002000
6	-0.921327000	-0.785528000	0.000004000
7	-0.325107000	1.276195000	0.000001000
7	-1.673002000	1.313420000	0.000001000
6	0.427650000	2.515473000	0.000003000
6	-3.410213000	-0.376291000	-0.000009000
9	-1.059042000	-2.102130000	0.000007000
1	1.073606000	2.544200000	-0.888879000
1	-0.286802000	3.345756000	-0.000004000
1	1.073594000	2.544206000	0.888893000
1	-3.627476000	-0.970749000	-0.896776000
1	-3.627449000	-0.970877000	0.896680000
1	-4.007422000	0.541222000	0.000066000
6	0.242452000	-0.000477000	0.000002000
34	2.027727000	-0.426050000	-0.000002000

MIC-Al-Sc

E (SCF) = -2965.89911159 a.u.

7	2.020386000	-0.490423000	-0.000742000
6	0.716559000	-0.869159000	-0.000383000
7	0.974661000	1.336678000	0.000297000
7	2.224406000	0.836143000	-0.000316000
6	0.757663000	2.774378000	-0.000361000
6	3.192073000	-1.361392000	0.000808000
13	-0.909141000	-2.094875000	-0.000407000
1	0.189536000	3.054752000	-0.897847000
1	0.178756000	3.053307000	0.890621000
1	1.731906000	3.273304000	0.005844000
1	4.089855000	-0.734698000	-0.013724000
1	3.178052000	-1.983875000	0.904358000
1	3.163434000	-2.005085000	-0.887273000
1	-1.172224000	-2.827616000	-1.393841000
1	-1.171925000	-2.828198000	1.392769000
6	0.026840000	0.348476000	0.000154000
34	-1.854810000	0.326496000	0.000247000

MIC-Si-Sc

E (SCF) = -3013.55757597 a.u.

7	-1.848155000	0.643920000	0.000000000
6	-0.951923000	-0.390404000	0.000000000
7	0.027060000	1.579475000	0.000000000
7	-1.287530000	1.845845000	0.000001000
6	0.992537000	2.662954000	0.000001000
6	-3.306280000	0.573837000	-0.000002000

14	-1.252867000	-2.235571000	0.000001000
1	1.632519000	2.572989000	0.888940000
1	1.632529000	2.572981000	-0.888931000
1	0.445825000	3.611727000	-0.000006000
1	-3.650513000	0.041020000	0.895512000
1	-3.688692000	1.599769000	0.000014000
1	-3.650512000	0.041047000	-0.895532000
1	-2.737353000	-2.434182000	-0.000009000
1	-0.666921000	-2.841068000	-1.226738000
1	-0.666938000	-2.841054000	1.226755000
6	0.327837000	0.218310000	-0.000001000
34	2.008163000	-0.526414000	0.000000000

MIC-P-Se

E (SCF) = -3064.82186499 a.u.

7	-1.847636000	0.615884000	-0.001997000
6	-0.950095000	-0.417978000	0.008426000
7	0.029675000	1.545842000	-0.005312000
7	-1.284997000	1.815441000	-0.003593000
6	0.990742000	2.633402000	-0.012659000
6	-3.305495000	0.541843000	0.017587000
15	-1.414184000	-2.175101000	-0.048661000
1	1.620233000	2.564351000	0.885467000
1	1.642002000	2.529130000	-0.891658000
1	0.437583000	3.578431000	-0.037266000
1	-3.648664000	-0.112033000	-0.793796000
1	-3.645712000	0.135849000	0.979303000
1	-3.689932000	1.557766000	-0.120504000
1	-0.230077000	-2.547837000	-0.764656000
1	-0.824979000	-2.533396000	1.207674000
6	0.336414000	0.186792000	0.005065000
34	2.024813000	-0.530890000	0.006798000

MIC-S-Se

E (SCF) = -3121.07843578 a.u.

7	-1.918707000	0.420435000	0.000000000
6	-0.908084000	-0.484536000	0.000000000
7	-0.152312000	1.562576000	0.000000000
7	-1.492796000	1.694773000	0.000000000
6	0.686946000	2.747306000	0.000000000
6	-3.346864000	0.146211000	0.000000000
16	-1.005663000	-2.210211000	0.000000000
1	1.329387000	2.733584000	-0.891325000
1	0.036065000	3.627934000	-0.000002000
1	1.329384000	2.733586000	0.891327000
1	-3.609742000	-0.432185000	-0.896356000

1	-3.609743000	-0.432178000	0.896361000
1	-3.874228000	1.105792000	-0.000004000
1	0.411693000	-2.184801000	0.000000000
6	0.297499000	0.261608000	0.000000000
34	2.019045000	-0.398717000	0.000000000

MIC-Cl-Se

E (SCF) = -3182.47439361 a.u.

7	-1.847517000	0.581515000	0.000114000
6	-0.931291000	-0.424347000	0.000015000
7	0.031987000	1.515289000	0.000087000
7	-1.285309000	1.788034000	0.000160000
6	0.991510000	2.603266000	0.000109000
6	-3.299224000	0.467202000	0.000170000
17	-1.371301000	-2.062601000	-0.000062000
1	1.632308000	2.517146000	-0.888645000
1	0.434831000	3.546643000	0.000188000
1	1.632383000	2.517042000	0.888799000
1	-3.624972000	-0.078017000	0.895494000
1	-3.708733000	1.482350000	0.000251000
1	-3.625050000	-0.077906000	-0.895192000
6	0.358498000	0.158313000	-0.000007000
34	2.045890000	-0.554809000	-0.000120000

MIC-Ga-Se

E (SCF) = -4648.53199415 a.u.

7	-0.953308000	1.634046000	0.000000000
6	-0.701513000	0.279845000	0.000000000
7	1.135289000	1.517429000	0.000000000
7	0.126425000	2.395181000	0.000000000
6	2.507896000	1.990021000	0.000000000
6	-2.251248000	2.303178000	0.000000000
31	-2.044855000	-1.141864000	0.000000000
1	3.022606000	1.597741000	0.888166000
1	3.022607000	1.597738000	-0.888164000
1	2.492931000	3.085137000	-0.000002000
1	-2.070815000	3.383113000	0.000005000
1	-2.816769000	2.011749000	-0.894103000
1	-2.816772000	2.011742000	0.894099000
1	-3.537249000	-0.633628000	0.000008000
1	-1.608947000	-2.634051000	-0.000008000
6	0.723519000	0.179448000	-0.000001000
34	1.878593000	-1.245980000	0.000000000

MIC-Ge-Se

E (SCF) = -4801.29370192 a.u.

7	0.872143000	1.724103000	-0.000001000
---	-------------	-------------	--------------

6	0.658647000	0.375331000	-0.000002000
7	-1.213356000	1.522651000	-0.000001000
7	-0.241807000	2.448282000	0.000000000
6	-2.606600000	1.928229000	0.000001000
6	2.145878000	2.436477000	0.000001000
32	1.956813000	-1.081125000	0.000000000
1	-3.101511000	1.512168000	-0.888750000
1	-3.101506000	1.512178000	0.888759000
1	-2.646485000	3.022599000	-0.000007000
1	2.720215000	2.167580000	-0.895797000
1	1.927131000	3.509279000	0.000006000
1	2.720216000	2.167573000	0.895796000
1	1.754874000	-1.921501000	1.272276000
1	1.754855000	-1.921521000	-1.272260000
1	3.364272000	-0.431622000	-0.000013000
6	-0.746488000	0.209211000	-0.000001000
34	-1.783457000	-1.311220000	0.000000000

MIC-As-Se

E (SCF) = -4959.56784533 a.u.

7	-0.935459000	1.659431000	0.007562000
6	-0.669590000	0.321141000	0.027561000
7	1.154743000	1.536804000	-0.011805000
7	0.149255000	2.426344000	-0.007611000
6	2.529256000	2.002265000	-0.033109000
6	-2.237946000	2.316181000	0.033397000
33	-2.013473000	-1.093402000	-0.050127000
1	3.048386000	1.634972000	0.863174000
1	3.035516000	1.582641000	-0.913645000
1	2.518876000	3.097118000	-0.064376000
1	-2.860065000	1.927176000	-0.782983000
1	-2.733651000	2.124152000	0.994335000
1	-2.071460000	3.390825000	-0.095240000
1	-0.896813000	-2.098420000	-0.391175000
1	-1.910710000	-1.438876000	1.446956000
6	0.745915000	0.205421000	0.011152000
34	1.868498000	-1.251924000	0.013121000

MIC-Se-Se

E (SCF) = -5124.64820271 a.u.

7	1.041985000	1.631848000	-0.000001000
6	0.694195000	0.317554000	-0.000002000
7	-1.060539000	1.606901000	-0.000001000
7	-0.016546000	2.454895000	-0.000001000
6	-2.415326000	2.126445000	0.000003000
6	2.372681000	2.217628000	0.000000000

34	1.769604000	-1.238260000	0.000001000
1	-2.942675000	1.754575000	0.889647000
1	-2.363038000	3.220246000	-0.000003000
1	-2.942683000	1.754568000	-0.889634000
1	2.919179000	1.898744000	-0.898239000
1	2.255654000	3.306432000	0.000010000
1	2.919184000	1.898727000	0.898231000
1	3.045196000	-0.464773000	-0.000002000
6	-0.716713000	0.264023000	-0.000001000
34	-1.835902000	-1.196385000	0.000000000

MIC-Br-Se

E (SCF) = -5296.64613881 a.u.

7	1.072760000	1.547924000	0.000164000
6	0.679702000	0.245322000	0.000045000
7	-1.026089000	1.581879000	0.000092000
7	0.045782000	2.394202000	0.000196000
6	-2.360152000	2.152040000	0.000090000
6	2.429602000	2.077478000	0.000254000
35	1.875039000	-1.177565000	-0.000028000
1	-2.901699000	1.798708000	0.888767000
1	-2.262902000	3.243121000	0.000196000
1	-2.901626000	1.798876000	-0.888698000
1	2.959927000	1.727436000	0.895333000
1	2.959990000	1.727579000	-0.894844000
1	2.355801000	3.169670000	0.000339000
6	-0.736132000	0.216515000	-0.000008000
34	-1.957681000	-1.149023000	-0.000164000

MIC-In-Se

E (SCF) = -2913.67256397 a.u.

7	1.652792000	1.621322000	-0.010154000
6	0.488712000	0.920800000	-0.003457000
7	2.285265000	-0.382621000	0.000520000
7	2.768233000	0.873137000	-0.007036000
6	3.193315000	-1.517483000	-0.006744000
6	1.806261000	3.072023000	0.014960000
49	-1.749631000	0.589978000	-0.002585000
1	2.996194000	-2.142772000	0.874786000
1	3.019947000	-2.115753000	-0.911906000
1	4.220996000	-1.140986000	0.012390000
1	2.845290000	3.317519000	-0.229292000
1	1.126864000	3.511291000	-0.724979000
1	1.555414000	3.452548000	1.014049000
1	-2.446512000	0.844496000	1.556020000
1	-2.445324000	0.836892000	-1.563056000

6	0.915329000	-0.414146000	0.002199000
34	-0.309020000	-1.841830000	0.005105000

MIC-Sn-Se

E (SCF) = -2938.42475296 a.u.

7	-0.090990000	2.027931000	0.000000000
6	0.155939000	0.685895000	0.000000000
7	-1.992527000	1.147325000	0.000000000
7	-1.383097000	2.343938000	0.000000000
6	-3.441552000	1.067091000	0.000001000
6	0.876897000	3.120207000	0.000000000
50	1.993227000	-0.423614000	0.000000000
1	-3.770311000	0.510841000	0.889048000
1	-3.843486000	2.085738000	0.000000000
1	-3.770312000	0.510840000	-0.889047000
1	1.508016000	3.054542000	-0.895605000
1	0.319139000	4.062377000	-0.000002000
1	1.508015000	3.054544000	0.895606000
1	2.069725000	-1.354559000	1.427803000
1	2.069723000	-1.354561000	-1.427801000
1	3.238847000	0.772968000	-0.000002000
6	-1.114977000	0.066485000	0.000000000
34	-1.575948000	-1.718660000	0.000000000

MIC-Sb-Se

E (SCF) = -2963.79470793 a.u.

7	-0.165946000	2.050714000	0.010688000
6	0.135762000	0.722179000	0.008796000
7	-2.027860000	1.081688000	-0.013855000
7	-1.474340000	2.306777000	-0.003685000
6	-3.471687000	0.934260000	-0.022719000
6	0.750086000	3.185844000	0.027283000
51	1.972945000	-0.406087000	-0.045541000
1	-3.763687000	0.331521000	-0.893953000
1	-3.785978000	0.398687000	0.884112000
1	-3.920292000	1.932291000	-0.064957000
1	1.427437000	3.093507000	0.885350000
1	1.338919000	3.201868000	-0.899016000
1	0.149896000	4.098139000	0.108606000
1	1.898756000	-0.738760000	1.645844000
1	2.902076000	1.039009000	0.274864000
6	-1.103028000	0.047293000	-0.004844000
34	-1.442855000	-1.766397000	0.011136000

MIC-Te-Se

E (SCF) = -2990.97582510 a.u.

7	-0.122209000	2.048913000	-0.000006000
---	--------------	-------------	--------------

6	0.150063000	0.717706000	-0.000010000
7	-1.999025000	1.096501000	-0.000002000
7	-1.435508000	2.319681000	-0.000001000
6	-3.444528000	0.963436000	0.000009000
6	0.817777000	3.159267000	0.000001000
52	1.905111000	-0.416388000	0.000002000
1	-3.753670000	0.398901000	0.890696000
1	-3.882834000	1.966797000	0.000012000
1	-3.753675000	0.398899000	-0.890675000
1	1.450217000	3.105295000	-0.896316000
1	0.239010000	4.088888000	-0.000019000
1	1.450183000	3.105314000	0.896344000
1	2.840439000	0.998161000	-0.000017000
6	-1.093038000	0.053992000	-0.000007000
34	-1.392350000	-1.765651000	-0.000001000

MIC-I-Se

E (SCF) = -3020.06026815 a.u.

7	-0.226025000	1.923980000	0.000000000
6	-0.244766000	0.561364000	0.000000000
7	1.787638000	1.331887000	0.000000000
7	1.005977000	2.425616000	0.000000000
6	3.231075000	1.480679000	-0.000001000
6	-1.356495000	2.842904000	0.000000000
53	-1.958043000	-0.582019000	0.000000000
1	3.643356000	0.982839000	-0.888779000
1	3.462279000	2.551427000	0.000004000
1	3.643358000	0.982829000	0.888771000
1	-1.968731000	2.671635000	-0.895007000
1	-1.968731000	2.671635000	0.895007000
1	-0.952979000	3.860632000	0.000000000
6	1.102985000	0.116890000	0.000000000
34	1.869053000	-1.548689000	0.000000000

MIC-Tl-Se

E (SCF) = -2896.05299998 a.u.

7	1.768042000	1.802964000	0.014277000
6	0.725653000	0.931475000	0.004049000
7	2.704390000	-0.075337000	0.000306000
7	2.988531000	1.239479000	0.010970000
6	3.776465000	-1.055769000	0.010952000
6	1.694346000	3.258901000	-0.022529000
1	3.679656000	-1.705670000	-0.869659000
1	4.733759000	-0.524994000	-0.006190000
1	3.694657000	-1.674267000	0.915621000
1	1.555734000	3.600115000	-1.057556000

1	0.840010000	3.577270000	0.585354000
1	2.625206000	3.670994000	0.382594000
1	-2.039918000	0.328937000	-1.634646000
1	-2.037182000	0.317456000	1.640980000
81	-1.537882000	0.258658000	0.002465000
6	1.354766000	-0.322271000	-0.003262000
34	0.411247000	-1.946615000	-0.007949000

MIC-Pb-Se

E (SCF) = -2916.98937207 a.u.

7	0.696914000	2.067003000	0.000000000
6	0.328407000	0.755175000	0.000000000
7	2.508314000	1.014207000	0.000000000
7	2.014312000	2.263216000	0.000000000
6	3.943554000	0.800140000	-0.000002000
6	-0.166330000	3.243221000	0.000001000
1	4.219572000	0.215555000	-0.888822000
1	4.437586000	1.777549000	-0.000024000
1	4.219581000	0.215593000	0.888842000
1	-0.800765000	3.236224000	-0.895728000
1	-0.800765000	3.236223000	0.895730000
1	0.475434000	4.130343000	0.000002000
1	-1.809261000	-1.141133000	1.479713000
1	-2.827249000	1.165536000	0.000006000
1	-1.809267000	-1.141123000	-1.479720000
82	-1.686430000	-0.204503000	0.000000000
6	1.534568000	0.018605000	0.000000000
34	1.841307000	-1.801156000	0.000000000

MIC-Bi-Se

E (SCF) = -2938.20302365 a.u.

7	-0.707377000	2.070933000	0.000000000
6	-0.335348000	0.760952000	0.000000000
7	-2.513921000	1.007735000	0.000001000
7	-2.025590000	2.260862000	0.000000000
6	-3.948555000	0.788233000	0.000001000
6	0.158802000	3.243809000	-0.000001000
1	-4.223003000	0.203588000	0.889194000
1	-4.445742000	1.764026000	0.000003000
1	-4.223005000	0.203590000	-0.889192000
1	0.795254000	3.226919000	0.894289000
1	0.795255000	3.226916000	-0.894291000
1	-0.478948000	4.133860000	-0.000004000
1	2.278988000	0.941903000	-1.265623000
1	2.278996000	0.941923000	1.265602000
83	1.687635000	-0.234471000	0.000000000

6	-1.536836000	0.019143000	0.000000000
34	-1.827991000	-1.806800000	-0.000001000