

Supporting Information:

Cooperativity of Halogen, Chalcogen, and Pnictogen Bonds in Infinite Molecular Chains by Electronic-Structure Theory

Janine George¹, Volker L. Deringer¹, and Richard Dronskowski^{1,2,*}

¹Institute of Inorganic Chemistry, Chair of Solid-State and Quantum Chemistry, RWTH Aachen University, Landoltweg 1, 52056 Aachen, Germany.

²Jülich-Aachen Research Alliance (JARA-HPC), RWTH Aachen University, 52056 Aachen, Germany.

*E-mail: drons@HAL9000.ac.rwth-aachen.de, Fax: +49 (0)241 80-92642, Phone: +49 (0)241 80-93642

Electrostatic Potential

We used the electrostatic potential including the exchange correlation potential (LVTOT-tag in VASP) to obtain the data shown in the article. The pure electrostatic potential (LVHAR-tag in VASP) was also calculated. The same percentage of the potential as in the publication is shown here. There is no visually recognizable difference in the resulting potentials.

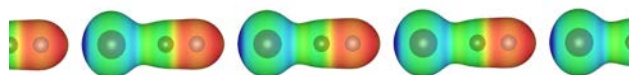


Figure S1. Charge-density isosurface ($0.05 \text{ electrons/\AA}^3$) plot for a structure-optimized infinite chain of ICN molecules, color-coded according to the pure electrostatic potential (red: most negative regions, blue: most positive regions).

Local densities-of-states

For the ICN chain, its monomeric, dimeric and trimeric fragments, the electronic structure was investigated by computing densities-of-states (DOS) and further resolving them according to atomic distributions, as depicted in Figure S2. The latter was achieved by projection of the plane-wave/PAW results onto an auxiliary local basis of Slater-type orbitals, as implemented in LOBSTER 1.1.0 and described in ref. 1. The spilling parameter was always in a similar range, between 10 and 11%, which ensures a reasonable projection for the present purpose. To describe a molecular system, one would normally choose a molecular orbital diagram. Nevertheless, the supercell approach reclaims a method for infinite systems. The discrete energy levels of the monomer's LDOS can be recognized in that of the dimer and trimer. The dimer and trimer LDOS of the different N and I atoms, respectively, are distinguished by a small energy shift. In the case of the infinite chain, discrete energy levels are also visible and they differ from the energy levels of the trimer. The absence of strong band dispersion is well in line with electrostatically dominated bonding. To sum up, the LDOS plots show the differences between clusters and infinite chains and hint toward the bonding mechanism.

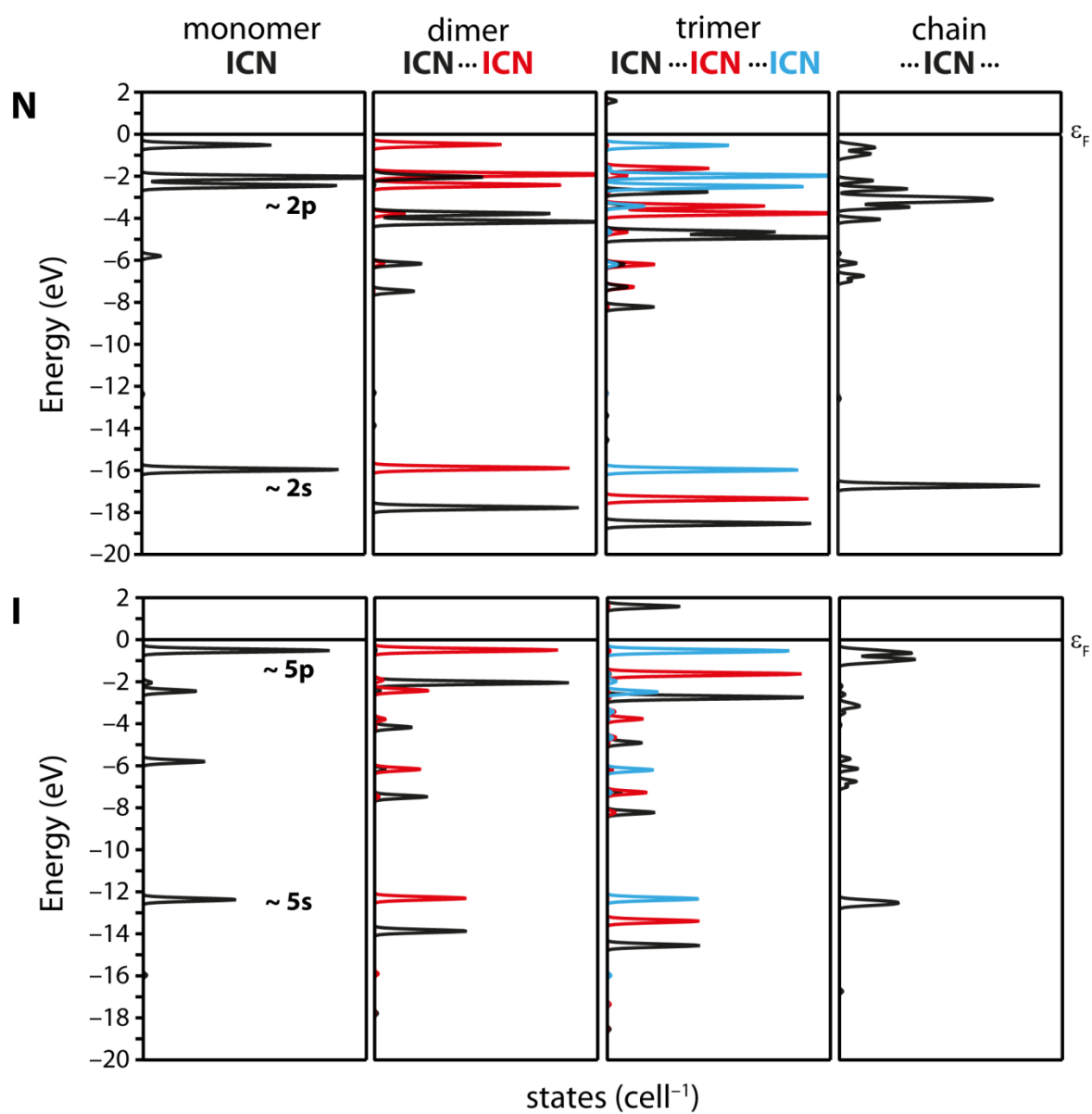


Figure S2. Atom-resolved density of states of N and I for the monomer, dimer, trimer and chain consisting of ICN molecules.

Influence of the Dispersion-Correction

Table S1. Interaction energies ΔE_{int} of all calculated systems with and without dispersion correction (D2). All chain structures are optimized at the PBE+D2/PAW level of theory. The dimers and trimers are cut from the chain.

System	ΔE_{int} /bond (kJ/mol)		$\Delta\Delta E_{\text{int}}$
	PBE//PBE+D2/PAW	PBE+D2/PAW	
FCN dimer	-3.9	-5.3	-1.4
FCN trimer	-4.2	-5.7	-1.4
FCN chain	-5.2	-6.6	-1.4
ClCN dimer	-12.3	-14.0	-1.8
ClCN trimer	-13.3	-15.1	-1.8
ClCN chain	-16.6	-18.4	-1.8
BrCN dimer	-16.4	-18.3	-2.0
BrCN trimer	-18.7	-20.7	-2.0
BrCN chain	-24.9	-26.9	-2.0
ICN dimer	-20.1	-22.8	-2.8
ICN trimer	-25.4	-28.2	-2.8
ICN chain	-38.0	-40.8	-2.8
O(CN) ₂ dimer	-6.8	-10.7	-3.9
O(CN) ₂ trimer	-7.2	-11.1	-3.9
O(CN) ₂ chain	-7.7	-11.7	-3.9
S(CN) ₂ dimer	-12.1	-15.9	-3.9
S(CN) ₂ trimer	-13.5	-17.4	-3.9
S(CN) ₂ chain	-16.0	-19.9	-3.9
Se(CN) ₂ dimer	-16.2	-20.4	-4.2
Se(CN) ₂ trimer	-19.3	-23.5	-4.2
Se(CN) ₂ chain	-25.3	-29.5	-4.2
Te(CN) ₂ dimer	-22.0	-27.3	-5.3
Te(CN) ₂ trimer	-29.9	-35.3	-5.3
Te(CN) ₂ chain	-46.4	-51.8	-5.4
N(CN) ₃ dimer	-7.1	-14.7	-7.6
N(CN) ₃ trimer	-7.3	-14.9	-7.6
N(CN) ₃ chain	-7.6	-15.3	-7.7
P(CN) ₃ dimer	-12.9	-19.3	-6.4
P(CN) ₃ trimer	-14.7	-21.1	-6.4
P(CN) ₃ chain	-17.8	-24.3	-6.5
As(CN) ₃ dimer	-17.5	-24.4	-6.9
As(CN) ₃ trimer	-21.7	-28.6	-6.9
As(CN) ₃ chain	-29.7	-36.6	-7.0
Sb(CN) ₃ dimer	-26.9	-35.0	-8.1
Sb(CN) ₃ trimer	-38.8	-47.0	-8.2
Sb(CN) ₃ chain	-63.0	-71.2	-8.2
PTK (Cl) dimer	-2.0	-14.6	-12.6
PTK (Cl) chain	-1.6	-14.3	-12.7

PTK (Br) dimer	-3.7	-20.1	-16.4
PTK (Br) chain	-3.6	-20.1	-16.6
PTK (I) dimer	-6.6	-26.9	-20.3
PTK (I) chain	-7.1	-27.6	-20.5
SAMDAL (Cl) dimer	-9.2	-18.0	-8.8
SAMDAL (Cl) chain	-12.1	-21.1	-8.9
SAMDAL (Br) dimer	-11.1	-26.7	-15.5
SAMDAL (Br) chain	-15.2	-31.0	-15.7
SAMDAL (I) dimer	-14.8	-40.7	-26.0
SAMDAL (I) chain	-22.7	-48.9	-26.2
Acetone/Chlorine dimer	-23.4	-27.9	-4.6
Acetone/Chlorine chain	-15.9	-20.9	-4.9
Acetone/Bromine dimer	-31.6	-37.4	-5.8
Acetone/Bromine chain	-21.0	-27.5	-6.5
Acetone/Iodine dimer	-30.5	-37.2	-6.7
Acetone/Iodine chain	-20.4	-28.6	-8.3
1,4-dioxane/Chlorine dimer	-22.6	-28.8	-6.2
1,4-dioxane/Chlorine chain	-16.8	-23.1	-6.3
1,4-dioxane/Bromine dimer	-29.1	-37.1	-8.0
1,4-dioxane/Bromine chain	-21.5	-29.6	-8.1
1,4-dioxane/Iodine dimer	-26.4	-36.0	-9.6
1,4-dioxane/Iodine chain	-20.2	-29.9	-9.7

All structures are given in POSCAR format.

Obtained Chain Structures:

ICN

```
1.0000000000000000
  5.8471372117388514 -0.0126414465006467 -0.0223758007642084
-0.0573180514640435 19.3141764636687370 -0.0011913757336467
-0.1059962928129393 -0.0011669645324599 19.2995084102811880
```

```
C      I      N
  1      1      1
```

Direct

```
0.1371907896697309 0.4999994006287949 0.5000151609455514
0.4843137793117762 0.5000434431011271 0.5000994003494696
0.9370684310184885 0.4999371562700929 0.4998964387049796
```

BrCN

```
1.0000000000000000
  5.7248317732051213 -0.0126735596260838 -0.0225205876332073
-0.0558394969210024 19.5194347494781866 -0.0012847425834574
-0.1035912716685999 -0.0012602947109527 19.5045381561304154
```

```
C      Br      N
  1      1      1
```

Direct

```
0.1495350561618463 0.4999960310379644 0.5000087050581660
0.4638435194823743 0.5000210354533059 0.5000562836171603
0.9451944243557748 0.4999629335087448 0.4999460113246743
```

ClCN

```
1.0000000000000000
  5.7118553409886914 -0.0128401237755961 -0.0229321923777709
-0.0563655055304705 19.5415489237353981 -0.0012602572907002
-0.1049484707039578 -0.0012371817308565 19.5267432696011412
```

```
C      Cl      N
  1      1      1
```

Direct

```
0.1599342432027540 0.4999948088945709 0.5000064393461383
0.4436289883861250 0.5000186137262802 0.5000514121967515
0.9550097684111170 0.4999665773791641 0.4999531484571109
```

FCN

```
1.0000000000000000
  5.4202700659407075 -0.0009993351516586 0.0002917152254225
-0.0036066516247508 20.0575839096037818 0.0027067221207500
-0.0038275624311887 0.0027250103115667 20.0472259358275444
```

```
C      F      N
  1      1      1
```

Direct

```
0.5262873405806374 0.4999971967227452 0.5000113639684187
0.2904527068764935 0.4998766936400401 0.4997805997933042
0.7418329525428646 0.5001061096372368 0.5002190362382848
```

O(CN)2

1.0000000000000000

5.4446303479251990 -0.4083304178235476 -0.0578764792635109

-1.9376470558809309 32.5431524164492316 0.0965050455288881

-0.2515731170644762 0.0967353233673049 23.3147518147821380

C O N
2 1 2

Direct

0.3196834402380311 0.3124179292811303 0.4876256431410182

0.6129126034294966 0.2694350889803185 0.4876625084408890

0.5555359050219864 0.3076630564405725 0.4876694307806526

0.1168586316712731 0.3200033952904696 0.4875962024814386

0.6766899121731211 0.2366866418296873 0.4876679176027411

S(CN)2

1.0000000000000000

5.7541589102228032 -0.3347754225875829 -0.0605547427212748

-1.7453506967098922 31.3605011164075691 0.0899721220959191

-0.2816283175143675 0.0858281332922631 22.8646707608639481

C S N
2 1 2

Direct

0.3048817418467687 0.3157687525069461 0.4876358223732125

0.6230881002482541 0.2653229288555080 0.4876510510577599

0.6008295843200760 0.3186758798131207 0.4876236770127492

0.1032142345119606 0.3175101597228179 0.4876436734974163

0.6496668316068561 0.2289283909237781 0.4876674785056014

Se(CN)2

1.0000000000000000

5.7503293002849318 -0.3160903933586147 -0.0604610867083272

-1.6265302788481613 31.7856119571806985 0.0897247152169796

-0.2839448428841354 0.0863335109845367 22.5643380143323817

C Se N
2 1 2

Direct

0.2945324246237178 0.3170805301646027 0.4876405258394314

0.6299352927025552 0.2631568532305906 0.4876481683904501

0.6224291643103896 0.3212887295574305 0.4876383358542924

0.0922075536940241 0.3179698942331086 0.4876420356408744

0.6425760572032289 0.2267101046364317 0.4876526367216911

Te(CN)2

1.0000000000000000

5.8051861350842380 -0.3088301695116047 -0.0602977333346752

-1.6077702993596794 31.5688974505362445 0.0966031290847942

-0.2864388918148267 0.0903327739962013 22.5022409005439989

C Te N
2 1 2

Direct

0.2799887772464336 0.3183471516918233 0.4876449328232621

0.6379414979057189 0.2606381579208969 0.4876462441788770

0.6495825566668257 0.3258120319017209 0.4876437677767595

0.0786639157819697 0.3178394490996426 0.4876405457966224

0.63550374449329674 0.2235693212080802 0.4876462118712186

N(CN)3

1.0000000000000000

5.2119786187571240	-0.1381658486918411	0.1251063650215833
-2.7991164240928850	32.0581035029411510	8.6434345423283414
13.2367149773374511	24.3553728995958494	41.2374085964229593

C N
3 4

Direct

0.3599122821806769	0.3357709962658821	0.3410545298164363
0.6375612532757735	0.2792363608684303	0.3526081502235268
0.5819665163801223	0.3127828615604242	0.3824799231338510
0.5286614478995417	0.3098021017393450	0.3583547229218763
0.2123804253612342	0.3575334417192194	0.3265486597048251
0.7274153502588906	0.2522949559691693	0.3482641803553011
0.6242936187458689	0.3144960530398760	0.4036378541853747

P(CN)3

1.0000000000000000

5.7817345319567828	-0.1166471115246691	0.0926254130926583
-3.0925695532564377	30.3429633431737891	8.0455772230577338
14.5921205714876674	22.8966018502875528	38.9891051535507600

C P N
3 1 3

Direct

0.3537398840371466	0.3367998610802161	0.3403388648915353
0.6617993560247086	0.2772894150113103	0.3479022306444151
0.5931790135055763	0.3186215300964221	0.3846057250533690
0.6837129623277391	0.3454068215245272	0.3346175198050432
0.1575338485803002	0.3391055851144600	0.3388174259458125
0.6699976558766565	0.2369560981853382	0.3519029556959907
0.5522281737499881	0.3077374601500722	0.4147632983050187

As(CN)3

1.0000000000000000

5.7689267712459191	-0.0849444528944823	0.0589330214621253
-2.9662770148158302	30.3945886530554326	8.0904625013846232
14.4638138411453898	23.0585176682160835	38.9265115278135383

C As N
3 1 3

Direct

0.3500693103819472	0.3400550373314744	0.3381684004794536
0.6663321116548104	0.2745461628027499	0.3480264510927427
0.5940652709483771	0.3180400163876271	0.3867087721188653
0.7182015061749993	0.3509987647628208	0.3308648157599237
0.1513923680273024	0.3415063935670872	0.3372024740825665
0.6561906831200943	0.2322148384907763	0.3538139708948265
0.5359396437945847	0.3045555578198176	0.4181631359127991

Sb(CN)3

1.0000000000000000

5.8313004540111839 -0.0430224214047412 0.0083909720676279

-2.8616920695633765 30.5083567118048435 8.5929912893841056

14.4700342791952590 23.8673374769836073 38.8412650593590243

C Sb N
3 1 3

Direct

0.3386973675775692 0.3415872774588430 0.3371112328471425

0.6757127074755837 0.2717942979318333 0.3471699388274980

0.5974352159939857 0.3186691241884748 0.3890112952078382

0.7617687823909075 0.3580521070935994 0.3260987868992187

0.1368521235234457 0.3408149552365539 0.3376314645457441

0.6436394022958424 0.2279222321044668 0.3544167938439802

0.5180852948447799 0.3030767771485821 0.4215085081697560

PTK

1.0000000000000000

34.5056386513662972 -0.1452806147553057 0.1258468436783611

-0.1725045261006212 39.3425826190039132 0.1717085136668151

0.0240843337083119 0.0271245264183442 6.0347085093705397

Cl C O N H
3 7 1 1 6

Direct

0.5948339187440134 0.6400517423081115 0.6756732461414466

0.6334816036795357 0.5767620501664292 0.5813205899042795

0.5751016556387384 0.6039224826829235 0.2750832832895773

0.4991813564001791 0.5333723326789559 0.9418907807894777

0.5552892220868207 0.5792191038793757 0.6867339479095708

0.5193937577710410 0.4929673273053496 0.6495918198506968

0.5478523074481936 0.5442544479759333 0.6255900143854568

0.5886880507982235 0.5993760930457975 0.5585562440658635

0.5446107705582938 0.4921286714086891 0.4677923235884930

0.5625542105435639 0.5241940342531444 0.4530673165418041

0.5370423048549471 0.5941178622511059 0.8316735471444855

0.5211681470569779 0.5241470903189855 0.7439637152212382

0.4827225815337917 0.5107948241301845 0.9967316682742782

0.4794867581107462 0.5543791331007646 0.9053946076341974

0.5004093415666544 0.4734462118454352 0.7197633464302938

0.5493325866297397 0.4705165709983294 0.3606188222378162

0.5839447316000265 0.5325841057660701 0.3315407712539296

0.5187566839999731 0.5414247938508943 0.0742840038115994

PTK with bromine

1.0000000000000000

35.9164618624034304	-0.1233995615709385	-0.1207922268902458
-0.1180639463066218	34.2919135543698417	-0.2026765983564864
-0.0207447537359230	-0.0367081901257885	6.1413261081806105

Br	C	O	N	H	
3	7	1	1	6	

Direct

0.5671920252973015	0.7703024844681485	0.7098586737524696
0.6137640241347246	0.6937317991121977	0.6084139383330591
0.5501037961454556	0.7234249640750811	0.2689433869649889
0.4846456167022668	0.6369892326355900	0.9418893401792499
0.5338954142394076	0.6931197215774580	0.6932356525639271
0.5065506351230359	0.5917402594561038	0.6519678090032723
0.5296560695906893	0.6524076771895152	0.6314132396328203
0.5644016843763624	0.7183194773470364	0.5769375904829736
0.5304373494971645	0.5921946757887503	0.4736142447141621
0.5450495594879033	0.6301020456721678	0.4612535303452645
0.5144790158141738	0.7089839851876110	0.8328789218473922
0.5059021377567897	0.6277434844199342	0.7462649054513650
0.4635310324197063	0.6590561961805984	0.9073357733197095
0.4901211273936136	0.5681760370493977	0.7198470569193528
0.5365041600901250	0.5675818960775046	0.3672007595007236
0.5646605364674486	0.6409452241455845	0.3426286974563945
0.5030688853698515	0.6484386197391272	0.0711699078185051
0.4713776471009771	0.6099038163952147	0.9962291332680255

PTK with iodine

1.0000000000000000

35.1470772807294409	-0.3678306192237103	-0.3342818725923976
-0.3784992000348787	36.0209379363974023	-0.7554543715495898
-0.0640495880981230	-0.1366481103427022	6.4636746115918013

I	C	O	N	H	
3	7	1	1	6	

Direct

0.5818161277274455	0.3713465400589392	0.7370308067861826
0.6403898567811784	0.2939335393246131	0.6386322479807620
0.5666217505700736	0.3192776413651512	0.2663723729782091
0.5058936132945350	0.2343161269986682	0.9332712959329756
0.5535894663349096	0.2898494350283046	0.7006485684219694
0.5293551224939905	0.1918340993718435	0.6544929232187336
0.5504831090125447	0.2507334547643570	0.6387579879462895
0.5828414278472390	0.3154175077304308	0.5936537764744549
0.5666768020523654	0.2297817035818860	0.4757509023955624
0.5533085434396923	0.1930001748270778	0.4850345738359740
0.5335595476168246	0.3037831113676630	0.8377474281219972
0.5275001506143738	0.2262935209982565	0.7465188960738316
0.4934034264685797	0.2079709916312640	0.9816174649314697
0.4834367030929302	0.2541544212449562	0.9027920418173457
0.5136380337048895	0.1687588973223865	0.7173433385873406
0.5602417731781983	0.1696033473367117	0.3823980987124808
0.5860420243793119	0.2406768261358585	0.3636062154008045
0.5245716510578752	0.2463913944198160	0.0576137998110337

SAMDAL

1.0000000000000000

6.3559973666825478 0.0438027902331531 -0.0223840963187842

-6.0867505048415476 36.6789645081997833 -0.1201307080329058

-4.3503644842628439 -11.6766493346281504 31.6612637927493417

Cl	C	O	N	H
6	4	2	1	1

Direct

0.1282834105990197 0.3816264604914303 0.3552160356892126

0.2827303211245249 0.4575353321631985 0.3496078210053222

0.4773201032685710 0.3918544821067777 0.3099916386526165

0.2086261946537099 0.4862082314383449 0.2284299876922991

0.4042123034806996 0.4210536181438969 0.1876176919751021

0.0022908804094281 0.4309805430227912 0.1444446509412995

0.2326092045741934 0.4057424881544475 0.3230045708005109

0.0593143392726867 0.3958944370191229 0.2811316864886385

0.0191120657608414 0.4117237831176166 0.2156629587588285

0.1547655776967490 0.4363161892002945 0.1937242263915605

0.876672555025058 0.3774274883964013 0.2758677307628582

0.8297378126142663 0.3960402948243731 0.2013728865738824

0.1401588288705642 0.4116036242354383 0.2527932008386601

0.3003313914263997 0.4250722188385601 0.2604531573487956

SAMDAL with bromine

1.0000000000000000

6.3624618091508287 0.0476485165853523 0.0676802178987373

-13.5727912378389100 38.7585790269978574 -0.4049447451198491

-14.6596071806833912 -11.1186669648608021 31.9254264205537659

Br	C	O	N	H
6	4	2	1	1

Direct

0.6416237267144353 0.3161680975221088 0.4299176468420711

0.1401739423049762 0.3273981606103646 0.3826847295668969

0.2214085432574819 0.2612685452809771 0.3377568775848303

0.9271571477086695 0.3565706542782294 0.2595702334951397

0.0205546557689118 0.2893778253413259 0.2202714502379237

0.2684822816428110 0.3681987381811993 0.2135381582942628

0.3895639065126204 0.3122112609408489 0.3762328225445302

0.5187403106028370 0.3368609803870442 0.3558286721217527

0.4068091051279765 0.3523276680912986 0.2907080280738441

0.1691470108694944 0.3428233235755798 0.2482560461907894

0.7459099232416762 0.3541243410061838 0.3720115315098838

0.6191610677682249 0.3714547771365631 0.2980847181416948

0.3463849224357034 0.3361290063841764 0.3177675319225770

0.1596100884772724 0.3213600519061899 0.3081928769088265

SAMDAL with iodine

1.0000000000000000

6.5880020428085073	-0.0085808217604963	0.1443474992015281
-12.4887743791423222	43.9769250048015081	-0.2709496627634027
-15.4486105809240950	-7.9416457021092466	35.4533709967492641

I	C	O	N	H
6	4	2	1	1

Direct

0.6862380526488820	0.2771666951742802	0.4451651418907758
0.8979760665241585	0.3562236324063974	0.4376448021589425
0.0774090908997280	0.2964615321710653	0.4013252539676628
0.7352870805184537	0.3878836463933695	0.3270567077364674
0.8985294956660397	0.3269527341664258	0.2893186592199370
0.3591770992785399	0.3376121129591709	0.2374021540144895
0.7957831501570922	0.3067773881372773	0.4109943720464457
0.5867041857895856	0.3016463038786270	0.3731414442044638
0.4936105026377504	0.3186026837863096	0.3129021759971522
0.6117515428454041	0.3404312777983307	0.2927727161455991
0.3893727734599679	0.2858029582720860	0.3669086129550578
0.2856409773166675	0.3043710811983473	0.2992397141327032
0.6462937168506073	0.3171660046248306	0.3477355710259644
0.8183551008315177	0.3289289239813797	0.3555995776193868

Acetone and Iodine

1.0000000000000000

30.0343566627585474	0.0008827443316180	-0.8109190809359871
0.0009349683114850	41.0861573028333851	0.0000608267107186
-5.2252496247594156	-0.0001656045894069	12.5091146248974852

I	O	C	H
4	2	6	12

Direct

0.6248831682087886	0.6282410990472023	0.9191808964497482
0.6251167317630854	0.6282377039404251	0.5808072491108374
0.6248766525534690	0.6680606720982915	0.4191920592469217
0.6251233926980511	0.6680580484987210	0.0808177472247885
0.6249996515615547	0.5865640423000327	0.7500028961828598
0.6250015619432493	0.7097314583632430	0.2499962194177290
0.6237892029609077	0.5374875556170666	0.8437651205672447
0.6249998872488749	0.5564925614516899	0.7500001721511785
0.6262101115929053	0.5374878912753072	0.6562351152842230
0.6237905096636053	0.7588068038126244	0.3437676033017768
0.6250000652341698	0.7398034776909462	0.2499973051424442
0.6262084968291112	0.7588067425014777	0.1562299054415438
0.6317065258170622	0.5532790669615050	0.9142026428201937
0.6493221128950815	0.5168434467180364	0.8637621931825965
0.5869131600735972	0.5270972313139024	0.8189688864887367
0.6630863924315580	0.5270955464368681	0.6810261755856377
0.6006784905030373	0.5168447618558747	0.6362325455245093
0.6182925275712350	0.5532800888873710	0.5858059003700162
0.6317208975620182	0.7430155394793150	0.4142102393759060
0.6493183726174158	0.7794537905442649	0.3637499982358186
0.5869150114461487	0.7691944128104247	0.3189796777258129
0.6630854171468199	0.7691938737870840	0.1810272068024412
0.6006796822875270	0.7794558704697334	0.1362534726961220
0.6182806085564517	0.7430174437112731	0.0857802187286619

Acetone and Bromine

1.0000000000000000

34.3102126797961873	0.0000571071251545	-0.6829350029455271
0.0007238321928861	39.8806762770417578	-0.0003287089480403
-5.2809494801077452	-0.0000176951753035	11.8740937932353834

Br	O	C	H
4	2	6	12

Direct

0.4998956300179529	0.4335350236114905	0.9240657673225456
0.5001066102549743	0.4335345574809608	0.5759371210606190
0.4998930463718381	0.4661769474762494	0.4240590765096499
0.5001056949183891	0.4661768051954240	0.0759397312251338
0.5000033863852735	0.3959376921885820	0.7500045976424232
0.4999974255837785	0.5037757927131139	0.2499945151865859
0.4988890257262995	0.3453168830356930	0.8476484285355781
0.5011120575365098	0.3453154331606711	0.6523525515523687
0.5000023147313897	0.3649686369419101	0.7500057005311760
0.4999973797866701	0.5347447969312782	0.2499991370252630
0.4988850690033289	0.5543969528137822	0.3476455125667712
0.5011126736759337	0.5543962441331516	0.1523521317738812
0.5209474895770754	0.3237746704492963	0.8683527441100694
0.4661752451029173	0.3350198677673433	0.8204941437843303
0.5338282052973824	0.3350159494852889	0.6795102400676214
0.4790533623289406	0.3237752590000582	0.6316468920913252
0.5063645389414475	0.3614291778038563	0.9220088397439952
0.4936393403766388	0.3614293567429527	0.5779940466637044
0.5063564854530540	0.5382835964278101	0.4220004781264493
0.4936394022626658	0.5382834405175458	0.0779939637061773
0.5209422611777015	0.5759375465734706	0.3683544099554013
0.4661685112398928	0.5646954081928115	0.3204823600993976
0.5338264310307963	0.5646936359926329	0.1795136239521327
0.4790534611193422	0.5759381190649790	0.1316434442821262

Acetone and Chlorine

1.0000000000000000

28.6757800945496157	0.0006991844582191	-0.4065282769044321
0.0009478130635196	41.6538100675617926	0.0000168494502102
-5.3625108326448965	-0.0001143663188832	11.4738324150637165

Cl	O	C	H
4	2	6	12

Direct

0.3748898098806492	0.5706109261621322	0.9308045494180348
0.3751105157307464	0.5706107993023579	0.5691924578666416
0.3748927578642451	0.5960622183096191	0.4308472740073910
0.3751066155839311	0.5960637901719039	0.0691508448438967
0.3750004672985554	0.5369359709933050	0.7500027798052358
0.3749997596745587	0.6297274862287239	0.2499964198307580
0.3739323153298102	0.4884090341946106	0.8504078989625654
0.3750006296394801	0.5073406752185292	0.7500008348703417
0.3760697950460354	0.4884087774972983	0.6495922025499610
0.3739313816402046	0.6782544040875749	0.3504079640088520
0.3749993050809621	0.6593224198613541	0.2499962369500963
0.3760666947670330	0.6782557755919711	0.1495946281181446
0.3822999005816285	0.5038984902970824	0.9265151322985190
0.4012263571626775	0.4681435417030571	0.8734624035583565
0.3348921050581382	0.4780013759908073	0.8211288051917691
0.4151100884753234	0.4780003833491335	0.6788702996085476
0.3487767208228476	0.4681441516150571	0.6265370156767318
0.3677007806305141	0.5038982846831530	0.5734887707610596
0.3823056585284945	0.6627690298056663	0.4265149902733683

0.4012209289594537	0.6985218473336516	0.3734423188694080
0.3348890137550384	0.6886612409784618	0.3211273288535779
0.4151082778796464	0.6886598376876094	0.1788709082154227
0.3487767844224834	0.6985225626285754	0.1265585013198773
0.3676924702965252	0.6627686545345313	0.0734757385458309

1,4-Dioxane and Iodine

1.0000000000000000

10.8964524766992543	-0.00000064245613678	-0.0011036152996072
-0.0000168374356888	25.1852929826029523	0.0000515458985241
10.3645489632269410	0.0000405812261486	22.6026143689172230

I	O	C	H
2	2	4	8

Direct

0.4779736976759281	0.4999691043926191	0.4893556217835027
0.2103308122870757	0.4999688189937785	0.5106358616778905
0.9377466161084698	0.4999922793703391	0.5261206169448158
0.7505698243242236	0.4999930645716404	0.4738773338311475
0.9156255902168340	0.5468525223440821	0.4980596936506458
0.9156256257951156	0.4531307437833831	0.4980596794559986
0.7726808431018100	0.4531315736354316	0.5019408434304751
0.7726826387346435	0.5468515324807939	0.5019398046414878
0.9325249221132239	0.4190026249697567	0.5216639050502749
0.9325223760062897	0.5809793458017580	0.5216664219209832
0.6985329962846194	0.5478384032278640	0.5487171842813510
0.6985341075638800	0.4521477742990143	0.5487207695816210
0.9897828485790257	0.4521441561825554	0.4512773944088408
0.9897842665311245	0.5478421767375821	0.4512812088066411
0.7557857905722400	0.4189980001155433	0.4783434884713671
0.7557905476060967	0.5809843750938626	0.4783401742605804

1,4-Dioxane and Bromine

1.0000000000000000

10.1557788696914013	0.0002869260064035	-0.0557790220676285
0.0009879850861118	35.2354129320260654	0.0014024459961847
11.8270723233925690	0.0014397891573343	27.4632925624979727

Br	O	C	H
2	2	4	8

Direct

0.1724225427952959	0.5000048520420393	0.5084724646717120
0.4207499463249817	0.5000069191154282	0.4915416040170726
0.8965280362331782	0.5000010295894270	0.5224374906051210
0.6966281926560924	0.5000036684496081	0.4775702309159868
0.7205856673554791	0.4665218645695219	0.5010431514764946
0.7205740371891665	0.5334833465485502	0.5010453434879167
0.8725871497299806	0.4665235008915403	0.4989637793290314
0.8725945368999746	0.5334797743975415	0.4989629299112792
0.6427364912326610	0.4658465465888355	0.5391931023566983
0.6427347593265367	0.5341527281214624	0.5392020801321991
0.8911560230583930	0.4421245201940849	0.5186307883273358
0.8911669512722895	0.5578807940912753	0.5186227895587265
0.7020316445151096	0.4421296508192327	0.4813717303110749
0.7020012296261058	0.5578855685177544	0.4813797022245012
0.9504395641441477	0.4658536570535716	0.4608119447923755
0.9504266835397530	0.5341509732958585	0.4608048593088157

1,4-Dioxane and Chlorine

1.0000000000000000

9.6871796178496048 0.0000227896945422 -0.0458426007681949

0.0000813166471703 35.3498785192377838 0.0000588823302336

13.2890966291926809 0.0000865096068461 32.3358930499571429

Cl O C H
2 2 4 8

Direct

0.0943317353070512	0.4999973996403995	0.5070166401038989
0.3203072666733959	0.4999978235373561	0.4929987135719927
0.8099183951587179	0.4999971421215648	0.5202087396950716
0.6047419848313638	0.4999978355119765	0.4797846373114609
0.7860624607154634	0.4666719119893656	0.4998431067334081
0.7860616369020619	0.5333209785786934	0.4998439327272166
0.6286068208875690	0.5333208471833402	0.5001423463163945
0.6286067771009982	0.4666726910081707	0.5001427496705588
0.8042640587846464	0.4423350193145623	0.5169331067627496
0.8042614956874701	0.5576579301165623	0.5169344688402475
0.5463657939313791	0.5340378370518764	0.5322528598629361
0.5463641106005284	0.4659571524558217	0.5322548588819203
0.8683105106375351	0.5340325160070378	0.4677333765668692
0.8683125540386882	0.4659624893496854	0.4677309253175750
0.6104253026693911	0.5576597186733494	0.4830498100384943
0.6104229588900125	0.4423347143173686	0.4830506854018992

Optimized Crystal Structures

ICN [ICN]

1.0000000000000000		
6.5520987258438597	0.0000012481234233	0.0000006520966954
-3.2760482813450413	5.6742841051537942	-0.0000005213663786
0.0000005620230887	-0.0000002017805483	5.8298277089695869

I	C	N
3	3	3

Direct

0.3333333742468446	0.6666666637683181	0.6619638730830516
0.6666667220966903	0.3333332704682946	0.3286195958265306
0.0000000777666297	0.0000000641851097	0.9952866815388685
0.6666666550254901	0.3333332895641968	0.6753089687547424
-0.0000000086817802	0.0000000517983605	0.3419684473221802
0.3333331899093829	0.6666666199732224	0.0086411553137185
0.6666666685338993	0.3333332861502611	0.8760769231087677
0.999999927763527	0.0000000835751820	0.5427325180050646
0.3333333283264977	0.6666666705170621	0.2094018370470765

ICN [BrCN]

1.0000000000000000		
5.8553232741247143	0.0000038807639573	0.0000037949864851
0.0000040785818133	6.0877966951183460	0.0000008472291478
0.0000028257188098	0.0000006185703088	4.2607614612208060

I	C	N
2	2	2

Direct

0.1500371897476944	0.2500004679260104	0.2500002042737514
0.8499303817805167	0.7499999364884797	0.7499996541802866
0.4948751373381913	0.2499995974889121	0.2499996930864422
0.5051368610308148	0.7500002803248441	0.7499997774753061
0.6948601625728325	0.2499997725513785	0.25000009487430273
0.3051602675299575	0.7499999452203820	0.7499997222412008

BrCN [ICN]

1.0000000000000000		
6.2571558554867828	-0.0000018870909976	0.0000001892804075
-3.1285795621138437	5.4188548461616524	0.0000002658959623
0.0000000819698000	0.0000003457383116	5.7041899529679707

Br	C	N
3	3	3

Direct

0.3333333207203512	0.6666666568061119	0.6821726491112713
0.6666666815156358	0.3333333068741838	0.3488362961974037
-0.0000000047656993	0.0000000205799407	0.0154986199206014
0.6666666657196932	0.3333332880178759	0.6630254997497764
0.0000000108280490	0.0000000369344689	0.3296898365031055
0.3333333065042675	0.6666666866160850	0.9963653448230685
0.6666666684675208	0.3333332698106306	0.8681354333760563
0.0000000290655703	0.0000000286259599	0.5348003904255081
0.3333333219446044	0.6666667057347364	0.2014759298932096

BrCN [BrCN]

1.0000000000000000		
5.7491598584121375	-0.0000030188230871	-0.0000055975972992
-0.0000029958400768	5.6789869922847283	0.0000015764219625
-0.0000039400208780	0.0000011547085191	4.0029470644517833

Br	C	N
2	2	2
Direct		
0.1454505390925795	0.2499945670878570	0.2500196171641500
0.8545519661481775	0.7500062700072786	0.7499923299537060
0.4567780089050107	0.2500088752991259	0.2499641729744591
0.5432199400114429	0.7499893295031720	0.7500124206883723
0.6603662449251596	0.2499954122972007	0.2500180988369508
0.3396333009176368	0.7500055458053658	0.7499933603823687

ClCN [ICN]

1.0000000000000000		
6.0471163088311544	0.0000027721023028	0.0000024516032229
-3.0235557502129202	5.2369562067006967	-0.0000019153719242
0.0000022619281923	-0.0000007768908851	5.6935126848024096

Cl	C	N
3	3	3

Direct

0.3333330749720226	0.6666666840007577	0.7025158693885865
0.6666663883497937	0.3333332991883639	0.3691959770238364
0.0000000396725258	0.0000001803471823	0.0358512168032410
0.6666666402350022	0.3333332964091135	0.6526057697379081
0.0000003077870089	0.0000001334246710	0.3192647203295769
0.3333334541199668	0.6666666663426228	0.9859311789077631
0.6666666835300474	0.3333332323153831	0.8582167116163036
0.0000000009068262	0.9999999151060079	0.5248759665179034
0.3333334104267994	0.6666665928658982	0.1915425896748954

ClCN [BrCN]

1.0000		
3.9491636178	0.0000000000	0.0000000000
0.0000023962	5.3286848401	0.0000000000
0.0000094358	-0.0000092484	5.7322911422

Cl	C	N
2	2	2

Direct

0.7499984075000000	0.7500022396000000	0.8462047667000000
0.2499990539000000	0.2499975309000000	0.1538025005000000
0.7500079567000000	0.7499939337000000	0.5648796236000000
0.2499985698000000	0.2500057570000000	0.4351200101000000
0.2500009003000000	0.2499968059000000	0.6393520248000000
0.7499951118000000	0.7500037329000000	0.3606410743000000

FCN [ICN]

1.0000000000000000		
5.2500490042823733	-0.0000389076474835	0.0000061995329690
-2.6250581922966041	4.5466447674408945	-0.0000064963558654
0.0000025416661760	-0.0000019841936414	5.4104458470733299

F	C	N
3	3	3

Direct

0.3333328301436822	0.6666757528570244	0.7314356888443356
0.6666569511885498	0.3333471767830787	0.3981091210676837
0.999995071675301	0.0000126738313213	0.0647929980910575
0.6666814821181433	0.3333114225700555	0.6330420594138815
0.0000032881218530	0.9999730940231970	0.2997260898457412
0.3333389703622913	0.6666440531683762	0.9663701853701809
0.6666585829161207	0.3333443406299850	0.8488368946556264
0.9999980142330003	0.0000137468559132	0.5155216740279087
0.3333303737488293	0.6666777392810417	0.1821652886836134

FCN [BrCN]

1.0000000000000000

5.3751935405941644	-0.0000032183896850	0.0000657803849463
0.0000002767891881	4.6240867534208245	0.0000016472693714
0.0000501749347597	-0.0000012446576690	4.0066053419062353

F	C	N
2	2	2

Direct

0.1866828378332190	0.2500011012385918	0.2500185847510830
0.8133146933861086	0.7499988739391870	0.7499814022219320
0.4227029398367874	0.2499971448990482	0.2500244585683065
0.5772984320373359	0.7500028720764700	0.7499839586877268
0.6401548063471497	0.2500017021865683	0.2499806689934640
0.3598462905594207	0.7499983056601277	0.7500109267775091

PTK

1.0000000000000000

11.2670747457083174	-0.0000000000803084	-0.0000005299155281
0.0000000011661146	12.9624789712166368	-0.0000003585801002
-0.0000002936995570	-0.0000001656047364	6.2322456204188921

Cl	C	O	N	H
12	28	4	4	24

Direct

0.0937738420180523	0.2403098389808775	0.9359976224526250
0.2246242210636069	0.4272794633239059	0.8475817704618791
0.7892346218498361	0.1939522472977160	0.7816147158476099
0.2107653083376846	0.6939522163100023	0.7183851432182209
0.7753757559981196	0.9272794989528350	0.6524183638946113
0.9062261626967540	0.7403098900705913	0.5640024122672926
0.4062261550420487	0.7596900877644472	0.4359974151328814
0.2753757271672654	0.5727204921326745	0.3475814030752318
0.7107653076511369	0.8060477469816618	0.2816146498839132
0.2892346472631147	0.3060477106537220	0.2183854943455472
0.7246242566890331	0.0727205307075707	0.1524184971188589
0.5937738420447118	0.2596901315246072	0.0640025521187439
0.8703410055794407	0.5233637546448762	0.9687440843354551
0.8102601098594704	0.4291788708089612	0.9626456447636826
0.2373148521395478	0.2998426728193024	0.9476357066888426
0.5021169653544248	0.5982962657441249	0.9435459233022101
0.3509537649171435	0.1310410931141348	0.8635491822352535
0.4465521147436249	0.9797716543757318	0.8539947940361117
0.3280822588156838	0.2361111885875502	0.8050942829457384
0.6719177355659625	0.7361112532816918	0.6949059485141547
0.5534479009184068	0.4797716870218380	0.6460052513606485
0.6490462468738869	0.6310411099900008	0.6364508949345122
0.4978830240298748	0.0982962524751159	0.5564541400126117
0.7626851389308698	0.7998427071451744	0.5523644125128229
0.1897398904429224	0.9291788331303437	0.5373542562040825
0.1296590156264443	0.0233637084404634	0.5312558785469150
0.6296590326769049	0.4766362485463134	0.4687441786281497
0.6897399082477449	0.5708211277050026	0.4626457165690780
0.2626851207043188	0.7001572796198232	0.4476353896238052
0.9978830555450671	0.4017037937410564	0.4435459296697957
0.1490462287302279	0.8689588884783674	0.3635490197373059
0.0534478747830605	0.0202283069385629	0.3539947851422767
0.1719177264546090	0.7638887501074905	0.3050938266352290
0.8280822507950631	0.2638888341973598	0.1949058855181036
0.9465521346194734	0.5202283429160701	0.1460051747084776

0.8509537741719413	0.3689589040065613	0.1364509021982272
0.0021169190313799	0.9017037769867713	0.0564539919091231
0.7373148535578551	0.2001573088349460	0.0523644993142582
0.3102601033137873	0.0708210952456838	0.0373543702241079
0.3703409902481454	0.9766362128616137	0.0312558659082782
0.6236468971699907	0.7817119665591861	0.8456986202253489
0.3763531841158638	0.2817119969615192	0.6543014308756767
0.8763531625980292	0.2182880550329358	0.3456988777362540
0.1236469346257607	0.7182881000717884	0.1543011052466454
0.4344287633380759	0.0714001967556115	0.7527010410019841
0.5655712441666765	0.5714002154168867	0.7472990325081099
0.0655712184127069	0.9285998009921386	0.2527009111799856
0.9344287798853159	0.4285998218779170	0.2472990073237753
0.4463176330571272	0.5323809607891192	0.9873611952884858
0.0648650519619025	0.8851853503877578	0.9262851087965629
0.4463541145047003	0.6664419763399678	0.9178044730891486
0.8615676861951655	0.5869103807968870	0.8568393127601439
0.7451646058332955	0.4056205209535264	0.8442777979501415
0.5094529743388989	0.9226001766423764	0.7964231823879544
0.4905470404498615	0.4226001956145851	0.7035768445272268
0.2548354070479490	0.9056204635223324	0.6557220839411286
0.1384323460573356	0.0869103345719253	0.6431606632476274
0.5536458747205515	0.1664419618442636	0.5821956093710909
0.9351349037702690	0.3851853577052040	0.5737147934399118
0.5536823503653210	0.0323809482075248	0.5126388205954839
0.0536823913815709	0.4676190991921843	0.4873612143733510
0.4351348643138024	0.1148147078510107	0.4262852869287812
0.0536458987946489	0.3335580760571091	0.4178045122828848
0.6384323579227456	0.4130895977895577	0.3568394517081330
0.7548354150564833	0.5943794711741646	0.3442778673627345
0.9905470031187491	0.0773998088870087	0.2964232364878754
0.0094530016535899	0.5773998269390219	0.2035767464884728
0.2451646074217564	0.0943794279623660	0.1557222236118534
0.3615676720764611	0.9130895639070076	0.1431605775734681
0.9463540799723802	0.8335580629346282	0.0821954116474757
0.5648651098225699	0.6148147147766920	0.0737148118979221
0.9463175813517992	0.9676190850202744	0.0126387721476675

Optimized Trimers

ICN

1.0000000000000000		
35.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C I N
3 3 3

Direct

0.6291303209216543	0.4994827222883476	0.4990720332629590
0.4573899852425508	0.5001136819461010	0.5002261971460551
0.2851538290552030	0.5007666276896937	0.5013703295919113
0.6858944342032157	0.4993514504676257	0.4987946377531220
0.5148370767630519	0.4998723273221796	0.4998209552711037
0.3427951633687864	0.5005412390344712	0.5009802425159069
0.5957181389332182	0.4995642990452940	0.4992660617468005
0.2516608027557850	0.5009139607926163	0.5015673741853416
0.4239631064708217	0.5002345989136764	0.5004794395268021

BrCN

1.0000000000000000		
37.2114065258000011	-0.0126735596000000	-0.0225205876000000
-0.3629567300000000	19.5194347495000002	-0.0012847426000000
-0.6733432658000000	-0.0012602947000000	19.5045381561000006

C Br N
3 3 3

Direct

0.3387342570625304	0.4988371224991718	0.4979158851895888
0.4964360283142034	0.4982765016407304	0.4969189284553791
0.6537260952646008	0.4976875143667247	0.4959654417062378
0.3871340446382208	0.4986542086056963	0.4975886233721753
0.5446902469359109	0.4980713575761485	0.4965863625230851
0.7017344005270197	0.4975429315637908	0.4956800369874440
0.3072572586984851	0.4989616695289995	0.4981430692580410
0.4650067545093304	0.4984235392511189	0.4971598025828992
0.6223125913979841	0.4977976248369371	0.4961793937479467

ClCN

1.0000000000000000		
39.9829873868999996	-0.0128401238000000	-0.0229321924000000
-0.3945585387000000	19.5415489236999989	-0.0012602573000000
-0.7346392949000000	-0.0012371817000000	19.5267432696000007

C Cl N
3 3 3

Direct

0.3184892552013496	0.4988193483469258	0.4978127099726108
0.4635744658403230	0.4982283444375566	0.4968295734466449
0.6082395411164212	0.4976328063887300	0.4958896048319466
0.3591222274557078	0.4986376586629754	0.4974463209764670
0.5041141259522740	0.4979914779420936	0.4964033579379962
0.6487374200449116	0.4974253922207351	0.4956042301241837
0.2891973302295660	0.4989497961160952	0.4980850055520512
0.4343124707372605	0.4984004847312870	0.4971420259169295

FCN

1.0000000000000000		
35.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	F	N
3	3	3

Direct

0.3494903199620898	0.5000774042945905	0.4999977415702407
0.5043264869725979	0.5000271930164184	0.5000414325837653
0.6592013833404596	0.4999772852970265	0.5000415763896563
0.3128842905697551	0.4999304300511248	0.4997906012692953
0.4677755094993703	0.4998803960918627	0.4997935556746488
0.6226193013145397	0.4998303361895073	0.4997936365564785
0.3828562902697440	0.5001809617405949	0.5002412684576277
0.5377040795491018	0.5001309360306226	0.5002443841550483
0.6925903910937808	0.5000809667882555	0.5002444413432222

Optimized Dimers

ICN

1.0000000000000000		
30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	I	N
2	2	2

Direct

0.3485537684573817	0.5004423340973616	0.5007705017312198
0.5517529658727676	0.4997958303580696	0.4996537829320298
0.6180321356493997	0.4996536697504273	0.4993624280736876
0.4156064117526567	0.5002085381607043	0.5003816256031330
0.3094857247883315	0.5005770274525146	0.5010273549523211
0.5127614168128020	0.4998839651809259	0.4998202157076045

BrCN

1.0000000000000000		
28.6241588659999984	-0.0126735596000000	-0.0225205876000000
-0.2791974846000000	19.5194347495000002	-0.0012847426000000
-0.5179563583000000	-0.0012602947000000	19.5045381561000006

C	Br	N
2	2	2

Direct

0.4376702775738175	0.4988922278053697	0.4980367146099674
0.6444507466130424	0.498358254517234	0.4970993821927975
0.5005308386012479	0.4987204185208504	0.4977299827472227
0.7069110850944897	0.4982051076679989	0.4968440380835077
0.3967523457327464	0.4990035756084545	0.4982363599167881
0.6036022270035198	0.4984534381953273	0.4972642297191616

ClCN

1.0000000000000000		
28.5592767049000003	-0.0128401238000000	-0.0229321924000000
-0.2818275277000000	19.5415489236999989	-0.0012602573000000
-0.5247423535000000	-0.0012371817000000	19.5267432696000007

C	Cl	N
2	2	2

Direct

0.4410060254390514	0.4988758214875087	0.4979870162485884
0.6453929275265730	0.4983264799644903	0.4970443418517240
0.4978963186114945	0.4987353585477669	0.4977101843455390
0.7021237375322258	0.4981892673542154	0.4968057070450110
0.3999959212856807	0.4989750448982653	0.4981870064734488
0.6044350215873483	0.4984293271334662	0.4972240077670463

FCN

1.0000000000000000		
30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	F	N
2	2	2

Direct

0.0618456889874380	0.0251857839952075	0.0252331415958688
0.2438328447091876	0.0251615358597019	0.0252697831209973
0.0191247285751118	0.0250382155519342	0.0250359911220865
0.2011370558516792	0.0250309044675828	0.0250388139884326
0.1007759781473558	0.0253060447366357	0.0254342531652076

0.2827867343959117 0.0252547883889402 0.0254607440074194

References

1. Maintz, S.; Deringer, V. L.; Tchougréeff, A. L.; Dronskowski, R., Analytic Projection from Plane-Wave and PAW Wavefunctions and Application to Chemical-Bonding Analysis in Solids. *J. Comput. Chem.* **2013**, 34 (29), 2557–2567.