Intermolecular X…X (X = C, N and O) Dipole Interaction between Atoms in Similar Chemical Environment

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Supporting Information

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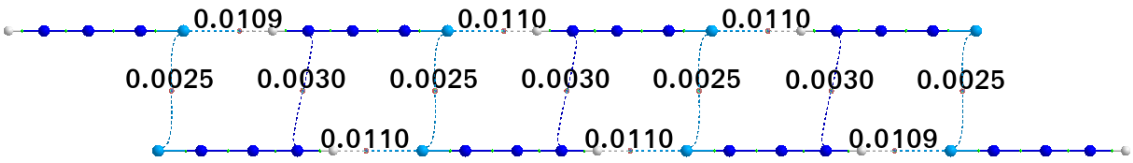

Figure S1: AIM plot of a part of the crystat structure CAACTY

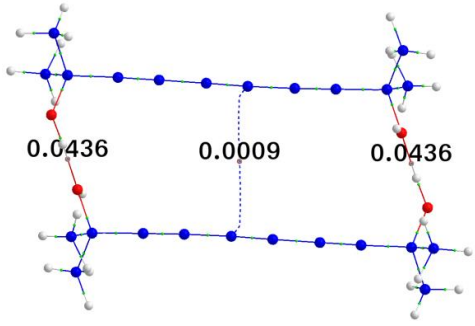

Figure S2: AIM plot of a part of the crystat structure LILJAR

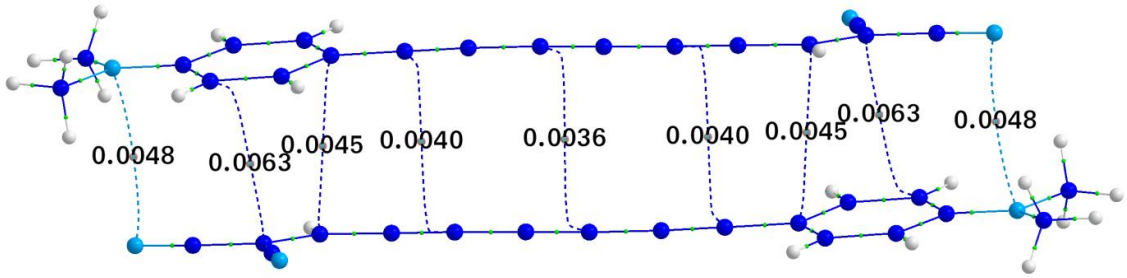

Figure S3: AIM plot of a part of the crystat structure AXEFOZ

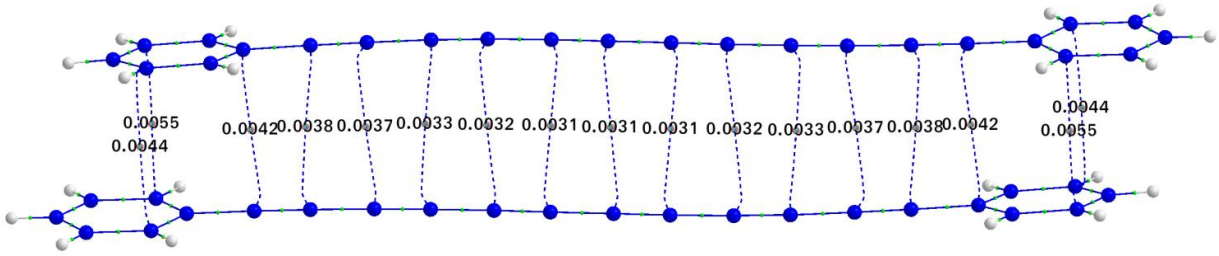

Figure S4: AIM plot of a part of the crystat structure FIFBOM

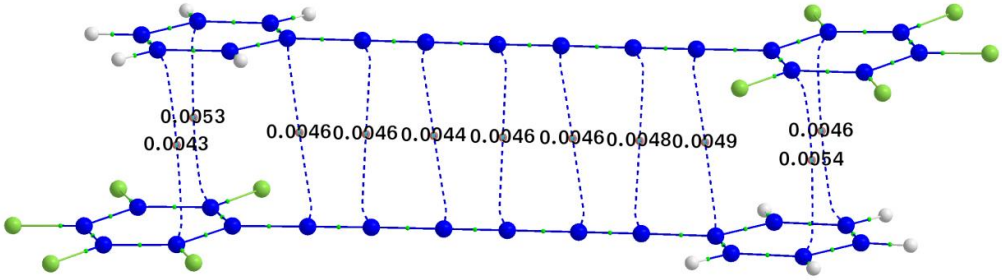

Figure S5: AIM plot of a part of the crystat structure IHUMII

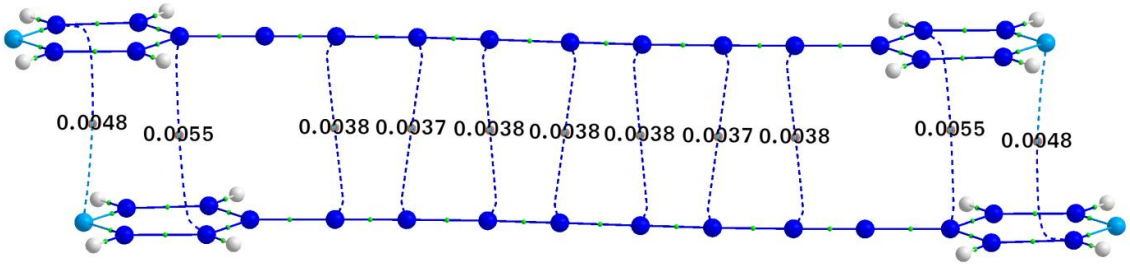

Figure S6: AIM plot of a part of the crystat structure MUPXIF

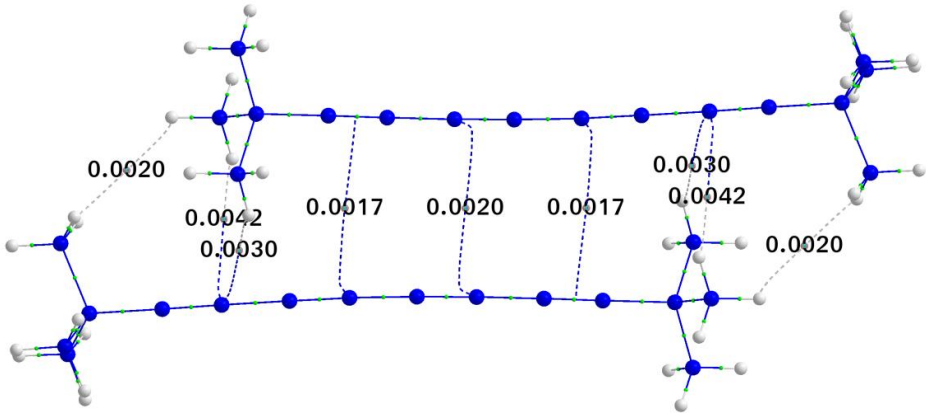

Figure S7: AIM plot of a part of the crystat structure YEXNIY01

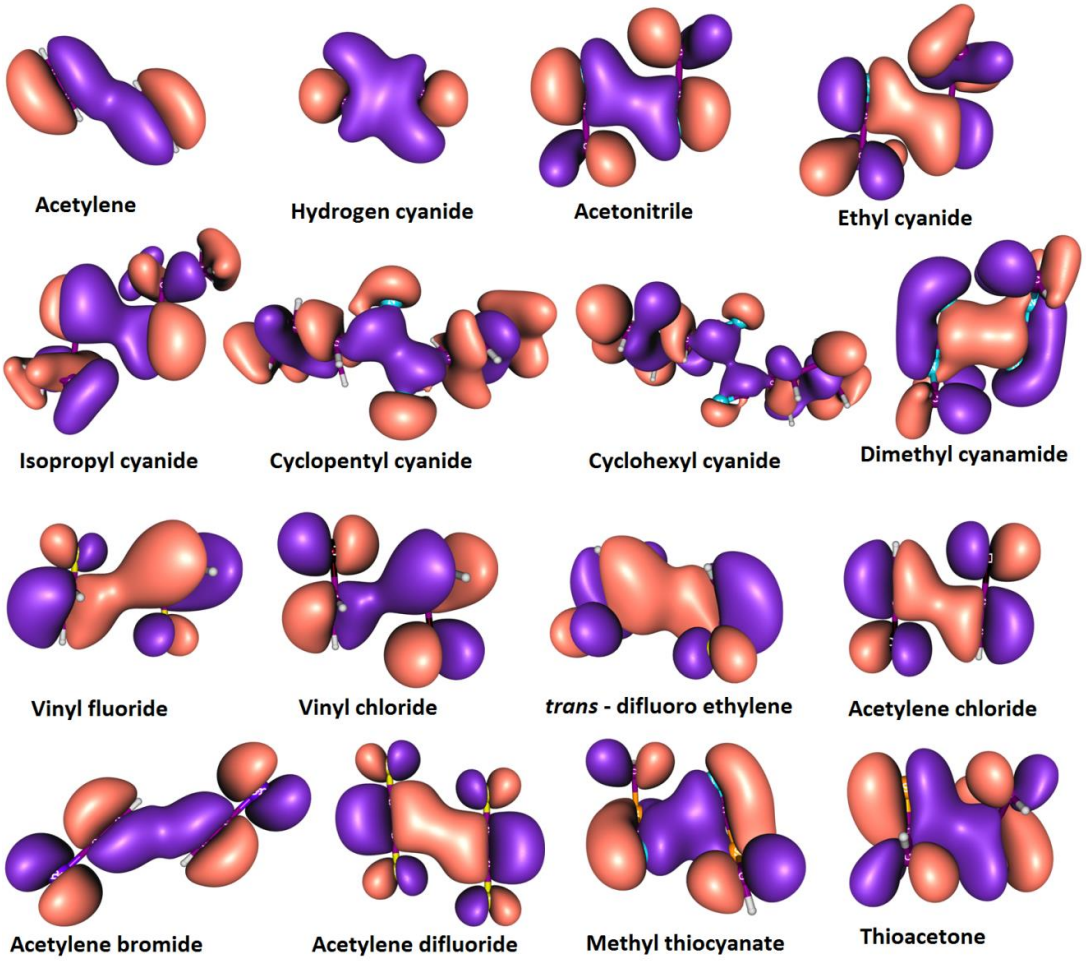

Figure S8**.** Occupied MOs corresponding to intermolecular Cé C interactions. The isosurface value is 0.018 a.u. in all the cases.

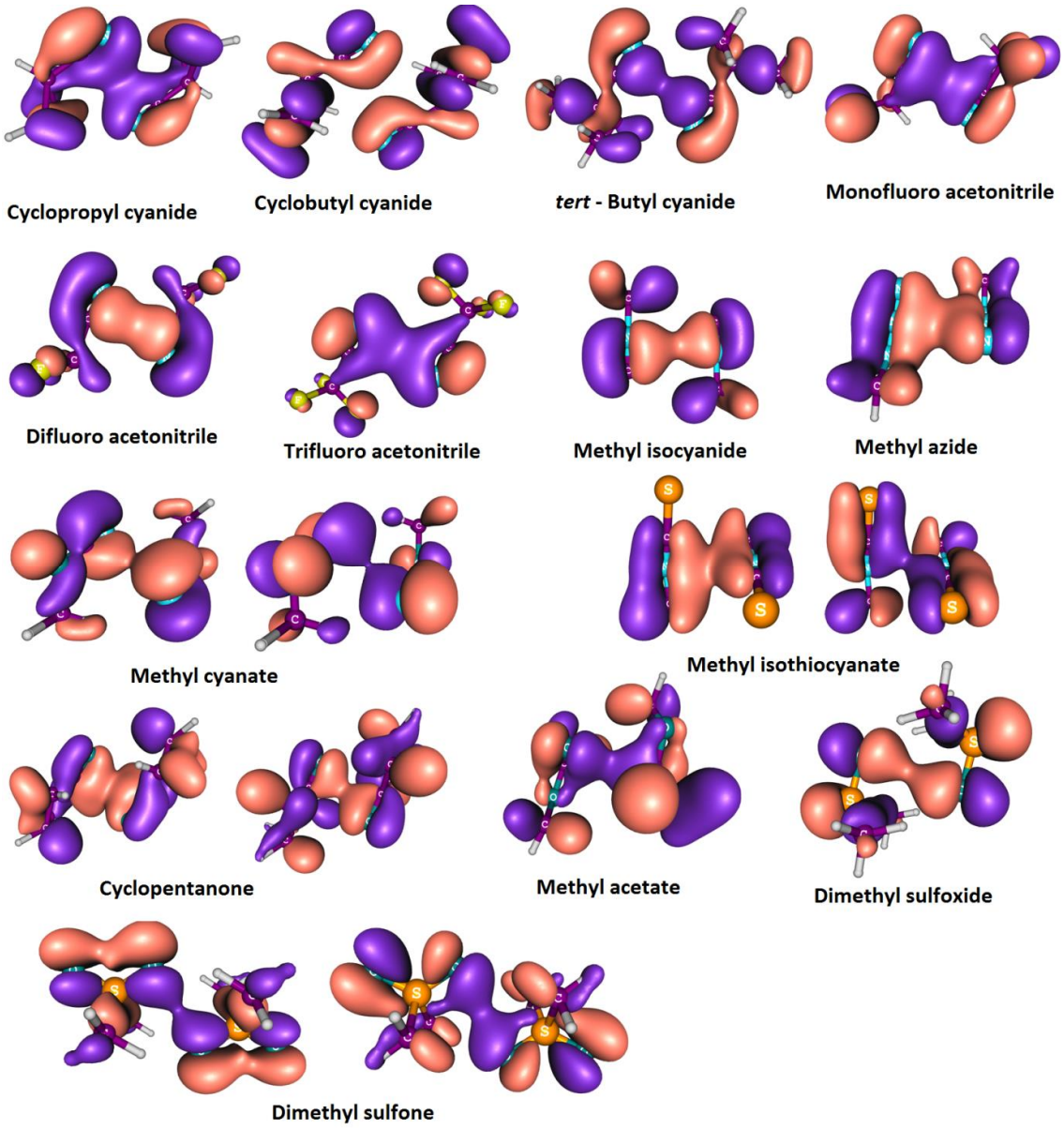

Figure S9: Occupied molecular orbitals corresponding to intermolecular Né N and Oé O interactions in the dimers studied.

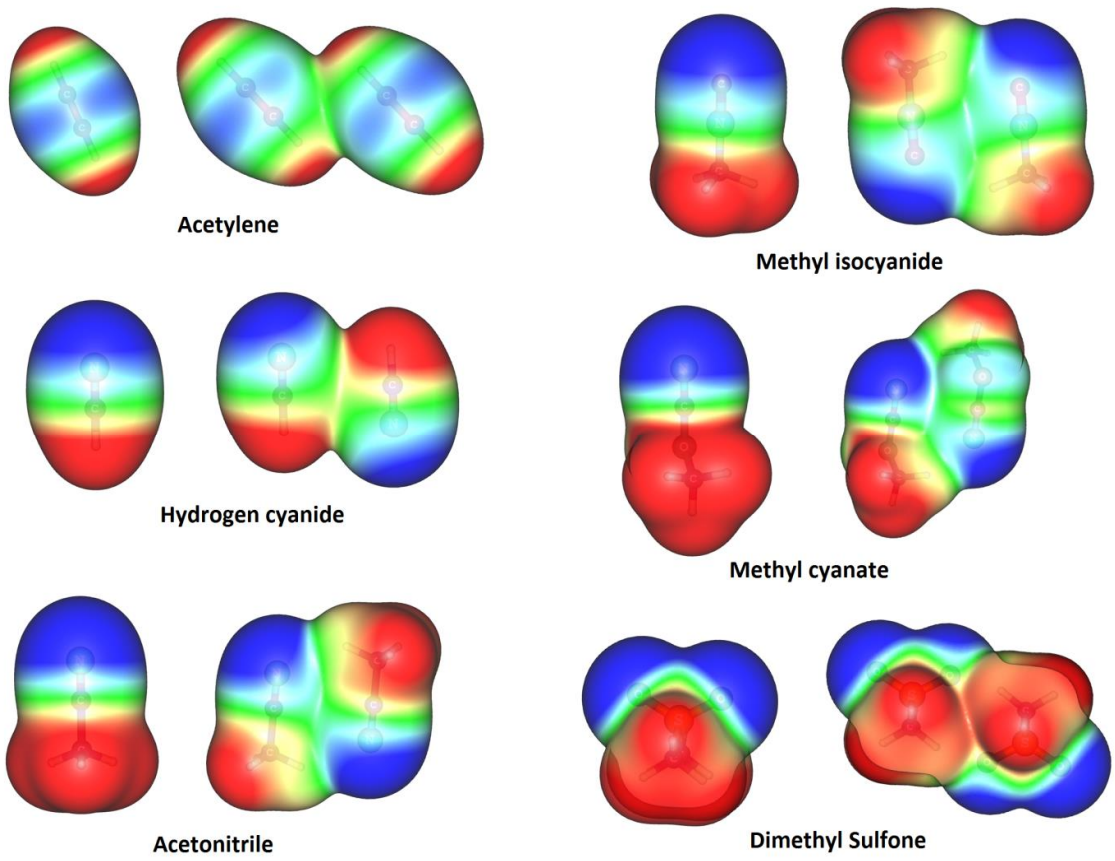

Figure S10: MESP plotted at 0.001 au isosurface before and after the interaction of some of the dimers with Cé C, Né N and Oé O interactions. Charge delocalization after the interaction is visualized. Range: from -0.03 (blue) to 0.03 (red).

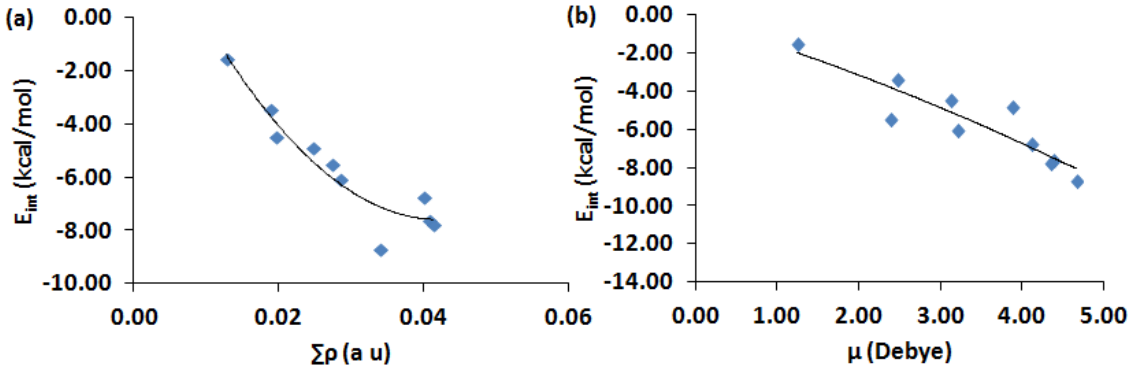

Figure S11: Variation of interaction energy (E_{int}) with (a) sum of electron density at in intermolecular BCPs (×ɟ) and (b) monomer dipole moments (ε) in the case of dimers with Né N interactions

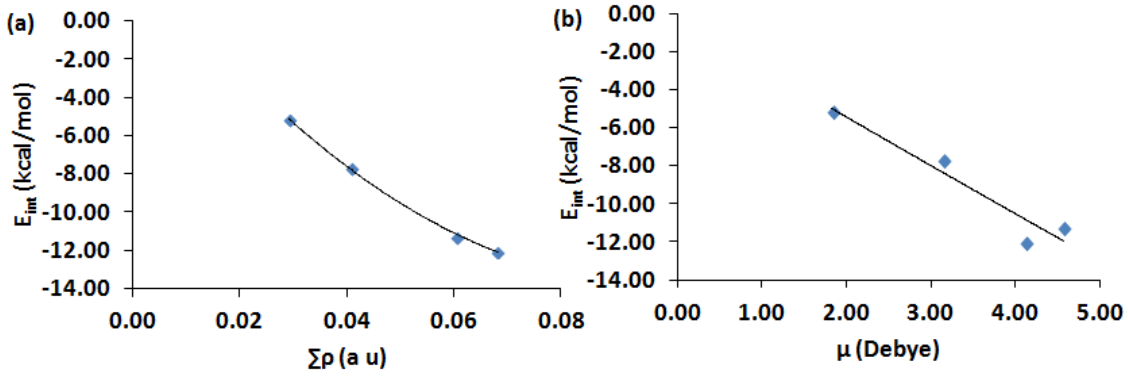

Figure S12: Variation of interaction energy (E_{int}) with (a) sum of electron density at in intermolecular BCPs (×ɟ) and (b) monomer dipole moments (ε) in the case of dimers with Oé O interactions

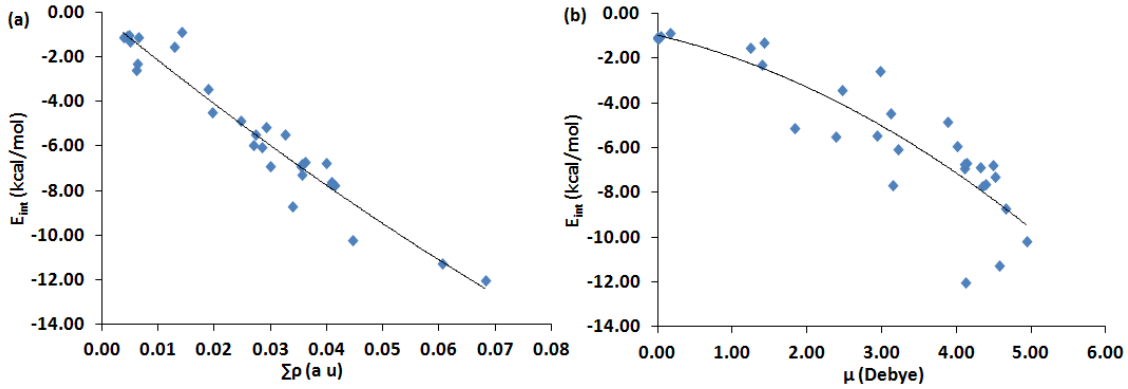

Figure S13: Variation of interaction energy (E_{int}) with (a) sum of electron density at in intermolecular BCPs (×ɟ) and (b) monomer dipole moments (ε) for all the dimers with Cé C, Né N and Oé O interactions

Table S1: Charge transfer corresponding to the intermolecular interactions in acetylene and acetonitrile dimers obtained in NBO analysis.

Acetylene (C2…C6)		
from unit 1 to unit 2		
Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (3) C1 - C2	BD*(3) C5 - C6	0.11
BD (3) C1 - C2	BD*(1) C 6 - H 8	0.09
BD (1) C2 - H4	RY*(2) C6	0.12
BD (1) C2 - H4	BD*(3) C5 - C6	0.1
from unit 2 to unit 1		
Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (3) C5 - C6	BD*(3) C1 - C 2	0.11
BD (3) C5 - C 6	BD*(1) C2 - H4	0.09
BD (1) C6 - H8	RY*(2) C2	0.12
BD (1) C6 - H8	BD*(3) C1 - C2	0.1

Acetonitrile (C8…C2), (N7…H4), (N3…H11)

from unit 1 to unit 2

C2é C8

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (1) C1 - C2	RY*(1) C8	0.06
BD (1) C2 - N3	RY*(2) C8	0.14
BD (3) C2 - N3	BD*(3) N7 - C8	0.27
BD (3) C2 - N3	RY*(2) C8	0.05

N3é H11

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (3) C2 - N3	RY*(1) H11	0.26
BD (3) C2 - N3	RY*(4) H11	0.08
BD (3) C2 - N3	BD*(1) C9 - H11	0.37
LP (1) N3	BD*(1) C9 - H11	0.68

N7é H4

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (1) C1 - H4	RY*(3) N7	0.11
BD (1) C1 - H4	BD*(3) N7 - C 8	0.26

from unit 2 to unit 1

C2é C8

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (1) N7 - C8	RY*(2) C2	0.14
. BD (3) N7 - C8	RY*(2) C2	0.05
. BD (3) N7 - C8	BD*(3) C2 - N3	0.27
BD (1) C8 - C9	RY*(1) C 2	0.06

N3é H11

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (1) C9 - H11	RY*(3) N3	0.11
BD (1) C9 - H11	BD*(3) C2 - N3	0.26

N7é H4

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
BD (3) N7 - C8	RY*(1) H 4	0.26
BD (3) N7 - C8	RY*(4) H 4	0.08
BD (3) N7 - C8	BD*(1) C1 - H4	0.37
LP (1) N7	BD*(1) C1 - H4	0.68

Table S2: Equations obtained by exempting each dimer in the 'leave one out' validation test for the multiple linear regression analysis method used for predicting the values of E_{int} of the monomers from their $\times$ and ε values.

Dimer exempted	Equation for E_{int}
acetylene	E_{int} (kcal/mol) = -137.713$\sum\rho$ (au) -0.557μ (Debye)
hydrogen cyanide	E_{int} (kcal/mol) = -139.383$\sum\rho$ (au) - 0.541μ (Debye)
acetonitrile	E_{int} (kcal/mol) = -138.436$\sum\rho$ (au) -0.550μ (Debye)
ethyl cyanide	E_{int} (kcal/mol) = -138.238$\sum\rho$ (au) - 0.555μ (Debye)

isopropyl cyanide	E_{int} (kcal/mol) = -138.152∑ρ (au) - 0.561μ (Debye)
cyclopentyl cyanide	E_{int} (kcal/mol) = -137.336∑ρ (au) - 0.569μ (Debye)
cyclohexyl cyanide	E_{int}(kcal/mol) = -138.123∑ρ (au) - 0.556μ (Debye)
dimethyl cyanamide	E_{int}(kcal/mol) = -138.514∑ρ (au) - 0.529μ (Debye)
vinyl flouride	E_{int}(kcal/mol) = -137.907∑ρ (au) - 0.556μ (Debye)
vinyl chloride	E_{int} (kcal/mol) = -139.787∑ρ (au) - 0.536μ (Debye)
trans - difluoro ethylene	E_{int}(kcal/mol) = -137.692∑ρ (au) - 0.557μ (Debye)
actylene chloride	E_{int} (kcal/mol) = -143.577∑ρ (au) - 0.505μ (Debye)
acetylene bromide	E_{int} (kcal/mol) = -137.862∑ρ (au) - 0.556μ (Debye)
acetylene difluoride	E_{int} (kcal/mol) = -137.912∑ρ (au) - 0.555μ (Debye)
methyl thiocyanate	E_{int} (kcal/mol) = -139.602∑ρ (au) - 0.535μ (Debye)
thioacetone	E_{int} (kcal/mol) = -139.819∑ρ (au) - 0.544μ (Debye)
cyclopropyl cyanide	E_{int} (kcal/mol) = -138.550∑ρ (au) - 0.556μ (Debye)
cyclobutyl cyanide	E_{int} (kcal/mol) = -138.649∑ρ (au) - 0.554μ (Debye)
tert - Butyl cyanide	E_{int} (kcal/mol) = -139.398∑ρ (au) - 0.556μ (Debye)
Monofluoro acetonitrile	E_{int} (kcal/mol) = -138.474∑ρ (au) - 0.547μ (Debye)
Difluoro acetonitrile	E_{int} (kcal/mol) = -137.626∑ρ (au) - 0.555μ (Debye)
Trifluoro acetonitrile	E_{int} (kcal/mol) = -138.882∑ρ (au) - 0.550μ (Debye)
methyl isocyanide	E_{int} (kcal/mol) = -135.728∑ρ (au) - 0.584μ (Debye)
methyl azide	E_{int}(kcal/mol) = -137.729∑ρ (au) - 0.561μ (Debye)
methyl cyanate	E_{int}(kcal/mol) = -142.698∑ρ (au) - 0.490μ (Debye)
Methyl isothiocyanate	E_{int} (kcal/mol) = -138.451∑ρ (au) - 0.550μ (Debye)
Cyclopentanone	E_{int} (kcal/mol) = -137.037∑ρ (au) - 0.560μ (Debye)
Methyl acetate	E_{int} (kcal/mol) = -137.989∑ρ (au) - 0.554μ (Debye)
Dimethyl sulfoxide	E_{int} (kcal/mol) = -133.170∑ρ (au) - 0.592μ (Debye)
Dimethylsulfone	E_{int}(kcal/mol) = -135.516∑ρ (au) - 0.571μ (Debye)

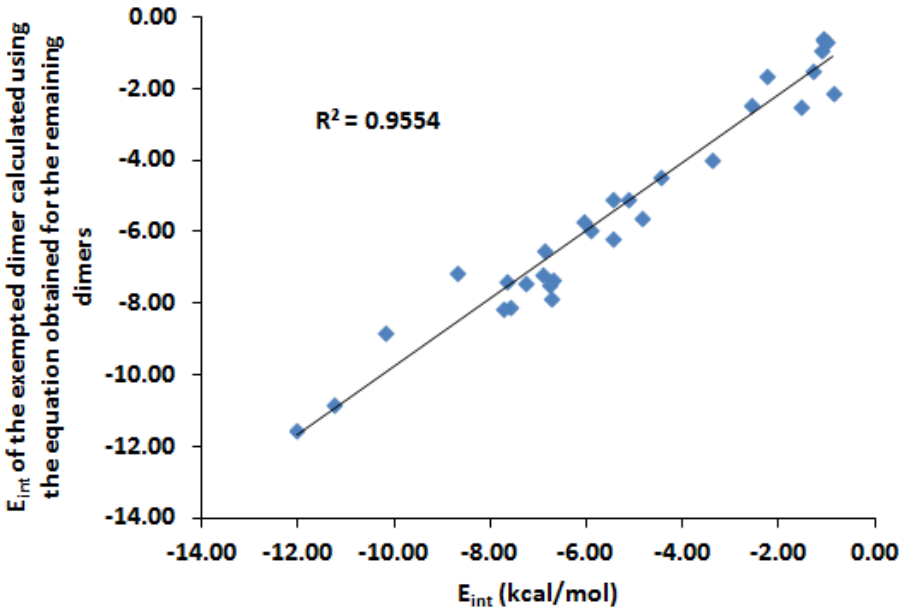

Figure S14: Correlation of E_{int} of each exempted dimer with its E_{int} value calculated from the equation obtained for the remaining dimers.

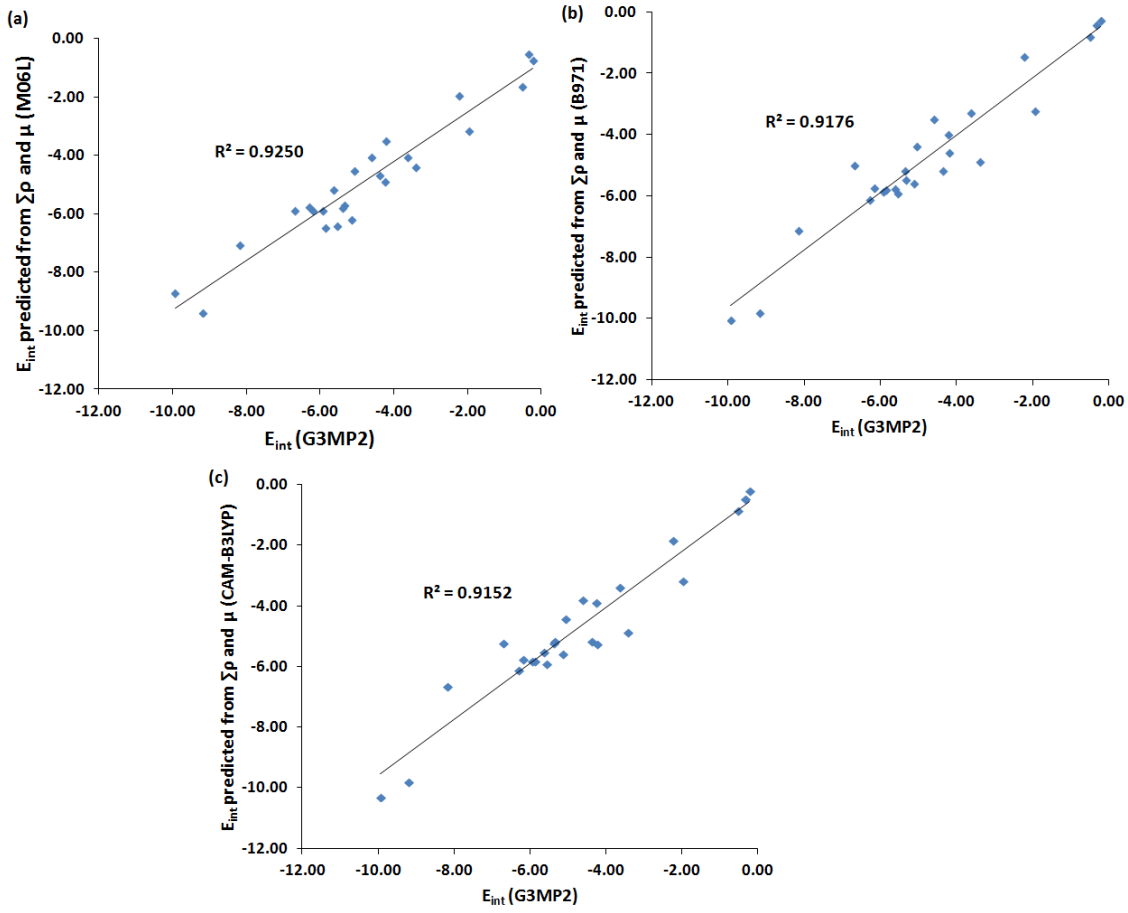

Figure S15: Correlation between E_{int} values obtained using G3MP2 method and those predicted from ×ɟ and ε values obtained from (a) M06L (b) B971 and (c) CAM-B3LYP calculations. Data for acetylene, hydrogen cyanide, Vinyl fluoride, vinyl chloride and trans-difluoro ethylene dimers are not included in the calculation since their geometry show deviation from the M06L geometry and do not possess Xé X interactions.

Table S3: Coordinates of acetylene dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	1.443442	2.178805	0.000000
6	1.443442	0.97775	0.000000
1	1.450449	3.241879	0.000000
1	1.434319	-0.08618	0.000000
6	-1.44344	-2.17881	0.000000
6	-1.44344	-0.97775	0.000000
1	-1.45045	-3.24188	0.000000
1	-1.43432	0.086179	0.000000

Table S4: Coordinates of hydrogen cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-1.52222	-0.56331	-0.00015
7	-1.83637	0.547119	0.000198
1	-1.21363	-1.58654	-0.00046
6	1.516169	0.561583	-0.00016
7	1.844336	-0.54481	0.000198
1	1.194144	1.580674	-0.00046

Table S5: Coordinates of acetonitrile dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	2.225574	-0.68765	-0.00014
6	1.528253	0.576385	0.00002
7	0.953332	1.58258	0.000179
1	1.495205	-1.50068	0.000515
1	2.857027	-0.77339	0.885907
1	2.85584	-0.77381	-0.88698
7	-0.95323	-1.58252	0.000176
6	-1.52829	-0.5764	0.000031
6	-2.22563	0.687615	-0.00014
1	-2.85646	0.773434	-0.88662
1	-1.49527	1.500661	-0.00022
1	-2.85651	0.773653	0.886279

Table S6: Coordinates of ethyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.16734	0.279403	0.621351
6	-1.11832	1.119058	0.073213
7	-0.28026	1.780687	-0.37929
1	-1.70947	-0.35876	1.384142
1	-2.88678	0.92761	1.13325
7	0.278815	-1.78066	0.373836
6	1.118641	-1.11905	-0.07544
6	2.169928	-0.27969	-0.61969
1	1.715148	0.35809	-1.38463
1	2.891391	-0.92815	-1.12837
6	2.84941	0.576974	0.44422
1	2.129481	1.251543	0.908887
1	3.30332	-0.03881	1.222785

1	3.633258	1.182573	-0.01258
6	-2.85103	-0.57672	-0.44028
1	-2.13282	-1.25074	-0.9084
1	-3.63279	-1.18288	0.019339
1	-3.30832	0.039481	-1.21654

Table S7: Coordinates of isopropyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	2.282662	-0.10274	-0.21814
6	1.314365	0.790008	0.408865
7	0.551136	1.501852	0.91513
1	1.815235	-0.43117	-1.15552
7	-0.5533	-1.50794	-0.90886
6	-1.31587	-0.79359	-0.40514
6	-2.28348	0.102471	0.218227
1	-1.81955	0.427471	1.158564
6	-2.5051	1.339345	-0.65335
1	-1.57028	1.875603	-0.81988
1	-2.93208	1.065455	-1.62153
1	-3.2012	2.017145	-0.15461
6	2.514135	-1.33729	0.654141
1	1.582482	-1.87721	0.826448
1	3.210484	-2.01293	0.152832
1	2.944922	-1.0601	1.619692
6	-3.58721	-0.63826	0.519427
1	-4.06832	-0.97422	-0.40247
1	-3.42155	-1.51207	1.151835
1	-4.27871	0.030763	1.035967
6	3.58148	0.643261	-0.52736
1	4.065925	0.982951	0.39143
1	4.273267	-0.02353	-1.0464
1	3.408648	1.515246	-1.16035

Table S8: Coordinates of cyclopentyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.34782	-0.88954	-0.58447
6	-2.19518	0.35526	0.342751
6	-3.83367	-0.93441	-0.96488
6	-3.57567	1.04427	0.337752

6	-4.53423	-0.11712	0.116451
1	-2.03597	-1.77851	-0.03295
1	-3.98993	-0.45566	-1.93801
1	-3.63743	1.746459	-0.50097
1	-1.96257	0.007207	1.355881
1	-3.75638	1.613113	1.252126
1	-5.53954	0.205651	-0.16391
1	-4.62697	-0.70578	1.037333
1	-4.21177	-1.95564	-1.05019
1	-1.69655	-0.82137	-1.45902
6	-1.10861	1.230179	-0.04941
7	-0.23777	1.921466	-0.3829
6	3.236591	-1.25845	-0.43051
6	2.082493	-0.33502	0.007299
6	4.416448	-0.30302	-0.70552
6	2.798277	0.826252	0.711857
6	3.958555	1.090303	-0.23826
1	2.962689	-1.87093	-1.29179
1	5.301553	-0.62913	-0.1532
1	3.158229	0.490557	1.691593
1	1.577836	0.07504	-0.8783
1	2.139972	1.683062	0.862404
1	4.761427	1.669332	0.222895
1	3.594379	1.677114	-1.08869
1	4.698802	-0.29932	-1.76073
1	3.47584	-1.94931	0.383079
6	1.062789	-0.98506	0.804849
7	0.241573	-1.49914	1.443604

Table S9: Coordinates of cyclohexyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-4.92682	-0.56996	-0.21035
6	-3.71291	-1.47404	-0.39351
6	-2.51276	-0.69706	-0.91666
6	-2.19172	0.48064	0.017478
6	-3.40895	1.402805	0.187389
6	-4.60417	0.608867	0.700047
1	-5.77169	-1.13947	0.189476
1	-5.24787	-0.1916	-1.19095
1	-3.94481	-2.29971	-1.07333
1	-3.44552	-1.93282	0.568091
1	-1.63561	-1.34415	-1.00177
1	-2.72423	-0.30442	-1.92008

1	-1.92051	0.063491	0.998325
1	-3.16443	2.226038	0.865171
1	-3.64836	1.85674	-0.78306
1	-5.4717	1.268393	0.800631
1	-4.38211	0.237189	1.709685
6	3.849057	1.417434	0.119076
6	2.673806	0.799424	0.862434
6	2.157982	-0.43332	0.100827
6	3.276708	-1.46686	-0.10429
6	4.452554	-0.833	-0.83488
6	4.965835	0.404451	-0.10593
1	4.221674	2.285034	0.672126
1	3.494435	1.799646	-0.8477
1	1.861905	1.521653	0.976953
1	2.981949	0.48969	1.869795
1	1.807732	-0.08909	-0.88386
1	2.893112	-2.33148	-0.65418
1	3.59866	-1.83842	0.877062
1	5.253181	-1.56893	-0.95831
1	4.135702	-0.55179	-1.84857
1	5.790044	0.859662	-0.66401
1	5.382127	0.103585	0.865597
6	1.001245	-1.02089	0.756472
7	0.07853	-1.49378	1.277661
6	-1.02191	1.205415	-0.4506
7	-0.08586	1.770526	-0.8394

Table S10: Coordinates of dimethyl cynamide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	1.068452	-1.12001	0.000442
7	0.108995	-1.78797	0.000265
7	2.193495	-0.42286	0.00014
6	2.547752	0.275798	1.235163
1	2.040478	1.244356	1.299251
1	2.27102	-0.33781	2.09175
1	3.629696	0.425936	1.248939
6	2.54755	0.274565	-1.23557
1	2.039206	1.242463	-1.30126
1	3.629305	0.426003	-1.24891
1	2.272086	-0.34052	-2.0915
6	-1.06837	1.11993	0.000743
7	-0.10896	1.787944	0.000223
7	-2.19341	0.422791	0.000142

6	-2.54817	-0.27585	1.234946
1	-2.04097	-1.24443	1.299285
1	-2.27182	0.337736	2.091664
1	-3.63011	-0.42599	1.248264
6	-2.54726	-0.27441	-1.2358
1	-2.03872	-1.24219	-1.30164
1	-3.62897	-0.42605	-1.24924
1	-2.27184	0.340967	-2.09156

Table S11: Coordinates of vinyl fluoride dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-1.57605	-0.37534	0.323232
1	-1.35665	0.565202	0.818031
6	-2.18809	-0.51827	-0.83798
1	-2.36808	-1.49258	-1.27397
1	-2.51738	0.36272	-1.37116
6	1.57605	0.375339	-0.32323
1	1.356646	-0.5652	-0.81803
6	2.188094	0.518273	0.837982
1	2.517377	-0.36272	1.371164
1	2.368078	1.492582	1.273967
9	-1.13095	-1.42858	1.032166
9	1.130946	1.42858	-1.03217

Table S12: Coordinates of vinyl chloride dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-1.54121	-0.40155	0.366221
1	-1.27432	0.548442	0.814216
6	-2.13545	-0.52955	-0.80923
1	-2.38671	-1.49347	-1.23511
1	-2.38038	0.361501	-1.37535
6	1.541207	0.401545	-0.36622
1	1.27432	-0.54844	-0.81422
6	2.13545	0.52955	0.809231
1	2.380377	-0.3615	1.375354
1	2.386709	1.493469	1.23511
17	-1.08022	-1.75159	1.356452
17	1.08022	1.75159	-1.35645

Table S13: Coordinates of *trans* – difluoro ethylene dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	1.927238	-0.70131	-0.51371
6	1.550459	-0.56477	0.749185
1	2.785505	-0.22305	-0.96917
9	1.220074	-1.48338	-1.34462
9	2.246669	0.222171	1.579208
1	0.69166	-1.04665	1.199925
6	-1.55046	0.564766	-0.74919
6	-1.92724	0.701308	0.513714
1	-0.69166	1.046654	-1.19993
9	-2.24667	-0.22217	-1.57921
9	-1.22007	1.483384	1.344617
1	-2.78551	0.223048	0.969171

Table S14: Coordinates of acetylene chloride dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-0.95483	1.222074	-0.79078
6	-1.82224	0.389763	-0.83463
1	-2.58085	-0.35154	-0.8689
6	0.95483	-1.22207	0.790777
6	1.822243	-0.38976	0.834634
1	2.580854	0.351537	0.8689
17	-0.21074	-2.36067	0.738735
17	0.210738	2.360674	-0.73874

Table S15: Coordinates of acetylene bromide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	0.427995	2.500607	0.000000
6	-0.428	1.65158	0.000000
1	-1.1741	0.894345	0.000000
6	-0.428	-2.50061	0.000000
6	0.427995	-1.65158	0.000000
1	1.174102	-0.89435	0.000000
35	-1.68997	-3.76466	0.000000
35	1.689965	3.764662	0.000000

Table S16: Coordinates of acetylene difluoride dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-1.97634	0.268403	-0.00002
6	-1.18593	1.153228	0.000058
9	-2.81421	-0.69739	-0.0002
9	-0.33697	2.10976	0.000157
6	2.006887	-0.29819	-5.5E-05
6	1.151512	-1.12038	0.000084
9	2.917782	0.599047	-0.00018
9	0.235972	-2.01346	0.000175

Table S17: Coordinates of methyl thiocyanate dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.78669	0.870001	0.558066
1	-3.4936	1.531702	0.057892
1	-3.28972	0.338057	1.363322
1	-1.93271	1.441008	0.919515
6	-1.14111	-1.20891	0.155015
16	-2.23971	-0.29857	-0.73037
7	-0.3677	-1.87212	0.723829
6	2.786668	-0.87003	0.558068
1	3.49364	-1.53168	0.057912
1	3.289642	-0.33808	1.363358
1	1.932714	-1.44109	0.919472
6	1.1411	1.208934	0.154977
16	2.239704	0.298561	-0.73037
7	0.367729	1.872153	0.723836

Table S18: Coordinates of thioacetone dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-0.38527	1.713969	0.000000
16	-1.96225	1.276975	0.000000
6	0.385269	1.934327	1.259988
6	0.385269	1.934327	-1.25999
1	-0.2247	1.780974	2.148416
1	-0.2247	1.780974	-2.14842
1	0.797415	2.950269	1.276016
1	1.247951	1.258056	1.291996
1	1.247951	1.258056	-1.292
1	0.797415	2.950269	-1.27602
6	0.385269	-1.71397	0.000000
16	1.962248	-1.27698	0.000000

6	-0.38527	-1.93433	-1.25999
6	-0.38527	-1.93433	1.259988
1	0.224699	-1.78097	-2.14842
1	0.224699	-1.78097	2.148416
1	-1.24795	-1.25806	-1.292
1	-0.79742	-2.95027	-1.27602
1	-0.79742	-2.95027	1.276016
1	-1.24795	-1.25806	1.291996

Table S19: Coordinates of cyclopropyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.54364	-0.7371	-0.0026
6	-2.85435	0.556433	-0.72573
6	-2.84732	0.536243	0.758117
1	-3.80001	0.590913	-1.25295
1	-2.02434	1.058467	-1.20671
1	-2.01314	1.024492	1.246099
1	-3.78739	0.556497	1.295961
6	2.544093	0.73815	-0.00124
6	2.846424	-0.53661	0.757781
6	2.855987	-0.55411	-0.72608
1	2.01116	-1.02535	1.243401
1	3.785628	-0.55795	1.297056
1	3.802584	-0.58784	-1.25169
1	2.026951	-1.05503	-1.20994
1	-3.31561	-1.49969	-0.00902
1	3.315651	1.501144	-0.00504
6	-1.21878	-1.266	-0.01477
7	-0.14599	-1.70997	-0.02385
6	1.218693	1.265604	-0.01435
7	0.14483	1.706927	-0.02385

Table S20: Coordinates of cyclobutyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	3.555552	-0.7633	-0.00246
6	2.733346	-0.03652	-1.07713
6	2.32006	0.996482	0.000782
6	2.734251	-0.03989	1.075145
1	4.602584	-0.44797	-0.00249
1	3.516043	-1.85317	-0.00412

1	1.874755	-0.63165	-1.39001
1	3.246945	0.354745	-1.95752
1	1.875902	-0.63611	1.386573
1	3.248549	0.348616	1.956341
6	0.961025	1.486446	0.001893
7	-0.13837	1.858898	0.002489
1	3.001486	1.853951	0.00179
6	-3.55527	0.763548	-0.0025
6	-2.73364	0.036049	-1.07712
6	-2.32024	-0.9966	0.001091
6	-2.73386	0.040319	1.075157
1	-4.60242	0.448628	-0.00205
1	-3.51531	1.853396	-0.00464
1	-1.875	0.630799	-1.39058
1	-3.24765	-0.35547	-1.95716
1	-1.87527	0.636412	1.386146
1	-3.24806	-0.34773	1.956612
6	-0.9612	-1.48657	0.002089
7	0.138221	-1.85893	0.002763
1	-3.0017	-1.85402	0.002684

Table S21: Coordinates of *tert* - Butyl cyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.60314	-0.03609	-0.00011
6	-1.49455	0.924156	0.000629
7	-0.63171	1.69917	0.001101
7	0.631854	-1.69936	0.00099
6	1.494479	-0.9241	0.000197
6	2.60306	0.036149	-0.00014
6	2.501405	0.910245	1.257203
1	1.569248	1.477954	1.261572
1	2.552904	0.307016	2.166659
1	3.336958	1.615604	1.268926
6	-2.50073	-0.90959	-1.25781
1	-1.56854	-1.47727	-1.26194
1	-3.33621	-1.61503	-1.27033
1	-2.55177	-0.30595	-2.16702
6	3.919965	-0.75262	-0.00059
1	4.006316	-1.38723	0.884315
1	4.005398	-1.38777	-0.8852
1	4.759555	-0.05235	-0.00126
6	-3.92005	0.75268	-9E-06
1	-4.00576	1.387977	-0.88447

1	-4.75965	0.052418	-0.00049
1	-4.00613	1.387142	0.885028
6	2.500663	0.910313	-1.25735
1	2.552987	0.307265	-2.16687
1	1.567879	1.477023	-1.26168
1	3.335439	1.616612	-1.26887
6	-2.5013	-0.91095	1.256677
1	-2.55292	-0.30838	2.166542
1	-3.3366	-1.61661	1.267955
1	-1.56891	-1.47825	1.260234

Table S22: Coordinates of monofluoro acetonitrile dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	2.293959	0.338146	0.401696
6	1.387416	-0.77982	0.179214
7	0.639532	-1.64669	0.008554
1	1.780001	1.266947	0.131527
1	2.571549	0.381776	1.45977
7	-0.63935	1.646386	-0.00605
6	-1.38694	0.779467	-0.17776
6	-2.29325	-0.33842	-0.40165
1	-1.78051	-1.26727	-0.12937
1	-2.56801	-0.38285	-1.46043
9	-3.43554	-0.19257	0.355243
9	3.434268	0.193376	-0.35836

Table S23: Coordinates of difluoro acetonitrile dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.39095	-0.24397	0.000297
6	-1.38645	0.834163	-0.00105
7	-0.54833	1.630223	-0.00167
1	-1.89749	-1.2232	0.001723
7	0.547333	-1.62906	0.002286
6	1.386235	-0.83382	0.001105
6	2.391331	0.243729	-0.00039
1	1.897968	1.222982	-0.00179
9	3.173254	0.130328	1.097601
9	-3.17275	-0.13076	-1.09785
9	3.173327	0.127162	-1.09802
9	-3.17321	-0.12768	1.097823

Table S24: Coordinates of trifluoro acetonitrile dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.86291	-0.02557	-0.0005
6	-1.65875	0.827729	0.001651
7	-0.71673	1.495701	0.003495
7	0.716743	-1.49573	0.00357
6	1.658607	-0.82754	0.001987
6	2.862893	0.025596	-0.00048
9	3.602534	-0.22064	1.083891
9	-3.60193	0.225417	-1.08424
9	3.60339	-0.2283	-1.08253
9	-3.60418	0.223309	1.082138
9	2.528972	1.311844	-0.00516
9	-2.52869	-1.31175	-0.00138

Table S25: Coordinates of methyl isocyanide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.26412	-0.6791	-0.00019
1	-2.89003	-0.76468	0.889472
1	-2.89341	-0.76252	-0.88767
1	-1.52261	-1.48209	-0.0025
7	-1.59719	0.567535	0.000037
6	-1.01118	1.584153	0.000257
6	2.272467	0.674415	-0.0002
1	2.899884	0.753749	0.888959
1	2.901709	0.752334	-0.88817
1	1.539181	1.484535	-0.00149
7	1.593982	-0.56589	0.000064
6	1.000789	-1.57827	0.000246

Table S26: Coordinates of methyl azide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.79023	0.680513	0.045859
1	-2.16885	1.431065	-0.45003
1	-3.49148	0.252402	-0.67698
1	-3.35673	1.157095	0.842256
7	-1.97021	-0.35858	0.679242

7	-1.23044	-0.99557	-0.05981
7	-0.49237	-1.66714	-0.61964
6	2.790229	-0.68059	0.045629
1	2.172058	-1.42083	-0.46941
1	3.505148	-0.24712	-0.66047
1	3.341735	-1.17118	0.844016
7	1.967298	0.355301	0.680409
7	1.230781	0.995932	-0.05879
7	0.494671	1.669911	-0.61832

Table S27: Coordinates of methyl cyanate dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	2.691349	-0.75541	-0.2753
1	3.569978	-1.12192	0.248076
1	1.872844	-1.47338	-0.23399
1	2.941161	-0.48485	-1.30162
6	1.270573	1.060016	0.027232
8	2.302395	0.449138	0.455716
7	0.343088	1.674016	-0.32179
6	-2.69036	0.756151	0.274033
1	-3.57213	1.119852	-0.24599
1	-2.93361	0.492027	1.303582
1	-1.87174	1.473246	0.223467
6	-1.27075	-1.06005	-0.02701
8	-2.30646	-0.45324	-0.45195
7	-0.34006	-1.67065	0.319303

Table S28: Coordinates of methyl isothiocyanate dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-0.20243	2.018938	1.380571
1	0.199221	1.580002	2.298069
1	0.619092	2.170086	0.67449
1	-0.64495	2.985009	1.634555
6	-1.59362	0.478543	-0.05877
7	-1.18876	1.16309	0.82753
16	-2.23609	-0.47409	-1.14235
6	0.20425	-2.02263	1.374985
1	-0.19443	-1.58591	2.294833
1	-0.61898	-2.16921	0.669959

1	0.644726	-2.99072	1.624767
6	1.59403	-0.47884	-0.06143
7	1.191926	-1.16743	0.82309
16	2.233577	0.478146	-1.14285

Table S29: Coordinates of cyclopentanone dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
6	-2.92907	0.631462	0.7271
6	-3.25683	-0.76404	0.182799
6	-2.01222	1.228096	-0.33508
6	-1.93847	-1.22725	-0.42782
6	-1.26846	0.041609	-0.91915
1	-2.37951	0.540215	1.669136
1	-2.58888	1.677161	-1.15539
1	-4.02569	-0.69179	-0.596
1	-2.00732	-1.97859	-1.2171
1	-3.64101	-1.44076	0.948563
1	-1.27671	-1.63227	0.350133
1	-1.31686	1.991903	0.017872
1	-3.81928	1.233678	0.920381
8	-0.2966	0.095333	-1.64182
6	2.929242	0.624759	-0.7327
6	3.256148	-0.76648	-0.17683
6	2.0132	1.231203	0.324548
6	1.938354	-1.22323	0.439847
6	1.26853	0.050481	0.918774
1	2.37956	0.526277	-1.67392
1	2.590323	1.686676	1.14104
1	4.026375	-0.68845	0.600045
1	2.00827	-1.96606	1.237056
1	3.638492	-1.45001	-0.93753
1	1.275892	-1.63718	-0.33257
1	1.318219	1.992389	-0.03489
1	3.820016	1.224558	-0.93096
8	0.296038	0.111236	1.639976

Table S30: Coordinates of methyl acetate dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
8	2.330216	-0.12769	-0.46857
6	1.582734	0.611459	0.372042

8	0.934155	0.145272	1.279859
6	1.659905	2.058947	0.003762
1	1.058577	2.220475	-0.89505
1	2.682548	2.353187	-0.23409
1	1.267942	2.673075	0.812171
6	2.224146	-1.54279	-0.29837
1	1.221567	-1.87238	-0.5782
1	2.963524	-1.97992	-0.96602
1	2.426749	-1.82699	0.736039
8	-2.40365	0.21049	0.33754
6	-1.52961	-0.63389	-0.24709
8	-0.84258	-0.32874	-1.19435
6	-1.5159	-1.95342	0.453118
1	-2.47492	-2.17837	0.918228
1	-0.75788	-1.90128	1.239645
1	-1.23583	-2.74215	-0.24425
6	-2.42129	1.535003	-0.19527
1	-3.25697	2.040155	0.284206
1	-1.48805	2.051205	0.040861
1	-2.55235	1.51644	-1.27857

Table S31: Coordinates of dimethyl sulfoxide dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
16	1.976019	0.963215	0.000000
8	0.603661	1.604104	0.000000
6	1.976019	-0.25584	1.349274
6	1.976019	-0.25584	-1.34927
1	1.885402	0.303388	2.280851
1	1.885402	0.303388	-2.28085
1	2.92228	-0.80031	1.339375
1	1.124108	-0.92443	1.203976
1	1.124108	-0.92443	-1.20398
1	2.92228	-0.80031	-1.33938
16	-1.97602	-0.96322	0.000000
8	-0.60366	-1.6041	0.000000
6	-1.97602	0.255835	-1.34927
6	-1.97602	0.255835	1.349274
1	-1.8854	-0.30339	-2.28085
1	-1.8854	-0.30339	2.280851
1	-1.12411	0.924433	-1.20398
1	-2.92228	0.800311	-1.33938
1	-2.92228	0.800311	1.339375

1	-1.12411	0.924433	1.203976

Table S32: Coordinates of dimethyl sulfone dimer optimized at M06L/6-311++g(d,p) level of DFT

Atom	x	y	z
16	2.112579	-0.00025	-0.16425
8	1.08433	-0.00146	-1.21177
6	1.797726	1.399047	0.900788
6	1.797788	-1.39719	0.903838
1	1.932692	2.288768	0.28559
1	1.933944	-2.28827	0.290875
1	2.524845	1.397547	1.712463
1	0.775178	1.327516	1.27166
1	0.774707	-1.32519	1.273117
1	2.524013	-1.39326	1.716295
16	-2.11268	-0.00021	0.164317
8	-1.08462	-0.00096	1.211925
6	-1.79735	-1.39706	-0.90365
6	-1.79754	1.398801	-0.90104
1	-1.93968	-2.2885	-0.29265
1	-1.93309	2.288765	-0.28632
1	-0.77241	-1.3274	-1.26818
1	-2.51945	-1.38956	-1.71978
1	-2.52381	1.396844	-1.71346
1	-0.77454	1.326976	-1.27059
8	3.519701	-0.00045	-0.53772
8	-3.51997	-0.00068	0.537595