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Supporting Material

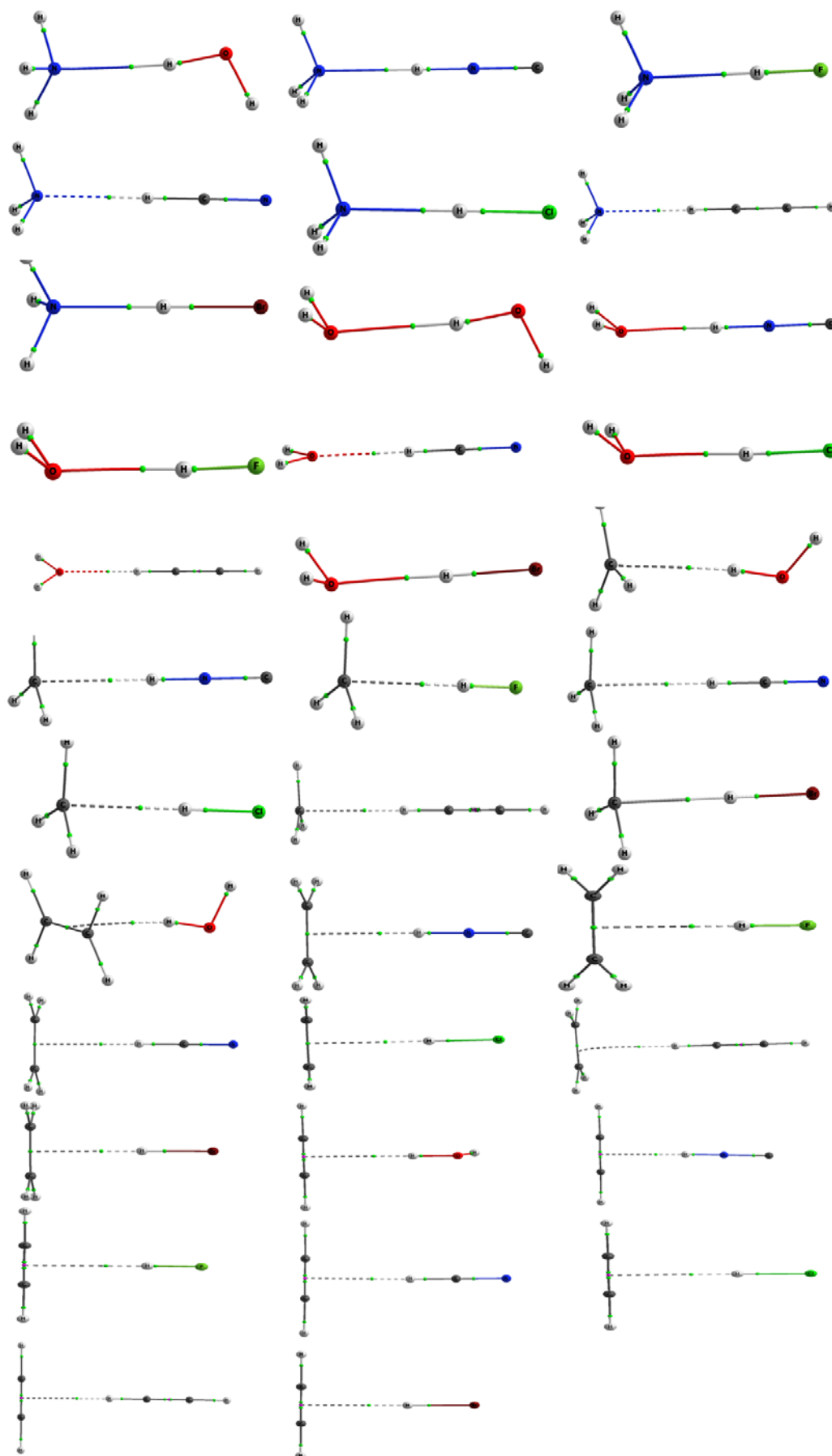
Hydrogen Bonding, Halogen Bonding and Lithium Bonding: An Atoms in Molecules and Natural Bond Orbital Perspective Towards Conservation of Total Bond Order, Inter- and Intra-molecular

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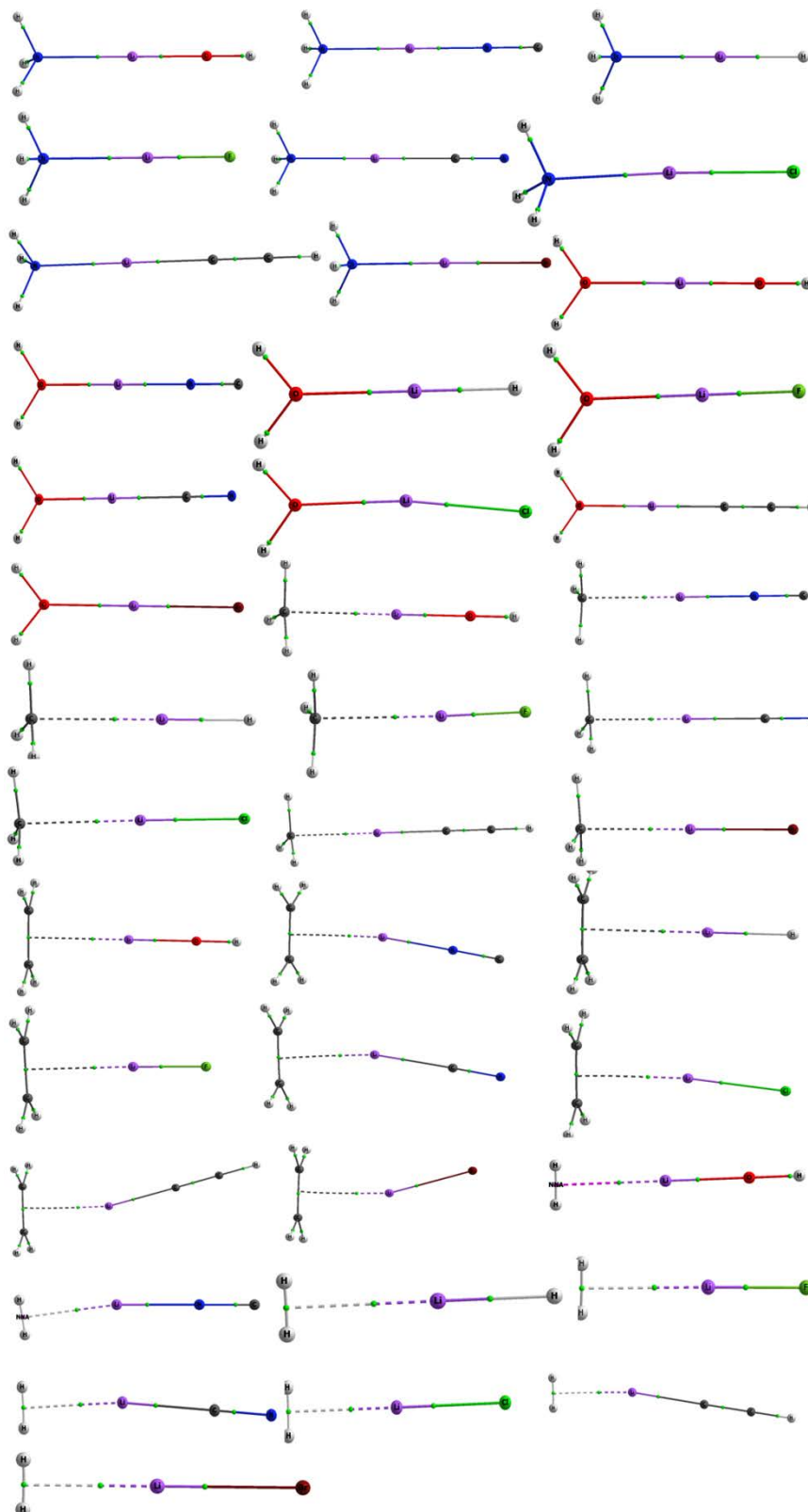
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a).



b).



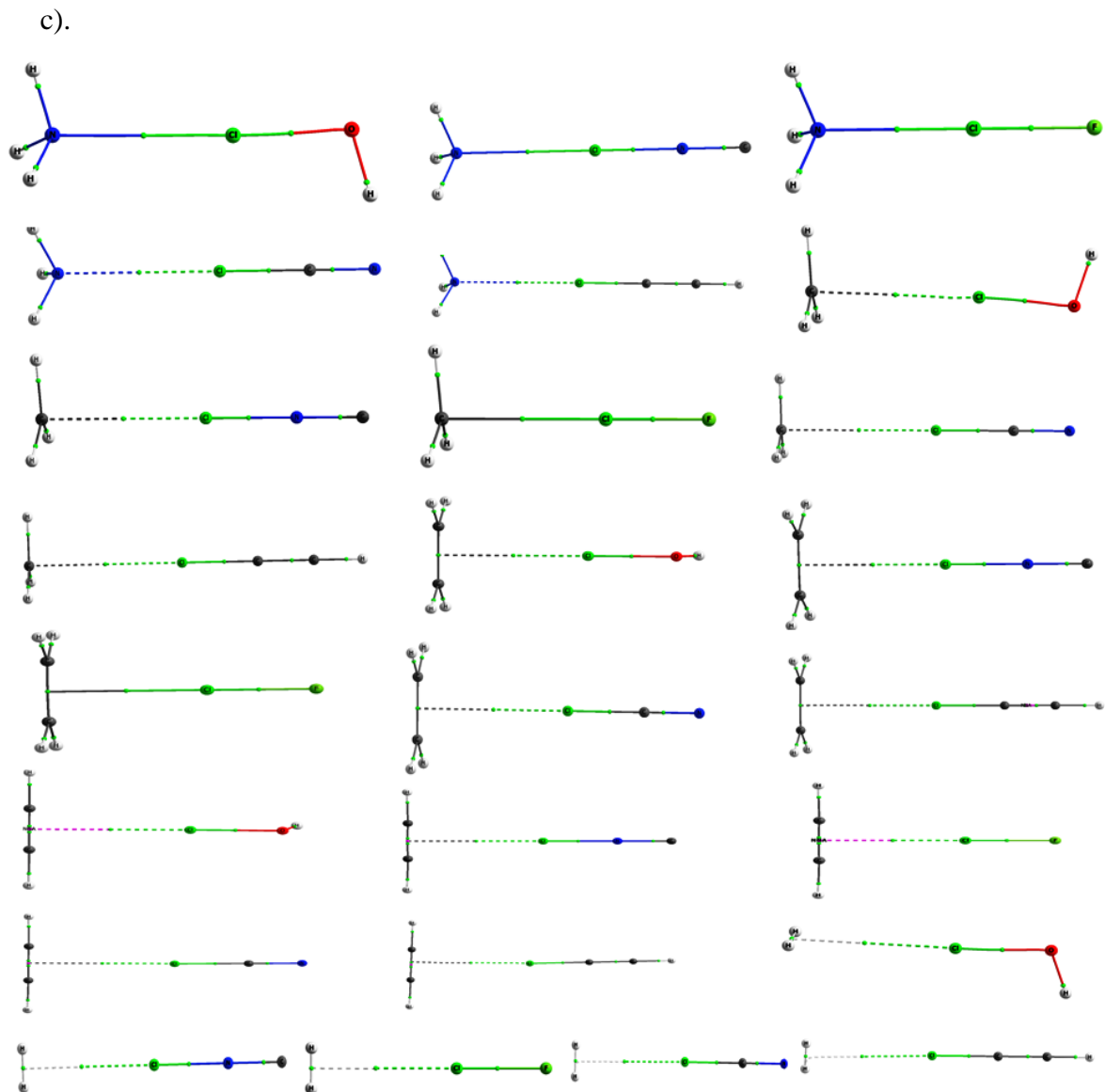


Figure S1. Structure of all complexes. a). hydrogen-bonding b). lithium-bonding and c). chlorine-bonding.

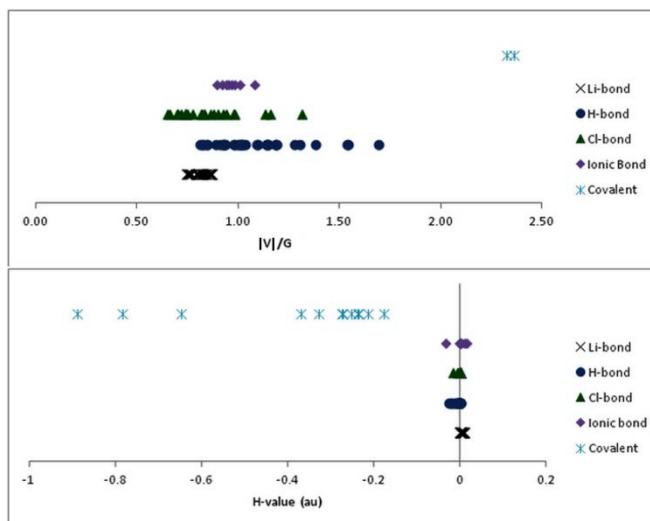


Figure S2. Criteria for interactions on the basis of $|V|/G$ values, H values. These figures include data for ionic and covalent bond.

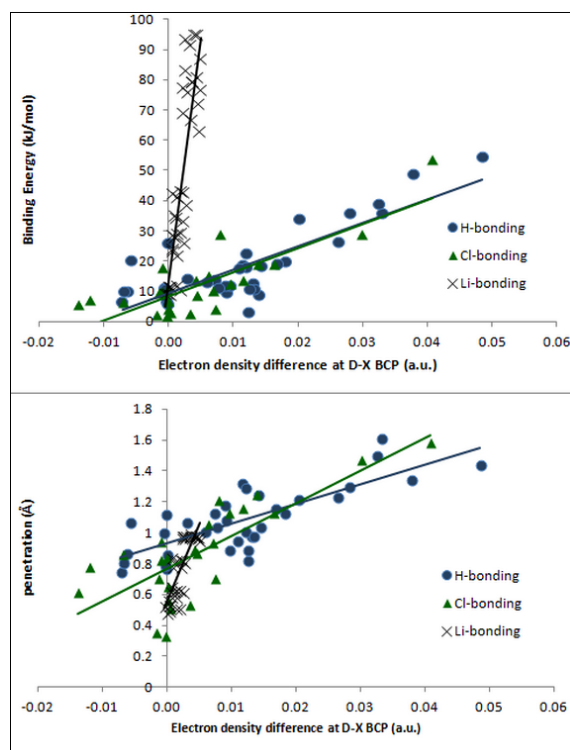


Figure S3. Correlation of differences in electron density of X-D on complex formation with binding energy (upper) and penetration (lower).

Table S1. Net charge, N(X), on the atom X, in complex, monomer and their difference $\Delta N(X)$ [N(X) in complex- N(X) in monomer].

Complexes	N(X) in Complexes	N(X) in monomer	$\Delta N(X)$
Hydrogen Bonding			
CH ₃ ---HBr	0.1461	0.0711	0.0749
CH ₃ ---HCl	0.3125	0.2961	0.0164
CH ₃ ---HF	0.7393	0.7539	-0.0146
CH ₃ ---HNC	0.5662	0.5668	-0.0006
CH ₃ ---HCN	0.2333	0.2378	-0.0045
CH ₃ ---HOH	0.6064	0.6331	-0.0267
CH ₃ ---HCCH	0.1834	0.1712	0.0123
H ₂ O---HBr	0.2217	0.0711	0.1506
H ₂ O---HCl	0.3860	0.2961	0.0898
H ₂ O---HF	0.7729	0.7539	0.0190
H ₂ O---HNC	0.6201	0.5668	0.0533
H ₂ O---HCN	0.2859	0.2378	0.0481
H ₂ O---HOH	0.6466	0.6331	0.0135
H ₂ O---HCCH	0.2284	0.1712	0.0572
NH ₃ ---HBr	0.3128	0.0711	0.2416
NH ₃ ---HCl	0.4230	0.2961	0.1269
NH ₃ ---HF	0.7586	0.7539	0.0047
NH ₃ ---HNC	0.6197	0.5668	0.0529
NH ₃ ---HCN	0.3036	0.2378	0.0658
NH ₃ ---HOH	0.6479	0.6331	0.0148
NH ₃ ---HCCH	0.2457	0.1712	0.0745
C ₂ H ₄ ---HBr	0.1505	0.0711	0.0794
C ₂ H ₄ ---HCl	0.3250	0.2961	0.0289
C ₂ H ₄ ---HF	0.7436	0.7539	-0.0103
C ₂ H ₄ ---HNC	0.5750	0.5668	0.0082
C ₂ H ₄ ---HCN	0.2439	0.2378	0.0061
C ₂ H ₄ ---HOH	0.6141	0.6331	-0.0190
C ₂ H ₄ ---HCCH	0.1928	0.1712	0.0216
C ₂ H ₂ ---HBr	0.1458	0.0711	0.0747
C ₂ H ₂ ---HCl	0.3257	0.2961	0.0295
C ₂ H ₂ ---HF	0.7485	0.7539	-0.0054
C ₂ H ₂ ---HNC	0.5784	0.5668	0.0117
C ₂ H ₂ ---HCN	0.2443	0.2378	0.0065
C ₂ H ₂ ---HOH	0.6168	0.6331	-0.0163
C ₂ H ₂ ---HCCH	0.1932	0.1712	0.0220
Chlorine Bonding			
CH ₃ --ClF	0.3824	0.528	-0.145
CH ₃ --ClCN	0.0271	0.012	0.015
CH ₃ --ClNC	0.3251	0.345	-0.020
CH ₃ --ClCCH	-0.0569	-0.057	0.000

CH ₃ --ClOH	0.2456	0.220	0.026
NH ₃ --ClF	0.3145	0.528	-0.213
NH ₃ --ClCN	0.0389	0.012	0.027
NH ₃ --ClNC	0.4415	0.345	0.096
NH ₃ --ClCCH	-0.0305	-0.057	0.026
NH ₃ --ClOH	0.2088	0.220	-0.011
C ₂ H ₂ --ClF	0.3775	0.528	-0.150
C ₂ H ₂ --ClCN	0.0171	0.012	0.005
C ₂ H ₂ --ClNC	0.3338	0.345	-0.011
C ₂ H ₂ --ClCCH	-0.0514	-0.057	0.005
C ₂ H ₂ --ClOH	0.2057	0.220	-0.014
C ₂ H ₄ --ClF	0.3195	0.528	-0.208
C ₂ H ₄ --ClCN	0.0155	0.012	0.003
C ₂ H ₄ --ClNC	0.3249	0.345	-0.020
C ₂ H ₄ --ClCCH	-0.0597	-0.057	-0.003
C ₂ H ₄ --ClOH	0.1970	0.220	-0.023
H ₂ --ClF	0.4204	0.528	-0.107
H ₂ --ClCN	0.0145	0.012	0.002
H ₂ --ClNC	0.3447	0.345	0.000
H ₂ --ClCCH	-0.0549	-0.057	0.002
H ₂ --ClOH	0.2161	0.220	-0.004

Lithium Bonding

CH ₃ ---LiCN	0.9099	0.9406	-0.0306
CH ₃ ---LiNC	0.9190	0.9408	-0.0218
CH ₃ ---LiBr	0.9030	0.9301	-0.0271
CH ₃ ---LiCl	0.9151	0.9340	-0.0189
CH ₃ ---LiCCH	0.9081	0.9333	-0.0252
CH ₃ ---LiH	0.8934	0.9122	-0.0188
CH ₃ ---LiF	0.9129	0.9437	-0.0308
CH ₃ ---LiOH	0.9043	0.9319	-0.0276
H ₂ O---LiCN	0.9155	0.9406	-0.0250
H ₂ O---LiNC	0.9206	0.9408	-0.0202
H ₂ O---LiBr	0.9070	0.9301	-0.0231
H ₂ O---LiCl	0.9105	0.9340	-0.0235
H ₂ O---LiCCH	0.9096	0.9333	-0.0236
H ₂ O---LiH	0.8955	0.9122	-0.0167
H ₂ O---LiF	0.9149	0.9437	-0.0287
H ₂ O---LiOH	0.9080	0.9319	-0.0239
NH ₃ ---LiCN	0.9071	0.9406	-0.0334
NH ₃ ---LiNC	0.9130	0.9408	-0.0278
NH ₃ ---LiBr	0.8994	0.9301	-0.0307
NH ₃ ---LiCl	0.9028	0.9340	-0.0312

NH ₃ ---LiCCH	0.9027	0.9333	-0.0305
NH ₃ ---LiH	0.8869	0.9122	-0.0253
NH ₃ ---LiF	0.9068	0.9437	-0.0369
NH ₃ ---LiOH	0.9008	0.9319	-0.0311
H ₂ ---LiCN	0.9240	0.9406	-0.0166
H ₂ ---LiNC	0.9284	0.9408	-0.0124
H ₂ ---LiBr	0.9115	0.9301	-0.0186
H ₂ ---LiCl	0.9161	0.9340	-0.0179
H ₂ ---LiCCH	0.9168	0.9333	-0.0164
H ₂ ---LiH	0.9021	0.9122	-0.0101
H ₂ ---LiF	0.9210	0.9437	-0.0227
H ₂ ---LiOH	0.9114	0.9319	-0.0205
C ₂ H ₄ ---LiCN	0.9099	0.9406	-0.0306
C ₂ H ₄ ---LiNC	0.9145	0.9408	-0.0263
C ₂ H ₄ ---LiBr	0.8987	0.9301	-0.0314
C ₂ H ₄ ---LiCl	0.9030	0.9340	-0.0310
C ₂ H ₄ ---LiCCH	0.9041	0.9333	-0.0292
C ₂ H ₄ ---LiH	0.8913	0.9122	-0.0209
C ₂ H ₄ ---LiF	0.9089	0.9437	-0.0348
C ₂ H ₄ ---LiOH	0.9006	0.9319	-0.0314

Table S2. Virial-based total energy, $K(X)$, on the atom X, in complex, monomer and their difference $\Delta K(X)$ [$K(X)$ in complex- $K(X)$ in monomer].

Complexes	$K(X)$ in Complex	$K(X)$ in monomers	$\Delta K(X)$
Hydrogen Bonding			
CH ₃ ---HBr	-0.5234	-0.5439	0.0204
CH ₃ ---HCl	-0.4692	-0.4827	0.0135
CH ₃ ---HF	-0.2535	-0.2533	-0.0002
CH ₃ ---HNC	-0.3579	-0.3651	0.0071
CH ₃ ---HCN	-0.5183	-0.5048	-0.0135
CH ₃ ---HOH	-0.3446	-0.3286	-0.0160
CH ₃ ---HCCH	-0.5428	-0.5485	0.0057
H ₂ O---HBr	-0.4981	-0.5439	0.0457
H ₂ O---HCl	-0.4413	-0.4827	0.0413
H ₂ O---HF	-0.2364	-0.2533	0.0169
H ₂ O---HNC	-0.3327	-0.3651	0.0324
H ₂ O---HCN	-0.4994	-0.5048	0.0054
H ₂ O---HOH	-0.3262	-0.3286	0.0024
H ₂ O---HCCH	-0.5272	-0.5485	0.0213
NH ₃ ---HBr	-0.4459	-0.5439	0.0980
NH ₃ ---HCl	-0.4122	-0.4827	0.0705
NH ₃ ---HF	-0.2382	-0.2533	0.0151
NH ₃ ---HNC	-0.3239	-0.3651	0.0412
NH ₃ ---HCN	-0.4851	-0.5048	0.0197
NH ₃ ---HOH	-0.3189	-0.3286	0.0098
NH ₃ ---HCCH	-0.5149	-0.5485	0.0336
C ₂ H ₄ ---HBr	-0.5239	-0.5439	0.0200
C ₂ H ₄ ---HCl	-0.4641	-0.4827	0.0185
C ₂ H ₄ ---HF	-0.2493	-0.2533	0.0040
C ₂ H ₄ ---HNC	-0.3514	-0.3651	0.0136
C ₂ H ₄ ---HCN	-0.5132	-0.5048	-0.0084
C ₂ H ₄ ---HOH	-0.3397	-0.3286	-0.0111
C ₂ H ₄ ---HCCH	-0.5384	-0.5485	0.0101
C ₂ H ₂ --HBr	-0.5273	-0.5439	0.0166
C ₂ H ₂ --HCl	-0.4656	-0.4827	0.0171
C ₂ H ₂ --HF	-0.2482	-0.2533	0.0052
C ₂ H ₂ --HNC	-0.3515	-0.3651	0.0136
C ₂ H ₂ --HCN	-0.5139	-0.5048	-0.0091
C ₂ H ₂ --HOH	-0.3399	-0.3286	-0.0113
C ₂ H ₂ --HCCH	-0.5390	-0.5485	0.0095

Chlorine Bonding

CH ₃ --ClF	-459.566	-459.277	-0.289
CH ₃ --ClCN	-459.763	-459.623	-0.140
CH ₃ --ClNC	-459.653	-459.414	-0.239
CH ₃ --ClCCH	-459.867	-459.598	-0.268
CH ₃ --ClOH	-459.469	-459.394	-0.074
NH ₃ --ClF	-459.599	-459.277	-0.323
NH ₃ --ClCN	-459.859	-459.623	-0.236
NH ₃ --ClNC	-459.473	-459.414	-0.059
NH ₃ --ClCCH	-459.865	-459.598	-0.267
NH ₃ --ClOH	-459.690	-459.394	-0.296
C ₂ H ₂ --ClF	-459.590	-459.277	-0.313
C ₂ H ₂ --ClCN	-459.872	-459.623	-0.249
C ₂ H ₂ --ClNC	-459.661	-459.414	-0.247
C ₂ H ₂ --ClCCH	-459.877	-459.598	-0.279
C ₂ H ₂ --ClOH	-459.703	-459.394	-0.308
C ₂ H ₄ --ClF	-459.612	-459.277	-0.335
C ₂ H ₄ --ClCN	-459.871	-459.623	-0.248
C ₂ H ₄ --ClNC	-459.662	-459.414	-0.248
C ₂ H ₄ --ClCCH	-459.763	-459.598	-0.165
C ₂ H ₄ --ClOH	-459.703	-459.394	-0.309
H ₂ --ClF	-459.545	-459.277	-0.268
H ₂ --ClCN	-459.845	-459.623	-0.222
H ₂ --ClNC	-459.630	-459.414	-0.216
H ₂ --ClCCH	-459.847	-459.598	-0.248
H ₂ --ClOH	-459.670	-459.394	-0.275

Lithium Bonding

CH ₃ ---LiCN	-7.3581	-7.3549	-0.0032
CH ₃ ---LiNC	-7.3536	-7.3343	-0.0193
CH ₃ ---LiBr	-7.3467	-7.3336	-0.0131
CH ₃ ---LiCl	-7.3513	-7.3339	-0.0174
CH ₃ ---LiCCH	-7.3678	-7.3639	-0.0039
CH ₃ ---LiH	-7.3800	-7.3628	-0.0173
CH ₃ ---LiF	-7.3629	-7.3432	-0.0197
CH ₃ ---LiOH	-7.3633	-7.3547	-0.0086
H ₂ O---LiCN	-7.3685	-7.3549	-0.0136

H ₂ O---LiNC	-7.3647	-7.3343	-0.0304
H ₂ O---LiBr	-7.3551	-7.3336	-0.0215
H ₂ O---LiCl	-7.3565	-7.3339	-0.0226
H ₂ O---LiCCH	-7.3779	-7.3639	-0.0140
H ₂ O---LiH	-7.3858	-7.3628	-0.0230
H ₂ O---LiF	-7.3736	-7.3432	-0.0304
H ₂ O---LiOH	-7.3734	-7.3547	-0.0187
NH ₃ ---LiCN	-7.3784	-7.3549	-0.0236
NH ₃ ---LiNC	-7.3741	-7.3343	-0.0398
NH ₃ ---LiBr	-7.3624	-7.3336	-0.0288
NH ₃ ---LiCl	-7.3664	-7.3339	-0.0325
NH ₃ ---LiCCH	-7.3859	-7.3639	-0.0220
NH ₃ ---LiH	-7.3942	-7.3628	-0.0314
NH ₃ ---LiF	-7.3831	-7.3432	-0.0399
NH ₃ ---LiOH	-7.3830	-7.3547	-0.0283
H ₂ ----LiCN	-7.3496	-7.3549	0.0052
H ₂ ----LiNC	-7.3455	-7.3343	-0.0112
H ₂ ----LiBr	-7.3384	-7.3336	-0.0048
H ₂ ----LiCl	-7.3382	-7.3339	-0.0043
H ₂ ----LiCCH	-7.3609	-7.3639	0.0030
H ₂ ----LiH	-7.3819	-7.3628	-0.0191
H ₂ ----LiF	-7.3552	-7.3432	-0.0120
H ₂ ----LiOH	-7.3578	-7.3547	-0.0031
C ₂ H ₄ ---LiCN	-7.3641	-7.3549	-0.0092
C ₂ H ₄ ---LiNC	-7.3605	-7.3343	-0.0262
C ₂ H ₄ ---LiBr	-7.3539	-7.3336	-0.0203
C ₂ H ₄ ---LiCl	-7.3542	-7.3339	-0.0204
C ₂ H ₄ ---LiCCH	-7.3733	-7.3639	-0.0094
C ₂ H ₄ ---LiH	-7.3814	-7.3628	-0.0186
C ₂ H ₄ ---LiF	-7.3698	-7.3432	-0.0266
C ₂ H ₄ ---LiOH	-7.3697	-7.3547	-0.0149

Table S3. Magnitude of dipole moment, $|\mu(X)|$, on the atom X, in complex, monomer and their difference $\Delta\mu(X)$ [$|\mu(X)|$ in complex - $|\mu(X)|$ in monomer].

Complexes	$ \mu(X) $ of complex	$ \mu(X) $ of monomer	$\Delta\mu(X)$
Hydrogen Bonding			
CH ₃ ---HBr	0.0631	0.0649	-0.0018
CH ₃ ---HCl	0.1203	0.1367	-0.0164
CH ₃ ---HF	0.1178	0.1176	0.0003
CH ₃ ---HNC	0.1411	0.1443	-0.0032
CH ₃ ---HCN	0.1203	0.1204	-0.0001
CH ₃ ---HOH	0.1610	0.1550	0.0060
CH ₃ ---HCCH	0.1271	0.1336	-0.0065
H ₂ O---HBr	0.0332	0.0649	-0.0318
H ₂ O---HCl	0.0836	0.1367	-0.0531
H ₂ O---HF	0.0839	0.1176	-0.0336
H ₂ O---HNC	0.1053	0.1443	-0.0390
H ₂ O---HCN	0.0955	0.1204	-0.0249
H ₂ O---HOH	0.1281	0.1550	-0.0269
H ₂ O---HCCH	0.1061	0.1336	-0.0275
NH ₃ ---HBr	0.0262	0.0649	-0.0387
NH ₃ ---HCl	0.0732	0.1367	-0.0635
NH ₃ ---HF	0.0852	0.1176	-0.0323
NH ₃ ---HNC	0.1043	0.1443	-0.0400
NH ₃ ---HCN	0.1024	0.1204	-0.0180
NH ₃ ---HOH	0.1289	0.1550	-0.0261
NH ₃ ---HCCH	0.1116	0.1336	-0.0221
C ₂ H ₄ ---HBr	0.0630	0.0649	-0.0019
C ₂ H ₄ ---HCl	0.1172	0.1367	-0.0195
C ₂ H ₄ ---HF	0.1127	0.1176	-0.0049
C ₂ H ₄ ---HNC	0.1365	0.1443	-0.0078
C ₂ H ₄ ---HCN	0.1172	0.1204	-0.0032
C ₂ H ₄ ---HOH	0.1557	0.1550	0.0006
C ₂ H ₄ ---HCCH	0.1246	0.1336	-0.0091
C ₂ H ₂ ---HBr	0.0598	0.0649	-0.0052
C ₂ H ₂ ---HCl	0.1144	0.1367	-0.0224
C ₂ H ₂ ---HF	0.1094	0.1176	-0.0081
C ₂ H ₂ ---HNC	0.1328	0.1443	-0.0115
C ₂ H ₂ ---HCN	0.1141	0.1204	-0.0063
C ₂ H ₂ ---HOH	0.1514	0.1550	-0.0036
C ₂ H ₂ ---HCCH	0.1219	0.1336	-0.0117

Chlorine Bonding

CH ₃ --ClF	0.823	0.971	-0.149
CH ₃ --ClCN	0.170	0.151	0.019
CH ₃ --ClNC	0.640	0.665	-0.025
CH ₃ --ClCCH	0.190	0.196	-0.007
CH ₃ --ClOH	0.759	0.734	0.025
NH ₃ --ClF	0.556	0.971	-0.415
NH ₃ --ClCN	0.103	0.151	-0.049
NH ₃ --ClNC	0.695	0.665	0.030
NH ₃ --ClCCH	0.143	0.196	-0.053
NH ₃ --ClOH	0.584	0.734	-0.151
C ₂ H ₂ --ClF	0.750	0.971	-0.221
C ₂ H ₂ --ClCN	0.137	0.151	-0.015
C ₂ H ₂ --ClNC	0.622	0.665	-0.044
C ₂ H ₂ --ClCCH	0.176	0.196	-0.021
C ₂ H ₂ --ClOH	0.667	0.734	-0.067
C ₂ H ₄ --ClF	0.698	0.971	-0.274
C ₂ H ₄ --ClCN	0.143	0.151	-0.008
C ₂ H ₄ --ClNC	0.621	0.665	-0.045
C ₂ H ₄ --ClCCH	0.182	0.196	-0.014
C ₂ H ₄ --ClOH	0.661	0.734	-0.073
H ₂ --ClF	0.817	0.971	-0.154
H ₂ --ClCN	0.143	0.151	-0.008
H ₂ --ClNC	0.650	0.665	-0.015
H ₂ --ClCCH	0.184	0.196	-0.012
H ₂ --ClOH	0.702	0.734	-0.032

Lithium Bonding

CH ₃ ---LiCN	0.0104	0.0024	0.0079
CH ₃ ---LiNC	0.0177	0.0056	0.0121
CH ₃ ---LiBr	0.0074	0.0033	0.0041
CH ₃ ---LiCl	0.0107	0.0006	0.0101
CH ₃ ---LiCCH	0.0120	0.0003	0.0117
CH ₃ ---LiH	0.0025	0.0008	0.0018
CH ₃ ---LiF	0.0295	0.0182	0.0114
CH ₃ ---LiOH	0.0318	0.0218	0.0100
H ₂ O---LiCN	0.0009	0.0024	-0.0015

H ₂ O---LiNC	0.0060	0.0056	0.0004
H ₂ O---LiBr	0.0052	0.0033	0.0019
H ₂ O---LiCl	0.0006	0.0006	0.0000
H ₂ O---LiCCH	0.0007	0.0003	0.0003
H ₂ O---LiH	0.0093	0.0008	0.0086
H ₂ O---LiF	0.0173	0.0182	-0.0009
H ₂ O---LiOH	0.0190	0.0218	-0.0028
NH ₃ ---LiCN	0.0033	0.0024	0.0008
NH ₃ ---LiNC	0.0099	0.0056	0.0043
NH ₃ ---LiBr	0.0014	0.0033	-0.0019
NH ₃ ---LiCl	0.0035	0.0006	0.0029
NH ₃ ---LiCCH	0.0044	0.0003	0.0041
NH ₃ ---LiH	0.0048	0.0008	0.0040
NH ₃ ---LiF	0.0214	0.0182	0.0033
NH ₃ ---LiOH	0.0228	0.0218	0.0010
H ₂ ---LiCN	0.0050	0.0024	0.0025
H ₂ ---LiNC	0.0126	0.0056	0.007
H ₂ ---LiBr	0.0025	0.0033	-0.0008
H ₂ ---LiCl	0.0068	0.0006	0.0062
H ₂ ---LiCCH	0.0071	0.0003	0.0067
H ₂ ---LiH	0.0020	0.0008	0.0012
H ₂ ---LiF	0.0248	0.0182	0.0067
H ₂ ---LiOH	0.0275	0.0218	0.0057
C ₂ H ₄ ---LiCN	0.0095	0.0024	0.0071
C ₂ H ₄ ---LiNC	0.0168	0.0056	0.0112
C ₂ H ₄ ---LiBr	0.0059	0.0033	0.0026
C ₂ H ₄ ---LiCl	0.0106	0.0006	0.0099
C ₂ H ₄ ---LiCCH	0.0110	0.0003	0.0106
C ₂ H ₄ ---LiH	0.0001	0.0008	-0.0006
C ₂ H ₄ ---LiF	0.0282	0.0182	0.0101
C ₂ H ₄ ---LiOH	0.0301	0.0218	0.0083

Table S4. Volume of bonded atom (X) at 0.001 a.u. isosurface value, Vol (X), in complex, monomer and their difference $\Delta\text{Vol}(X)$ [Vol(x) in complex-Vol(x) in monomer]

Complexes	Vol (X) of complex	Vol (X) of monomer	diff.Vol(X)
Hydrogen Bonding			
CH ₃ ---HBr	36.5	47.0	-10.5
CH ₃ ---HCl	30.4	36.0	-5.6
CH ₃ ---HF	11.4	13.9	-2.5
CH ₃ ---HNC	20.1	22.1	-2.1
CH ₃ ---HCN	37.1	38.5	-1.3
CH ₃ ---HOH	19.6	19.4	0.2
CH ₃ ---HCCH	39.8	41.1	-1.3
H ₂ O---HBr	31.6	47.0	-15.4
H ₂ O---HCl	23.7	36.0	-12.3
H ₂ O---HF	7.0	13.9	-6.9
H ₂ O---HNC	13.4	22.1	-8.7
H ₂ O---HCN	30.4	38.5	-8.1
H ₂ O---HOH	13.6	19.4	-5.8
H ₂ O---HCCH	34.4	41.1	-6.7
NH ₃ ---HBr	25.1	47.0	-21.9
NH ₃ ---HCl	20.5	36.0	-15.5
NH ₃ ---HF	7.2	13.9	-6.7
NH ₃ ---HNC	12.9	22.1	-9.2
NH ₃ ---HCN	29.4	38.5	-9.1
NH ₃ ---HOH	13.2	19.4	-6.2
NH ₃ ---HCCH	33.4	41.1	-7.7
C ₂ H ₄ ---HBr	37.5	47.0	-9.5
C ₂ H ₄ ---HCl	29.4	36.0	-6.6
C ₂ H ₄ ---HF	9.8	13.9	-4.1
C ₂ H ₄ ---HNC	18.2	22.1	-3.9
C ₂ H ₄ ---HCN	36.0	38.5	-2.5
C ₂ H ₄ ---HOH	17.6	19.4	-1.8
C ₂ H ₄ ---HCCH	39.0	41.1	-2.1
C ₂ H ₂ ---HBr	38.6	47.0	-8.3
C ₂ H ₂ ---HCl	29.8	36.0	-6.2
C ₂ H ₂ ---HF	9.7	13.9	-4.2
C ₂ H ₂ ---HNC	17.9	22.1	-4.2
C ₂ H ₂ ---HCN	35.5	38.5	-3.0
C ₂ H ₂ ---HOH	17.3	19.4	-2.1
C ₂ H ₂ ---HCCH	38.7	41.1	-2.4

Chlorine Bonding

CH ₃ --ClF	195.2	199.1	-3.9
CH ₃ --ClCN	202.5	204.2	-1.7
CH ₃ --ClNC	196.5	199.7	-3.2
CH ₃ --ClCCH	211.0	209.6	1.4
CH ₃ --ClOH	203.1	209.3	-6.2
NH ₃ --ClF	190.8	199.1	-8.3
NH ₃ --ClCN	201.5	204.2	-2.7
NH ₃ --ClNC	187.2	199.7	-0.1
NH ₃ --ClCCH	207.6	209.6	-2.0
NH ₃ --ClOH	200.9	209.3	-8.4
C ₂ H ₂ --ClF	194.4	199.1	-4.7
C ₂ H ₂ --ClCN	202.9	204.2	-1.3
C ₂ H ₂ --ClNC	194.8	199.7	-4.9
C ₂ H ₂ --ClCCH	210.0	209.6	0.4
C ₂ H ₂ --ClOH	204.5	209.3	-4.8
C ₂ H ₄ --ClF	188.7	199.1	-0.1
C ₂ H ₄ --ClCN	202.8	204.2	-1.4
C ₂ H ₄ --ClNC	193.7	199.7	-6.0
C ₂ H ₄ --ClCCH	206.9	209.6	-2.7
C ₂ H ₄ --ClOH	202.3	209.3	-7.0
H ₂ --ClF	201.2	199.1	2.1
H ₂ --ClCN	205.1	204.2	0.9
H ₂ --ClNC	199.0	199.7	-0.7
H ₂ --ClCCH	211.3	209.6	1.7
H ₂ --ClOH	209.2	209.3	-0.1

Lithium Bonding

CH ₃ ---LiCN	31.0	26.6	4.4
CH ₃ ---LiNC	30.0	26.7	3.3
CH ₃ ---LiBr	33.1	28.0	5.2
CH ₃ ---LiCl	30.6	27.4	3.2
CH ₃ ---LiCCH	31.8	26.9	4.8
CH ₃ ---LiH	36.0	30.4	5.6
CH ₃ ---LiF	30.2	25.4	4.8
CH ₃ ---LiOH	32.0	26.7	5.4
H ₂ O---LiCN	28.5	26.6	1.8

H ₂ O---LiNC	27.3	26.7	0.6
H ₂ O---LiBr	29.8	28.0	1.8
H ₂ O---LiCl	29.0	27.4	1.6
H ₂ O---LiCCH	29.0	26.9	2.1
H ₂ O---LiH	32.5	30.4	2.1
H ₂ O---LiF	27.4	25.4	2.0
H ₂ O---LiOH	28.6	26.7	1.9
NH ₃ ---LiCN	29.5	26.6	2.9
NH ₃ ---LiNC	28.3	26.7	1.7
NH ₃ ---LiBr	30.7	28.0	2.8
NH ₃ ---LiCl	30.1	27.4	2.7
NH ₃ ---LiCCH	30.0	26.9	3.1
NH ₃ ---LiH	33.4	30.4	3.0
NH ₃ ---LiF	28.4	25.4	3.0
NH ₃ ---LiOH	29.6	26.7	3.0
H ₂ ----LiCN	29.2	26.6	2.6
H ₂ ----LiNC	28.3	26.7	1.7
H ₂ ----LiBr	31.2	28.0	3.2
H ₂ ----LiCl	30.4	27.4	3.0
H ₂ ----LiCCH	29.9	26.9	2.9
H ₂ ----LiH	33.5	30.4	3.1
H ₂ ----LiF	28.5	25.4	3.1
H ₂ ----LiOH	30.3	26.7	3.6
C ₂ H ₄ ---LiCN	30.6	26.6	4.0
C ₂ H ₄ ---LiNC	29.9	26.7	3.2
C ₂ H ₄ ---LiBr	31.6	28.0	3.6
C ₂ H ₄ ---LiCl	31.9	27.4	4.5
C ₂ H ₄ ---LiCCH	30.9	26.9	4.0
C ₂ H ₄ ---LiH	35.4	30.4	5.0
C ₂ H ₄ ---LiF	30.2	25.4	4.8
C ₂ H ₄ ---LiOH	31.8	26.7	5.1

Table S5. Eigen values of Hessian matrix at intermolecular, λ_1 , λ_2 , and λ_3 are presented.

Complexes	λ_1	λ_2	λ_3
Lithium Bonding			
CH ₃ ---LiCN	-0.017	-0.017	0.095
CH ₃ ---LiNC	-0.017	-0.017	0.097
CH ₃ ---LiBr	-0.019	-0.018	0.103
CH ₃ ---LiCl	-0.017	-0.017	0.097
CH ₃ ---LiCCH	-0.016	-0.016	0.090
CH ₃ ---LiH	-0.016	-0.016	0.088
CH ₃ ---LiF	-0.016	-0.016	0.089
CH ₃ ---LiOH	-0.014	-0.014	0.081
H ₂ O---LiCN	-0.064	-0.060	0.372
H ₂ O---LiNC	-0.065	-0.060	0.374
H ₂ O---LiBr	-0.066	-0.062	0.386
H ₂ O---LiCl	-0.064	-0.060	0.373
H ₂ O---LiCCH	-0.063	-0.058	0.362
H ₂ O---LiH	-0.062	-0.058	0.361
H ₂ O---LiF	-0.060	-0.056	0.351
H ₂ O---LiOH	-0.057	-0.053	0.336
NH ₃ ---LiCN	-0.053	-0.053	0.291
NH ₃ ---LiNC	-0.053	-0.053	0.291
NH ₃ ---LiBr	-0.056	-0.056	0.307
NH ₃ ---LiCl	-0.053	-0.053	0.292
NH ₃ ---LiCCH	-0.051	-0.051	0.277
NH ₃ ---LiH	-0.052	-0.052	0.285
NH ₃ ---LiF	-0.050	-0.050	0.277
NH ₃ ---LiOH	-0.047	-0.047	0.263
H ₂ ---LiCN	-0.017	-0.015	0.093
H ₂ ---LiNC	-0.018	-0.016	0.097
H ₂ ---LiBr	-0.020	-0.018	0.109
H ₂ ---LiCl	-0.018	-0.016	0.099
H ₂ ---LiCCH	-0.016	-0.015	0.091
H ₂ ---LiH	-0.016	-0.014	0.088
H ₂ ---LiF	-0.017	-0.015	0.092
H ₂ ---LiOH	-0.015	-0.014	0.085
C ₂ H ₄ ---LiCN	-0.022	-0.016	0.115
C ₂ H ₄ ---LiNC	-0.022	-0.016	0.115
C ₂ H ₄ ---LiBr	-0.024	-0.017	0.125

C ₂ H ₄ ---LiCl	-0.022	-0.016	0.116
C ₂ H ₄ ---LiCCH	-0.021	-0.015	0.111
C ₂ H ₄ ---LiH	-0.020	-0.015	0.106
C ₂ H ₄ ---LiF	-0.020	-0.015	0.107
C ₂ H ₄ ---LiOH	-0.019	-0.014	0.102
C ₂ H ₂ ---LiCN	-0.023	-0.017	0.134
C ₂ H ₂ ---LiNC	-0.023	-0.017	0.136
C ₂ H ₂ ---LiBr	-0.024	-0.019	0.140
C ₂ H ₂ ---LiCl	-0.023	-0.017	0.137
C ₂ H ₂ ---LiCCH	-0.022	-0.015	0.131
C ₂ H ₂ ---LiH	-0.021	-0.016	0.128
C ₂ H ₂ ---LiF	-0.020	-0.013	0.122
C ₂ H ₂ ---LiOH	-0.019	-0.013	0.118
Hydrogen Bonding			
CH ₃ ---HBr	-0.035	-0.035	0.115
CH ₃ ---HCl	-0.024	-0.024	0.089
CH ₃ ---HF	-0.023	-0.023	0.086
CH ₃ ---HNC	-0.018	-0.018	0.072
CH ₃ ---HCN	-0.010	-0.010	0.049
CH ₃ ---HOH	-0.013	-0.013	0.058
CH ₃ ---HCCH	-0.010	-0.009	0.047
H ₂ O---HBr	-0.057	-0.055	0.208
H ₂ O---HCl	-0.057	-0.055	0.208
H ₂ O---HF	-0.083	-0.080	0.267
H ₂ O---HNC	-0.060	-0.057	0.217
H ₂ O---HCN	-0.028	-0.026	0.133
H ₂ O---HOH	-0.039	-0.038	0.161
H ₂ O---HCCH	-0.020	-0.018	0.102
NH ₃ ---HBr	-0.116	-0.116	0.277
NH ₃ ---HCl	-0.093	-0.093	0.247
NH ₃ ---HF	-0.103	-0.103	0.275
NH ₃ ---HNC	-0.072	-0.072	0.215
NH ₃ ---HCN	-0.030	-0.030	0.126
NH ₃ ---HOH	-0.045	-0.044	0.159
NH ₃ ---HCCH	-0.022	-0.022	0.102
C ₂ H ₄ ---HBr	-0.022	-0.015	0.082
C ₂ H ₄ ---HCl	-0.021	-0.015	0.078
C ₂ H ₄ ---HF	-0.029	-0.020	0.094
C ₂ H ₄ ---HNC	-0.020	-0.014	0.075

C ₂ H ₄ ---HCN	-0.012	-0.008	0.051
C ₂ H ₄ ---HOH	-0.015	-0.010	0.063
C ₂ H ₄ ---HCCH	-0.010	-0.007	0.047
C ₂ H ₂ --HBr	-0.019	-0.014	0.080
C ₂ H ₂ --HCl	-0.019	-0.014	0.079
C ₂ H ₂ --HF	-0.026	-0.020	0.096
C ₂ H ₂ --HNC	-0.020	-0.015	0.082
C ₂ H ₂ --HCN	-0.011	-0.009	0.056
C ₂ H ₂ --HOH	-0.015	-0.011	0.067
C ₂ H ₂ --HCCH	-0.010	-0.007	0.050
Chlorine Bonding			
CH ₃ ---ClF	-0.020	-0.020	0.104
CH ₃ ---ClCN	-0.004	-0.004	0.035
CH ₃ ---ClNC	-0.009	-0.009	0.061
CH ₃ ---ClCCH	-0.004	-0.004	0.031
CH ₃ ---ClOH	-0.007	-0.007	0.056
NH ₃ --ClF	-0.071	-0.071	0.284
NH ₃ --ClCN	-0.011	-0.011	0.077
NH ₃ --ClNC	-0.022	-0.022	0.144
NH ₃ --ClCCH	-0.008	-0.008	0.061
NH ₃ --ClOH	-0.024	-0.024	0.143
C ₂ H ₂ --ClF	-0.017	-0.009	0.101
C ₂ H ₂ --ClCN	-0.005	-0.003	0.042
C ₂ H ₂ --ClNC	-0.009	-0.005	0.065
C ₂ H ₂ --ClCCH	-0.005	-0.003	0.037
C ₂ H ₂ --ClOH	-0.009	-0.005	0.064
C ₂ H ₄ --ClF	-0.035	-0.013	0.139
C ₂ H ₄ --ClCN	-0.006	-0.004	0.042
C ₂ H ₄ --ClNC	-0.012	-0.006	0.069
C ₂ H ₄ --ClCCH	-0.005	-0.003	0.039
C ₂ H ₄ --ClOH	-0.013	-0.006	0.074
H ₂ --ClF	-0.008	-0.006	0.057
H ₂ --ClCN	-0.003	-0.003	0.026
H ₂ --ClNC	-0.005	-0.004	0.038
H ₂ --ClCCH	-0.003	-0.003	0.024
H ₂ --ClOH	-0.005	-0.004	0.037

Table S6. Correlation coefficient (CC), slope and intercept for the all complexes, case I and case II type of complexes. This result from correlation plot of binding energy with electron density.

Complex	Li-Bonding			H-Bonding			Cl-bonding		
	CC	Slope	Intercept	CC	Slope	intercept	CC	slope	intercept
Overall	0.97	3271	-17.6	0.88	777	-0.4	0.96	776	-0.3
	(CASE-I) Same Donor (X-D), Different acceptor								
A•••X-F	0.97	3150	-18.2	0.99	1037	-5.7	0.99	849	-5.2
A•••X-Cl	0.97	3337	-18.2	0.97	748	-2.5	XXX		
A•••X-Br	0.97	3416	-22.5	0.95	566	-1.7	XXX		
A•••X-CN	0.97	3424	-17.7	0.99	1425	-7.6	1	1577	-5.2
A•••X-NC	0.97	3445	-19	0.99	1189	-4.6	0.98	1337	-7
A•••X-CCH	0.97	3225	-16	0.78	903	-2.8	0.98	1259	-3.7
A•••X-OH	0.97	3150	-18.2	0.99	987	-4.4	0.98	748	-1.8
A•••X-H	0.97	3057	-14.5	XXX			XXX		
	(CASE-II) Same acceptor (A), Different Donor								
CH3 •••X-D	0.86	2928	-10.3	0.53	257	3.9	0.98	458	1.4
NH3•••X-D	0.88	5080	-63.2	0.76	601	9.9	0.97	706	4.5
H2O•••X-D	0.95	5093	-83	0.78	692	2.4	XXX		
C2H4•••X-D	0.89	3767	-19.9	0.82	865	-1.5	0.98	660	2.4
C2H2•••X-D	XXX			0.75	671	2.3	0.96	698	2.1
H2•••X-D	0.68	1002	-0.3	XXX			0.97	335	0.2

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Table S7. Correlation coefficient (C.C.) for the correlation between mutual penetration and binding energy.

Complex	Li-Bonding	H-Bonding	Cl-bonding
	CC=0.96# MP=0.001*BE+0.4	CC=0.80 MP=0.01*BE+0.7	CC=0.87 MP=0.02*BE+0.6
Overall	CC (CASE-I) Same Donor (X-D), Different acceptor	CC	CC
A•••X-F	0.96	0.96	0.90
A•••X-Cl	0.95	0.97	xxx
A•••X-Br	0.96	0.96	xxx
A•••X-CN	0.96	0.98	0.94
A•••X-NC	0.96	0.99	0.92
A•••X-CCH	0.96	0.77	0.95
A•••X-OH	0.96	0.97	0.95
A•••X-H	0.96	xxx	xxx
	(CASE-II) Same acceptor (X), Different Donor		
CH3 •••X-D	0.79	0.48	0.95
NH3•••X-D	0.72	0.68	0.91
H2O•••X-D	0.74	0.59	Xxx
C2H4•••X-D	0.83	0.64	0.95
C2H2•••X-D	xxx	0.55	0.93
H2•••X-D	0.66	xxx	0.95

#There are two type of correlation for Li-bonding. For Li-bonding in figure 7 (main text), Lower part shows linear dependence and upper part plateau. The correlation coefficient of the lower part is presented.

Table S8. : Correlation coefficient for the correlation between electron density (in a.u.) and mutual penetration (in Å).

Complex Overall	Li-Bond CC=0.97# MP=55.6*ρ-0.1 CC#	H-Bond CC=0.94\$ MP=13.9*ρ+0.7 CC	Cl-bond CC=0.92 MP=30.9*ρ+0.4 CC**
	(CASE-I) Same Donor (X-D) , Different acceptor		
A•••X-F	0.94	0.96	0.99
A•••X-Cl	0.94	0.98	xxx
A•••X-Br	0.93	0.98	xxx
A•••X-CN	0.94	0.97	0.99
A•••X-NC	0.94	0.86	1.00
A•••X-CCH	0.94	0.96	0.99
A•••X-OH	0.94	0.85	0.99
A•••X-H	0.94	xxx	xxx
	(CASE-II) Same acceptor (X) , Different Donor		
CH3 •••X-D	0.96	0.99	0.96
NH3•••-X-D	0.81	0.99	0.95
H2O•••X-D	0.73	0.94	xxx
C2H4•••X-D	0.93	0.96	0.97
C2H2•••X-D	xxx	0.95	0.98
H2•••X-D	0.97	xxx	0.98

\$ Without the values of C2H2•••H-D complexes. ** Without the values of NH3•••Cl-D complexes for case 1 only. # Figure 7 of main text for Li-bonding, lower part depends linearly and upper part plateau. The correlation coefficient and equation are presented only for the lower part.

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Table S9. Comparison of slope from other studies and present work.

Level of theory	Comparison of slopes from different studies			References ^S
	Li-bonding	H-bonding	Cl-bonding	
MP2(full)/aug-cc-PVTZ	3271(-17.6) [*]	777(-0.4)	776(-0.3)	This work
MP2(full)/aug-cc-PVTZ	2951(-9.1)	1001(-3.8)	855(-3.8)	[16]
B3LYP/6-311++G(d,p)	----	911(-2.9)	1623(-21.9)	[19]
MP2/6-311G++(d,p)	2435(11.9)/5316(-47.8)	717(-4.5)/708(-1.1)	----	[20]

*In parentheses, intercept are presented. ^Sreferences are from main text.

Table S10. Radii of bonded (r_A and r_D), non-bonded (r_A^0 and r_X^0) atoms, differences between them (Del r_A , Del r_X) and summation of both differences i.e. mutual penetration (Del r_A + Del r_X).

Complexes	r_A^0	r_A	Del r_A	r_X^0	r_X	Del r_X	Del r_A + Del r_X
Hydrogen Bond							
CH ₃ •••HBr	1.98	1.26	0.72	1.27	0.74	0.53	1.25
CH ₃ •••HCl	1.98	1.34	0.64	1.22	0.78	0.44	1.08
CH ₃ •••HF	1.98	1.38	0.61	1.11	0.74	0.37	0.98
CH ₃ •••HNC	1.98	1.43	0.55	1.13	0.80	0.33	0.89
CH ₃ •••HCN	1.98	1.53	0.46	1.21	0.92	0.30	0.75
CH ₃ •••HOH	1.98	1.48	0.50	1.17	0.86	0.32	0.82
CH ₃ •••HCCH	1.98	1.53	0.46	1.25	0.94	0.32	0.77
H ₂ O•••HBr	1.88	1.20	0.68	1.27	0.63	0.64	1.32
H ₂ O•••HCl	1.88	1.20	0.68	1.22	0.62	0.61	1.29
H ₂ O•••HF	1.88	1.16	0.72	1.11	0.53	0.58	1.30
H ₂ O•••HNC	1.88	1.20	0.68	1.13	0.59	0.54	1.22
H ₂ O•••HCN	1.88	1.28	0.60	1.21	0.74	0.47	1.07
H ₂ O•••HOH	1.88	1.26	0.62	1.17	0.67	0.50	1.13
H ₂ O•••HCCH	1.88	1.33	0.55	1.25	0.80	0.45	1.00
NH ₃ •••HBr	2.00	1.14	0.86	1.27	0.52	0.75	1.61
NH ₃ •••HCl	2.00	1.18	0.82	1.22	0.54	0.68	1.50
NH ₃ •••HF	2.00	1.17	0.83	1.11	0.50	0.61	1.44
NH ₃ •••HNC	2.00	1.23	0.77	1.13	0.57	0.57	1.34
NH ₃ •••HCN	2.00	1.36	0.64	1.21	0.73	0.49	1.12
NH ₃ •••HOH	2.00	1.30	0.70	1.17	0.65	0.52	1.23
NH ₃ •••HCCH	2.00	1.41	0.59	1.25	0.78	0.47	1.07
C ₂ H ₄ •••HBr	2.14	1.41	0.74	1.27	0.82	0.45	1.18
C ₂ H ₄ •••HCl	2.14	1.43	0.71	1.22	0.80	0.42	1.13
C ₂ H ₄ •••HF	2.14	1.39	0.76	1.11	0.71	0.40	1.16
C ₂ H ₄ •••HNC	2.14	1.46	0.69	1.13	0.81	0.32	1.01
C ₂ H ₄ •••HCN	2.14	1.56	0.58	1.21	0.92	0.29	0.87
C ₂ H ₄ •••HOH	2.14	1.50	0.64	1.17	0.84	0.34	0.98
C ₂ H ₄ •••HCCH	2.14	1.58	0.56	1.25	0.95	0.30	0.86
Lithium Bond							
CH ₃ •••LiCN	1.98	1.50	0.48	1.00	0.86	0.14	0.63
CH ₃ •••LiNC	1.98	1.49	0.49	1.00	0.86	0.14	0.63
CH ₃ •••LiBr	1.98	1.48	0.51	0.98	0.85	0.14	0.65
CH ₃ •••LiCl	1.98	1.51	0.48	0.99	0.85	0.14	0.62
CH ₃ •••LiCCH	1.98	1.51	0.47	1.00	0.87	0.13	0.61

CH ₃ •••LiH	1.98	1.52	0.47	0.98	0.87	0.12	0.58
CH ₃ •••LiF	1.98	1.50	0.48	1.01	0.87	0.14	0.62
CH ₃ •••LiOH	1.98	1.53	0.45	1.01	0.88	0.12	0.58
H ₂ O•••LiCN	1.88	1.17	0.71	1.00	0.72	0.28	0.98
H ₂ O•••LiNC	1.88	1.17	0.71	1.00	0.72	0.28	0.99
H ₂ O•••LiBr	1.88	1.17	0.71	0.98	0.72	0.27	0.98
H ₂ O•••LiCl	1.88	1.17	0.71	0.99	0.72	0.27	0.98
H ₂ O•••LiCCH	1.88	1.18	0.70	1.00	0.73	0.28	0.98
H ₂ O•••LiH	1.88	1.18	0.70	0.98	0.73	0.26	0.96
H ₂ O•••LiF	1.88	1.18	0.70	1.01	0.73	0.28	0.98
H ₂ O•••LiOH	1.88	1.19	0.69	1.01	0.73	0.27	0.96
NH ₃ •••LiCN	2.00	1.28	0.72	1.00	0.74	0.26	0.98
NH ₃ •••LiNC	2.00	1.28	0.72	1.00	0.74	0.26	0.98
NH ₃ •••LiBr	2.00	1.27	0.73	0.98	0.73	0.25	0.98
NH ₃ •••LiCl	2.00	1.28	0.72	0.99	0.74	0.25	0.97
NH ₃ •••LiCCH	2.00	1.29	0.71	1.00	0.74	0.26	0.97
NH ₃ •••LiH	2.00	1.28	0.72	0.98	0.74	0.24	0.96
NH ₃ •••LiF	2.00	1.29	0.71	1.01	0.75	0.26	0.98
NH ₃ •••LiOH	2.00	1.30	0.70	1.01	0.75	0.25	0.95
H ₂ •••LiCN	1.56	1.18	0.38	1.00	0.87	0.13	0.51
H ₂ •••LiNC	1.56	1.17	0.39	1.00	0.86	0.14	0.53
H ₂ •••LiBr	1.56	1.14	0.42	0.98	0.85	0.14	0.56
H ₂ •••LiCl	1.56	1.17	0.40	0.99	0.86	0.13	0.53
H ₂ •••LiCCH	1.56	1.19	0.38	1.00	0.87	0.13	0.51
H ₂ •••LiH	1.56	1.19	0.37	0.98	0.87	0.11	0.48
H ₂ •••LiF	1.56	1.17	0.39	1.01	0.87	0.14	0.52
H ₂ •••LiOH	1.56	1.19	0.37	1.01	0.88	0.12	0.49
C ₂ H ₄ •••LiCN	2.14	1.49	0.65	1.00	0.83	0.17	0.82
C ₂ H ₄ •••LiNC	2.14	1.49	0.66	1.00	0.83	0.17	0.83
C ₂ H ₄ •••LiBr	2.14	1.46	0.68	0.98	0.82	0.16	0.84
C ₂ H ₄ •••LiCl	2.14	1.48	0.66	0.99	0.83	0.16	0.82
C ₂ H ₄ •••LiCCH	2.14	1.50	0.65	1.00	0.84	0.16	0.81
C ₂ H ₄ •••LiH	2.14	1.51	0.63	0.98	0.84	0.14	0.78
C ₂ H ₄ •••LiF	2.14	1.50	0.65	1.01	0.85	0.16	0.81
C ₂ H ₄ •••LiOH	2.14	1.51	0.63	1.01	0.85	0.15	0.78
Chlorine Bond							
CH ₃ •••ClF	1.98	1.28	0.70	1.79	1.33	0.46	1.16
CH ₃ •••ClCN	1.98	1.62	0.36	1.87	1.61	0.25	0.61
CH ₃ •••ClNC	1.98	1.46	0.53	1.82	1.48	0.34	0.87

CH ₃ •••CICCH	1.98	1.64	0.34	1.88	1.66	0.22	0.56
CH ₃ •••CIOH	1.98	1.49	0.50	1.85	1.49	0.36	0.86
NH ₃ •••CIF	2.00	1.12	0.88	1.79	1.09	0.70	1.58
NH ₃ •••CICN	2.00	1.47	0.53	1.87	1.46	0.41	0.94
NH ₃ •••CINC	2.00	1.34	0.66	1.82	1.27	0.54	1.21
NH ₃ •••CICCH	2.00	1.52	0.48	1.88	1.51	0.36	0.84
NH ₃ •••CIOH	2.00	1.31	0.69	1.85	1.29	0.56	1.25
C ₂ H ₂ •••CIF	2.04	1.36	0.68	1.79	1.34	0.45	1.13
C ₂ H ₂ •••CICN	2.04	1.62	0.42	1.87	1.59	0.28	0.70
C ₂ H ₂ •••CINC	2.04	1.50	0.54	1.82	1.46	0.35	0.89
C ₂ H ₂ •••CICCH	2.04	1.65	0.39	1.88	1.62	0.26	0.65
C ₂ H ₂ •••CIOH	2.04	1.49	0.54	1.85	1.47	0.38	0.93
C ₂ H ₄ •••CIF	2.14	1.21	0.93	1.79	1.25	0.54	1.47
C ₂ H ₄ •••CICN	2.14	1.61	0.53	1.87	1.58	0.29	0.82
C ₂ H ₄ •••CINC	2.14	1.46	0.68	1.82	1.44	0.37	1.05
C ₂ H ₄ •••CICCH	2.14	1.66	0.49	1.88	1.59	0.29	0.78
C ₂ H ₄ •••CIOH	2.14	1.43	0.71	1.85	1.43	0.42	1.13
H ₂ •••CIF	1.57	1.18	0.39	1.79	1.48	0.31	0.70
H ₂ •••CICN	1.57	1.38	0.19	1.87	1.70	0.16	0.35
H ₂ •••CINC	1.57	1.28	0.28	1.82	1.59	0.22	0.51
H ₂ •••CICCH	1.57	1.39	0.18	1.88	1.73	0.15	0.33
H ₂ •••CIOH	1.57	1.28	0.28	1.85	1.60	0.25	0.53