Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information For

Towards Developing a Quantitative Criterion to Characterize Non-covalent Bonds: A Quantum Mechanical Study

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Figure S2: Linear fitting of interaction energy with electron density at a critical point for (a) covalent, (b) ionic, and (c) coordinate bonds. Values are calculated at MP2/6-311++G** level of theory.

Table S1: Details of charge and multiplicity used in this study for the considered covalent, ionic, and coordinate systems.

S. No.	Covalent	Charge	Multiplicity
1.	H_2	0	1
2.	N_2	0	1
3.	O_2	0	3
4.	Cl_2	0	1
5.	HF	0	1
6.	HCl	0	1
7.	FCl	0	1
8.	BH_3	0	1
9.	NH_3	0	1
10.	CH_4	0	1
11.	H_2O	0	1
12.	PH_3	0	1
13.	H_2S	0	1
14.	BCl_3	0	1
15.	NCl_3	0	1
16.	Cl_2O	0	1
17.	PCl_3	0	1
18.	SCl_2	0	1
19.	CCl_4	0	1
20.	C_2H_6	0	1
21.	C_2H_4	0	1
22.	C_2H_2	0	1
23.	CH_3OH	0	1
24.	CH_3SH	0	1
	Ionic		
25.	NaCl	0	1
26.	LiH	0	1
27.	NaH	0	1
25.	KH	0	1
29.	CaS	0	1
30.	AlN	0	1
31.	$MgCl_2$	0	1
32.	MgH_2	0	1
33.	CaH_2	0	1
	Coordinate		
34.	NH_3-BH_3	0	1
35.	NH_3-BF_3	0	1
36.	PH_3-BH_3	0	1
37.	PH_3-AlH_3	0	1
38.	H_2S-BH_3	0	1
39.	H_2S-AlH_3	0	1
40.	CO-BH_3	0	1
41.	$(CH_3)NH_2$-BH_3	0	1
42.	HF-BH_3	0	1

Table S2: Details of charge and multiplicity used in this study for the considered non-covalent systems.

S. No.	Non-covalent	Charge	Multiplicity	S. No.	Non-covalent	Charge	Multiplicity
1.	H_2O-H_2O	0	1	23.	LiH-$ClCF_3$	0	1
2.	NH_3-NH_3	0	1	24.	C_2H_4-CH_3CN	0	1
3.	NH_3-NH_4^+	1	1	25.	LiF-CH_3F	0	1
4.	H_2O-NH_4^+	1	1	26.	H_2O-CH_3OH	0	1
5.	H_2O-Li^+	1	1	27.	FH_2P-NH_2F	0	1
6.	NH_3-Li^+	1	1	28.	FH_2P-NH_2Me	0	1
7.	C_2H_2-HCN	0	1	29.	F(Me)S-NH_3	0	1
8.	C_2H_2-HNC	0	1	30.	OH(Me)S-NH_3	0	1
9.	NH_3-C_2H_4	0	1	31.	$CN(H_3)Si$-$CN(H_3)Si$	0	1
10.	CH_4-Bz	0	1	32.	$NC(H_3)Si$-$NC(H_3)Si$	0	1
11.	NH_3-Bz	0	1	33.	C_2H_4-LiF	0	1
12.	H_2O-CNBz	0	1	34.	H_2O-LiF	0	1
13.	Cl^--FBz	-1	1	35.	H_3N-LiF	0	1
14.	Li^+-Bz	1	1	36.	He_2	0	1
15.	Bz-Bz	0	1	37.	Ne_2	0	1
16.	Pyridine-Bz	0	1	38.	Ar_2	0	1
17.	Li^+-C_2H_6	1	1	39.	$Propane_2$	0	1
18.	Li^+-CH_4	1	1	40.	DHB-Me	0	1
19.	CH_3NH_2-I_2	0	1	41.	DHB-Et	0	1
20.	$(CH_3)_3N$-I_2	0	1	42.	HBeCHN(H)-Be(H)CHN(H)	0	1
21.	C_2H_2-ClCN	0	1	43.	FBeCHN(H)-Be(F)CHN(H)	0	1
22.	H_3N-ClCN	0	1				

Table S3: Details of charge (Icharg) and multiplicity (Mult) used in the LMO-EDA calculation for the considered covalent, ionic, and coordinate systems. Mmult is the multiplicity for each moiety. Bond distance (BD) has been shown in Å.

S. No.	Covalent	Icharg	Mult	Mcharg	Mmult	BD
1.	H_2	0	1	0, 0	2, -2	0.738
2.	N_2	0	1	0, 0	4, -4	1.120
3.	O_2	0	1	0, 0	3, -3	1.224
4.	Cl_2	0	1	0, 0	2, -2	2.025
5.	HF	0	1	0, 0	2, -2	0.917
6.	HCl	0	1	0, 0	2, -2	1.273
7.	FCl	0	1	0, 0	2, -2	1.673
8.	BH_3	0	1	0, 0	2, -2	1.191
9.	NH_3	0	1	0, 0	2, -2	1.014
10.	CH_4	0	1	0, 0	2, -2	1.091
11.	H_2O	0	1	0, 0	2, -2	0.959
12.	PH_3	0	1	0, 0	2, -2	1.409
13.	H_2S	0	1	0, 0	2, -2	1.333
14.	BCl_3	0	1	0, 0	2, -2	1.740
15.	NCl_3	0	1	0, 0	2, -2	1.768
16.	OCl_2	0	1	0, 0	2, -2	1.728
17.	PCl_3	0	1	0, 0	2, -2	2.058
18.	SCl_2	0	1	0, 0	2, -2	2.045
19.	CCl_4	0	1	0, 0	2, -2	1.772
20.	C_2H_6	0	1	0, 0	2, -2	1.530
21.	C_2H_4	0	1	0, 0	1, -1	1.339
22.	C_2H_2	0	1	0, 0	2, -2	1.216
23.	CH_3OH	0	1	0, 0	2, -2	1.423
24.	CH_3SH	0	1	0, 0	2, -2	1.812
	Ionic					
25.	NaCl	0	1	1, -1	1, 1	2.381
26.	LiH	0	1	1, -1	1, 1	1.600
27.	NaH	0	1	1, -1	1, 1	1.908
28.	KH	0	1	1, -1	1, 1	2.245
29.	CaS	0	1	2, -2	1, 1	2.369
30.	AlN	0	1	3, -3	1, 1	1.640
31.	$MgCl_2$	0	1	1, -1	1, 1	2.181
32.	MgH_2	0	1	1, -1	1, 1	1.704
33.	CaH_2	0	1	1, -1	1, 1	2.050
	Coordinate					
34.	NH_3-BH_3	0	1	0, 0	1, 1	1.656
35.	NH_3-BF_3	0	1	0, 0	1, 1	1.668
36.	PH_3-BH_3	0	1	0, 0	1, 1	1.941
37.	PH_3-AlH_3	0	1	0, 0	1, 1	2.561
38.	H_2S-BH_3	0	1	0, 0	1, 1	2.024
39.	H_2S-AlH_3	0	1	0, 0	1, 1	2.565
40.	CO-BH_3	0	1	0, 0	1, 1	1.553
41.	$(CH_3)NH_2$-BH_3	0	1	0, 0	1, 1	1.640
42.	HF-BH_3	0	1	0, 0	1, 1	2.286

Table S4: Details of charge (Icharg) and multiplicity (Mult) used in the LMO-EDA calculation for the considered non-covalentsystems.Mmult is the multiplicity for each moiety. Bond distance (BD) has been shown in Å.

S. No.	Non-covalent	Icharg	Mult	Mcharg	Mmult	BD	S. No.	Non-covalent	Icharg	Mult	Mcharg	Mmult	BD
1.	H_2O-H_2O	0	1	0, 0	1, 1	1.950	23.	LiH-$ClCF_3$	0	1	0, 0	1, 1	2.835
2.	NH_3-NH_3	0	1	0, 0	1, 1	2.263	24.	C_2H_4-CH_3CN	0	1	0, 0	1, 1	3.644
3.	NH_3-NH_4^+	1	1	0, 1	1, 1	1.815	25.	LiF-CH_3F	0	1	0, 0	1, 1	2.844
4.	H_2O-NH_4^+	1	1	1, 0	1, 1	1.649	26.	H_2O-CH_3OH	0	1	0, 0	1, 1	3.104
5.	H_2O-Li^+	1	1	0, 1	1, 1	1.866	27.	FH_2P-NH_2F	0	1	0, 0	1, 1	2.664
6.	NH_3-Li^+	1	1	0, 1	1, 1	1.997	28.	FH_2P-NH_2Me	0	1	0, 0	1, 1	2.534
7.	C_2H_2-HCN	0	1	0, 0	1, 1	2.598	29.	F(Me)S-NH_3	0	1	0, 0	1, 1	2.836
8.	C_2H_2-HNC	0	1	0, 0	1, 1	2.300	30.	OH(Me)S-NH_3	0	1	0, 0	1, 1	3.196
9.	NH_3-C_2H_4	0	1	0, 0	1, 1	2.711	31.	$CN(H_3)Si$-$CN(H_3)Si$	0	1	0, 0	1, 1	3.021
10.	CH_4-Bz	0	1	0, 0	1, 1	2.575	32.	$NC(H_3)Si$-$NC(H_3)Si$	0	1	0, 0	1, 1	3.025
11.	NH_3-Bz	0	1	0, 0	1, 1	2.476	33.	C_2H_4-LiF	0	1	0, 0	1, 1	2.377
12.	H_2O-CNBz	0	1	0, 0	1, 1	2.946	34.	H_2O-LiF	0	1	0, 0	1, 1	1.957
13.	Cl^--FBz	-1	1	0, -1	1, 1	3.099	35.	H_3N-LiF	0	1	0, 0	1, 1	2.076
14.	Li^+-Bz	1	1	0, 1	1, 1	1.869	36.	He_2	0	1	0, 0	1, 1	3.335
15.	Bz-Bz	0	1	0, 0	1, 1	3.635	37.	Ne_2	0	1	0, 0	1, 1	3.171
16.	Pyridine-Bz	0	1	0, 0	1, 1	3.578	38.	Ar_2	0	1	0, 0	1, 1	4.085
17.	Li^+-C_2H_6	1	1	0, 1	1, -1	2.141	39.	$Propane_2$	0	1	0, 0	1, 1	2.610
18.	Li^+-CH_4	1	1	0, 1	1, 1	2.157	40.	DHB-Me	0	1	0, 0	1, 1	2.001
19.	CH_3NH_2-I_2	0	1	0, 0	1, 1	2.623	41.	DHB-Et	0	1	0, 0	1, 1	2.022
20.	$(CH_3)_3N$-I_2	0	1	0, 0	1, 1	2.540	42.	HBeCHN(H)-Be(H)CHN(H)	0	1	0, 0	1, 1	1.751
21.	C_2H_2-ClCN	0	1	0, 0	1, 1	3.371	43.	FBeCHN(H)-Be(F)CHN(H)	0	1	0, 0	1, 1	1.765
22.	H_3N-ClCN	0	1	0, 0	1, 1	3.001							

Table S5: Comparison of the calculated interaction energy of covalent, ionic, and coordinate bonds at MP2, B3LYP, and M05-2X from the corresponding CSSD(T) results. It also has shown the mean absolute value of the MP2, B3LYP, and M05-2X results from the corresponding CCSD(T) values. Energies in kcal/mol.

S. No.	Covalent	MP2	B3LYP	M05-2X	CCSD(T)	M1	M2	M3
1.	H_2	-100.82	-109.84	-106.97	-105.87	-5.06	3.96	1.10
2.	N_2	-375.55	-351.12	-355.90	-337.87	**37.68**	13.25	18.03
3.	O_2	-116.91	-119.36	-113.69	-105.64	11.27	13.72	8.05
4.	Cl_2	-43.08	-47.41	-49.43	-41.91	1.17	5.50	7.51
5.	HF	-137.73	-137.75	-138.45	-134.08	3.65	3.67	4.37
6.	HCl	-99.74	-103.40	-103.84	-100.49	-0.76	2.90	3.35
7.	FCl	-50.32	-52.63	-51.54	-46.42	3.90	6.21	5.13
8.	BH_3	-105.21	-110.71	-112.12	-107.94	-1.35	16.71	16.60
9.	NH_3	-112.15	-113.40	-114.99	-110.65	-1.14	22.78	22.34
10.	CH_4	-114.13	-117.91	-119.07	-115.14	-2.41	21.50	24.48
11.	H_2O	-122.54	-121.76	-123.16	-119.54	3.16	10.13	11.39
12.	PH_3	-81.03	-85.56	-85.20	-83.27	-8.59	17.93	17.50
13.	H_2S	-88.99	-92.46	-92.76	-90.62	-4.06	8.37	9.93
14.	BCl_3	-120.07	-113.11	-119.93	-115.66	26.87	-12.59	13.00
15.	NCl_3	-39.61	-27.80	-34.61	-30.56	14.23	-3.00	9.27
16.	OCl_2	-42.20	-31.47	-35.90	-30.66	15.08	5.46	16.31
17.	PCl_3	-66.84	-64.07	-68.79	-63.12	22.41	7.57	34.55
18.	SCl_2	-49.93	-49.86	-53.51	-47.18	17.14	13.20	33.51
19.	CCl_4	-77.90	-65.52	-74.62	-71.42	23.90	-22.53	6.97
20.	C_2H_6	-113.99	-109.69	-116.54	-110.70	3.29	-1.01	5.84
21.	C_2H_4	-215.73	-208.63	-211.43	-203.27	12.46	5.36	8.16
22.	C_2H_2	-243.80	-233.57	-237.52	-227.80	16.00	5.77	9.72
23.	CH_3OH	-105.85	-100.52	-106.24	-99.88	5.97	0.64	6.36
24.	CH_3SH	-84.28	-80.05	-86.43	-81.45	2.82	-1.40	4.98
	Mean Absolute Value					**6.42**	**3.90**	**5.48**
	Ionic							
25.	NaCl	-91.01	-92.45	-101.75	-89.22	1.79	3.23	12.53
26.	LiH	-48.22	-58.17	-58.70	-53.20	-4.98	4.97	5.50
27.	NaH	-35.02	-45.00	-47.46	-40.46	-5.44	4.54	7.00
28.	KH	-30.27	-42.67	-45.71	-35.13	-4.86	7.54	10.58
29.	CaS	-98.13	-114.30	-109.04	-83.52	14.60	30.78	25.52
30.	AlN	-94.19	-96.85	-93.88	-100.31	-6.13	-3.46	-6.43
31.	$MgCl_2$	-106.88	-105.51	-114.05	-104.83	2.05	0.68	9.22
32.	MgH_2	-65.44	-72.03	-71.70	-69.21	-3.10	7.30	0.15
33.	CaH_2	-52.37	-59.86	-62.03	-55.93	-4.11	14.70	8.74
	Mean Absolute Value					**5.24**	**6.88**	**9.49**
	Coordinate							
34.	NH_3-BH_3	-45.25	-41.78	-43.40	-44.28	0.96	-2.50	-0.89
35.	NH_3-BF_3	-48.17	-44.72	-51.33	-48.32	-0.15	-3.60	3.01
36.	PH_3-BH_3	-39.15	-34.34	-36.50	-37.36	1.79	-3.01	-0.86
37.	PH_3-AlH_3	-18.54	-16.15	-20.17	-18.39	0.15	-2.23	1.79
38.	H_2S-BH_3	-24.68	-20.00	-21.92	-23.96	0.73	-3.96	-2.03
39.	H_2S-AlH_3	-14.67	-12.11	-16.23	-14.60	0.07	-2.49	1.63
40.	CO-BH_3	-36.52	-39.59	-36.41	-33.57	2.95	6.02	2.84
41.	$(CH_3)NH_2$-BH_3	-51.44	-46.56	-49.46	-50.19	1.25	-3.63	-0.73
42.	HF-BH_3	-3.49	-3.13	-4.62	-3.63	-0.13	-0.49	1.00
	Mean Absolute Value					**0.91**	**3.11**	**1.64**

M1 = $IE_{CCSD(T)} - IE_{MP2;}$ **M2** = $IE_{CCSD(T)} - IE_{B3LYP;}$ **M3** = $IE_{CCSD(T)} - IE_{M05\text{-}2X}$

Table S6: Comparison of the calculated interaction energy at MP2, B3LYP, and M05-2X from the corresponding CSSD(T) results. It also has shown the mean absolute value of the MP2, B3LYP, and M05-2X results from the corresponding CCSD(T) values. Energies in kcal/mol.

S. No.	Non-covalent	MP2	B3LYP	M05-2X	CCSD(T)	M1	M2	M3
1.	H_2O- H_2O	-6.11	-5.79	-6.47	-4.13	1.98	1.65	2.34
2.	NH_3 - NH_3	-3.80	-3.33	-3.94	-3.72	0.08	-0.39	0.22
3.	NH_3 - NH_4^+	-31.59	-32.00	-32.29	-30.86	0.73	1.14	1.43
4.	H_2O- NH_4^+	-22.17	-22.39	-22.76	-21.79	0.37	0.60	0.96
5.	H_2O-Li^+	-35.50	-36.55	-37.00	-35.34	0.16	1.21	1.66
6.	NH_3-Li^+	-40.84	-41.78	-42.06	-40.64	0.21	1.14	1.42
7.	C_2H_2-HCN	-2.77	-1.81	-2.62	-2.61	0.16	-0.80	0.01
8.	C_2H_2-HNC	-4.44	-3.09	-3.98	-3.92	0.52	-0.83	0.06
9.	NH_3-C_2H_4	-1.84	-0.59	-1.78	-1.74	0.10	-1.15	0.05
10.	CH_4-Bz	-2.66	0.79	-1.39	-2.32	0.34	-3.11	-0.93
11.	NH_3-Bz	-3.53	-0.21	-2.64	-3.17	0.36	-2.96	-0.53
12.	H_2O-CNBz	-6.90	-3.47	-5.91	-6.71	0.19	-3.24	-0.80
13.	Cl^--FBz	-18.55	-11.36	-15.59	-18.60	-0.05	-7.25	-3.01
14.	Li^+-Bz	-38.85	-38.91	-42.51	-38.35	0.50	0.56	4.16
15.	Bz-Bz	-7.45	4.26	-2.04	-5.00	2.45	-9.26	-2.96
16.	Pyridine-Bz	-7.98	3.65	-2.79	-5.51	2.47	-9.16	-2.72
17.	Li^+-C_2H_6	-16.50	-17.81	-18.38	-16.40	0.10	1.41	1.98
18.	Li^+-CH_4	-12.90	-13.82	-13.99	-12.84	0.06	0.98	1.15
19.	CH_3NH_2-I_2	-13.66	-11.44	-14.15	-11.75	1.91	-0.31	2.40
20.	$(CH_3)_3N$-I_2	-20.66	-12.74	-19.04	-17.16	3.30	-4.42	1.88
21.	C_2H_2-ClCN	-2.23	-1.09	-2.24	-2.05	0.18	-0.96	0.19
22.	H_3N-ClCN	-4.61	-4.37	-5.46	-4.55	0.06	-0.18	0.91
23.	LiH-$ClCF_3$	-3.24	-2.92	-3.60	-3.25	-0.01	-0.33	0.34
24.	C_2H_4-CH_3CN	-1.51	-0.02	-1.27	-1.46	0.05	-1.44	-0.18
25.	LiF-CH_3F	-4.49	-3.97	-5.49	-4.70	-0.21	-0.73	0.79
26.	H_2O-CH_3OH	-1.63	-0.78	-1.85	-1.70	-0.07	-0.92	0.16
27.	FH_2P- NH_2F	-6.31	-5.88	-7.58	-5.85	0.46	0.03	1.73
28.	FH_2P- NH_2Me	-9.99	-8.60	-11.56	-9.31	0.68	-0.72	2.24
29.	F(Me)S-NH_3	-5.78	-4.98	-7.08	-5.50	0.27	-0.52	1.58
30.	OH(Me)S-NH_3	-3.91	-2.48	-4.38	-3.84	0.07	-1.35	0.54
31.	$CN(H_3)Si$- $CN(H_3)Si$	-5.42	-3.67	-5.14	-5.09	0.33	-1.43	0.05
32.	$NC(H_3)Si$- $NC(H_3)Si$	-4.70	-3.25	-4.98	-4.62	0.08	-1.36	0.36
33.	C_2H_4-LiF	-10.24	-9.13	-10.22	-10.26	-0.01	-1.12	-0.03
34.	H_2O-LiF	-19.14	-18.55	-19.32	-19.23	-0.09	-0.68	0.09
35.	NH_3-LiF	-22.50	-21.73	-22.41	-22.62	-0.12	-0.90	-0.22
36.	He_2	-0.01	0.03	0.00	-0.01	0.00	-0.03	-0.01
37.	Ne_2	-0.13	-0.06	-v0.15	-0.15	-0.01	-0.09	0.00
38.	Ar_2	-0.16	0.11	-0.20	-0.16	0.00	-0.27	0.04
39.	Propen2	-2.13	0.95	-1.84	-2.13	0.00	-3.08	-0.29
40.	DHB-Me	-16.25	-12.57	-16.11	-16.09	0.15	-3.52	0.02
41.	DHB-Et	-16.27	-11.85	-15.75	-16.15	0.12	-4.31	-0.40
42.	HBeCHN(H)-Be(H)CHN(H)	-41.07	-38.80	-43.50	-40.70	0.36	-1.90	2.80
43.	FBeCHN(H)-Be(F)CHN(H)	-42.22	-39.79	-45.26	-42.33	-0.11	-2.55	2.92
	Mean Absolute Value					**0.45**	**1.86**	**1.08**

M1 = $IE_{CCSD(T)} - IE_{MP2;}$ **M2** = $IE_{CCSD(T)} - IE_{B3LYP;}$ **M3** = $IE_{CCSD(T)} - IE_{M05\text{-}2X}$

Table S7: Calculated interaction energy (kcal/mol) at MP2 and the available experimental values[142] of interaction energy for covalent, ionic, and non-covalent bonds. All values are in kcal/mol.

Systems	MP2	Exp
H_2	-100.82	-109.30
N_2	-375.55	-228.53
O_2	-116.91	-119.90
Cl_2	-43.08	-59.70
HF	-137.73	-140.90
HCl	-99.74	-106.54
ClF	-50.32	-58.34
LiH	-48.22	-58.02
NaH	-35.02	-49.0 + 4.6
KH	-30.27	- 44.3 + 3.5
Li^+-Bz	-38.85	-38.5 ± 3.2
Na^+-Bz	-23.98	-22.1 ± 1.4
K^+-Bz	-19.48	-17.5 ± 0.9
H_2O-Li^+	-35.50	-32.62 ± 3.3
NH_3-Bz	-3.53	-1.84 ± 0.12
Ne_2	-0.13	-0.08

Table S8(a): Contribution of interaction energy components (kcal/mol) at MP2/6-311++G** level using LMO-EDA approach for the covalent systems.

S. No.	Covalent	Electrostatic	Exchange	Repulsion	Polarization	Dispersion
1.	H_2	-1.13	0.00	0.00	-82.24	-17.44
2.	N_2	-311.89	-449.97	1208.73	-552.09	-108.71
3.	O_2	-142.35	-302.39	755.95	-282.58	-110.64
4.	Cl_2	-43.82	-110.38	238.27	-94.98	-28.49
5.	HF	-112.42	-226.46	570.43	-327.14	-39.13
6.	HCl	-65.99	-98.83	227.10	-137.62	-21.58
7.	FCl	-41.85	-121.28	272.60	-107.30	-48.48
8.	BH_3	-55.75	-39.07	88.77	-82.01	-16.65
9.	NH_3	-89.48	-172.66	382.71	-203.34	-27.23
10.	CH_4	-63.81	-76.54	161.15	-112.49	-21.57
11.	H_2O	-122.33	-242.30	597.50	-318.99	-33.45
12.	PH_3	-60.11	-80.95	175.35	-97.33	-16.24
13.	H_2S	-93.91	-200.61	473.33	-246.19	-18.14
14.	BCl_3	-155.37	-185.48	430.96	-176.68	-26.30
15.	NCl_3	-88.15	-176.36	389.40	-119.52	-37.08
16.	OCl_2	-60.50	-142.18	313.33	-100.92	-46.39
17.	PCl_3	-98.26	-162.36	358.73	-134.88	-23.63
18.	SCl_2	-65.05	-133.40	289.65	-110.25	-25.54
19.	CCl_4	-96.39	-163.17	359.25	-137.82	-30.60
20.	C_2H_6	-142.01	-180.23	381.03	-141.30	-28.08
21.	C_2H_4	-447.34	-667.79	1866.75	-928.95	-30.20
22.	C_2H_2	-454.01	-679.44	2002.73	-1047.60	-59.15
23.	CH_3OH	-195.50	-321.72	786.15	-332.59	-36.95
24.	CH_3SH	-115.84	-165.71	357.29	-128.26	-26.52

Table S8(b): Contribution of interaction energy components (%) at MP2/6-311++G** level using LMO-EDA approach for the covalent systems.

S. No.	Covalent	Electrostatic	Exchange	Polarization	Dispersion
1.	H_2	1.12	0.00	81.58	17.30
2.	N_2	21.92	31.63	38.81	7.64
3.	O_2	16.99	36.09	33.72	13.20
4.	Cl_2	15.78	39.75	34.21	10.26
5.	HF	15.94	32.12	46.39	5.55
6.	HCl	20.37	30.50	42.47	6.66
7.	FCl	13.12	38.03	33.65	15.20
8.	BH_3	28.81	20.19	42.39	8.61
9.	NH_3	18.16	35.04	41.27	5.53
10.	CH_4	23.25	27.89	40.99	7.86
11.	H_2O	17.06	33.79	44.49	4.66
12.	PH_3	23.61	31.79	38.22	6.38
13.	H_2S	16.80	35.90	44.05	3.25
14.	BCl_3	28.57	34.11	32.49	4.84
15.	NCl_3	20.93	41.88	28.38	8.81
16.	OCl_2	17.29	40.62	28.84	13.25
17.	PCl_3	23.44	38.74	32.18	5.64
18.	SCl_2	19.46	39.91	32.99	7.64
19.	CCl_4	22.52	38.13	32.20	7.15
20.	C_2H_6	28.89	36.66	28.74	5.71
21.	C_2H_4	21.57	32.19	44.78	1.46
22.	C_2H_2	20.27	30.33	46.76	2.64
23.	CH_3OH	22.05	36.28	37.51	4.17
24.	CH_3SH	26.55	37.98	29.40	6.08

Table S9 (a): Contribution of interaction energy components (kcal/mol) at MP2/6-311++G** level using LMO-EDA approach for the ionic systems.

S. No.	Ionic	Electrostatic	Exchange	Repulsion	Polarization	Dispersion
25.	NaCl	-143.83	-17.93	45.10	-10.69	-71.03
26.	LiH	-393.70	-12.53	40.37	-44.12	7.41
27.	NaH	-168.49	-26.91	68.69	-15.77	-0.97
25.	KH	-160.26	-41.54	96.02	-13.31	-3.13
29.	CaS	-359.40	-46.71	133.97	-222.90	-184.02
30.	AlN	-860.91	-12.74	48.03	-676.90	-159.89
31.	$MgCl_2$	-206.51	-28.59	77.14	-44.52	1.73
32.	MgH_2	-431.39	-30.46	75.82	-64.86	8.54
33.	CaH_2	-221.54	-60.97	145.20	-36.98	1.17

Table S9 (b): Contribution of interaction energy components (%) at MP2/6-311++G** level using LMO-EDA approach for the ionic systems.

S. No.	Ionic	Electrostatic	Exchange	Polarization	Dispersion
25.	NaCl	59.07	7.36	4.39	29.17
26.	LiH	88.88	2.83	9.96	-1.67
27.	NaH	79.42	12.69	7.43	0.46
25.	KH	73.43	19.03	6.10	1.43
29.	CaS	44.21	5.75	27.42	22.63
30.	AlN	50.33	0.74	39.57	9.35
31.	$MgCl_2$	74.31	10.29	16.02	-0.62
32.	MgH_2	83.25	5.88	12.52	-1.65
33.	CaH_2	69.60	19.15	11.62	-0.37

Table S10 (a): Contribution of interaction energy components (kcal/mol) at MP2/6-311++G** level using LMO-EDA approach for the coordinate systems.

S. No.	Systems	Electrostatic	Exchange	Repulsion	Polarization	Dispersion
34.	NH_3-BH_3	-80.40	-121.33	233.85	-65.81	-7.18
35.	NH_3-BF_3	-96.59	-110.87	232.14	-72.12	5.65
36.	PH_3-BH_3	-67.95	-142.92	271.17	-83.27	-11.11
37.	PH_3-AlH_3	-35.21	-49.22	93.19	-22.35	-2.01
38.	H_2S-BH_3	-46.17	-101.27	191.44	-53.33	-10.20
39.	H_2S-AlH_3	-26.67	-38.68	73.09	-17.10	-2.43
40.	CO-BH_3	-67.69	-148.25	291.17	-94.24	-14.66
41.	$(CH_3)NH_2$-BH_3	-88.62	-130.00	250.47	-70.11	-8.68
42.	HF-BH_3	-6.99	-10.87	19.61	-2.75	-1.27

Table S10 (b): Contribution of interaction energy components (%) at MP2/6-311++G** level using LMO-EDA approach for the coordinate systems.

S. No.	Systems	Electrostatic	Exchange	Polarization	Dispersion
34.	NH_3-BH_3	29.27	44.16	23.96	2.61
35.	NH_3-BF_3	35.26	40.47	26.33	-2.06
36.	PH_3-BH_3	22.26	46.82	27.28	3.64
37.	PH_3-AlH_3	32.37	45.24	20.54	1.85
38.	H_2S-BH_3	21.88	48.00	25.28	4.83
39.	H_2S-AlH_3	31.42	45.57	20.15	2.86
40.	CO-BH_3	20.84	45.64	29.01	4.51
41.	$(CH_3)NH_2$-BH_3	29.80	43.71	23.57	2.92
42.	HF-BH_3	31.95	49.68	12.57	5.80

Table S11 (a): Contribution of interaction energy components (kcal/mol) at MP2/6-311++G** level using LMO-EDA approach for the non-covalent systems.

S. No.	Non-covalent	Electrostatic	Exchange	Repulsion	Polarization	Dispersion
1.	H_2O-H_2O	-8.75	-8.46	15.23	-2.19	-0.29
2.	NH_3-NH_3	-5.69	-7.49	12.74	-1.47	-0.80
3.	NH_3-NH_4^+	-39.54	-38.99	77.49	-25.52	-2.57
4.	H_2O-NH_4^+	-26.41	-18.27	36.06	-10.88	-0.75
5.	H_2O-Li^+	-36.00	-5.75	16.96	-10.98	2.15
6.	NH_3-Li^+	-43.10	-7.69	23.28	-13.01	1.52
7.	C_2H_2-HCN	-3.34	-3.68	6.60	-1.04	-0.36
8.	C_2H_2-HNC	-5.37	-6.76	12.47	-2.33	-1.27
9.	NH_3-C_2H_4	-2.03	-3.53	5.89	-0.41	-0.95
10.	CH_4-Bz	-1.13	-5.32	8.23	-0.35	-2.29
11.	NH_3-Bz	-2.11	-5.46	8.77	-0.60	-2.20
12.	H_2O-CNBz	-5.43	-6.28	10.21	-0.96	-1.75
13.	Cl^--FBz	-20.48	-26.25	43.09	-6.48	-2.48
14.	Li^+-Bz	-18.92	-6.22	18.14	-31.96	-3.13
15.	Bz-Bz	-4.09	-21.13	33.66	-1.38	-9.79
16.	Pyridine-Bz	-5.05	-21.11	33.99	-1.44	-9.77
17.	Li^+-C_2H_6	-3.59	-3.74	10.98	-18.87	-0.56
18.	Li^+-CH_4	-4.44	-2.89	8.63	-13.08	-0.49
19.	CH_3NH_2-I_2	-58.59	-49.03	94.93	-23.66	-3.49
20.	$(CH_3)_3N$-I_2	-74.32	-79.26	152.18	-30.51	-9.42
21.	C_2H_2-ClCN	-2.57	-3.65	6.39	-0.57	-0.78
22.	H_3N-ClCN	-6.99	-7.01	12.45	-1.48	-0.38
23.	LiH-$ClCF_3$	-5.38	-6.68	11.61	-1.53	-0.68
24.	C_2H_4-CH_3CN	-1.20	-2.42	3.97	-0.20	-0.92
25.	LiF-CH_3F	-5.79	-4.18	6.94	-1.12	0.36
26.	H_2O-CH_3OH	-1.60	-2.43	3.94	-0.30	-0.42
27.	FH_2P- NH_2F	-14.00	-21.91	38.94	-5.02	-2.40
28.	FH_2P- NH_2Me	-24.61	-39.11	70.52	-10.71	-3.48
29.	F(Me)S-NH_3	-11.45	-16.61	28.72	-3.47	-1.34
30.	OH(Me)S-NH_3	-5.33	-7.52	12.44	-1.07	-1.09
31.	$CN(H_3)Si$- $CN(H_3)Si$	-7.79	-11.92	20.23	-2.44	-2.75
32.	$NC(H_3)Si$- $NC(H_3)Si$	-6.24	-7.24	12.24	-1.59	-0.94
33.	C_2H_4-LiF	-10.57	-3.95	10.82	-5.01	0.77
34.	H_2O-LiF	-21.07	-4.43	11.94	-4.37	1.71
35.	NH_3-LiF	-26.73	-6.49	17.83	-5.39	1.34
36.	He_2	0.00	0.00	0.01	0.00	0.00
37.	Ne_2	-0.01	-0.06	0.12	0.00	0.00
38.	Ar_2	-0.03	-0.20	0.32	0.00	-0.06
39.	Propen2	-0.77	-4.23	6.65	-0.21	-2.58
40.	DHB-Me	-19.86	-23.68	40.91	-6.29	-5.43
41.	DHB-Et	-19.46	-24.11	41.46	-6.22	-5.78
42.	HBeCHN(H)-Be(H)CHN(H)	-63.16	-65.08	125.90	-34.93	0.10
43.	FBeCHN(H)-Be(F)CHN(H)	-60.58	-54.12	108.66	-34.27	2.96

Table S11 (b): Contribution of interaction energy components (in %) at MP2/6-311++G** level using LMO-EDA approach for the non-covalent systems.

S. No.	Non-covalent	Electrostatic	Exchange	Polarization	Dispersion
1.	H_2O-H_2O	44.44	42.97	11.12	1.47
2.	NH_3 - NH_3	36.83	48.48	9.51	5.18
3.	NH_3 - NH_4^+	37.08	36.57	23.94	2.41
4.	H_2O- NH_4^+	46.90	32.45	19.32	1.33
5.	H_2O-Li^+	71.17	11.37	21.71	-4.25
6.	NH_3-Li^+	69.20	12.35	20.89	-2.44
7.	C_2H_2-HCN	39.67	43.71	12.35	4.28
8.	C_2H_2-HNC	34.14	42.98	14.81	8.07
9.	NH_3-C_2H_4	29.34	51.01	5.92	13.73
10.	CH_4-Bz	12.43	58.53	3.85	25.19
11.	NH_3-Bz	20.35	52.65	5.79	21.22
12.	H_2O-CNBz	37.66	43.55	6.66	12.14
13.	Cl^--FBz	36.78	47.14	11.64	4.45
14.	Li^+-Bz	31.41	10.33	53.06	5.20
15.	Bz-Bz	11.24	58.07	3.79	26.90
16.	Pyridine-Bz	13.51	56.49	3.85	26.14
17.	Li^+-C_2H_6	13.42	13.98	70.52	2.09
18.	Li^+-CH_4	21.24	13.83	62.58	2.34
19.	CH_3NH_2-I_2	43.47	36.38	17.56	2.59
20.	$(CH_3)_3N$-I_2	38.41	40.96	15.77	4.87
21.	C_2H_2-ClCN	33.95	48.22	7.53	10.30
22.	H_3N-ClCN	44.07	44.20	9.33	2.40
23.	LiH-$ClCF_3$	37.70	46.81	10.72	4.77
24.	C_2H_4-CH_3CN	25.32	51.05	4.22	19.41
25.	LiF-CH_3F	53.96	38.96	10.44	-3.36
26.	H_2O-CH_3OH	33.68	51.16	6.32	8.84
27.	FH_2P- NH_2F	32.31	50.57	11.59	5.54
28.	FH_2P- NH_2Me	31.59	50.20	13.75	4.47
29.	F(Me)S-NH_3	34.83	50.53	10.56	4.08
30.	OH(Me)S-NH_3	35.51	50.10	7.13	7.26
31.	$CN(H_3)Si$- $CN(H_3)Si$	31.29	47.87	9.80	11.04
32.	$NC(H_3)Si$- $NC(H_3)Si$	38.98	45.22	9.93	5.87
33.	C_2H_4-LiF	56.34	21.06	26.71	-4.10
34.	H_2O-LiF	74.82	15.73	15.52	-6.07
35.	NH_3-LiF	71.72	17.41	14.46	-3.60
36.	He_2	0.00	0.00	0.00	0.00
37.	Ne_2	14.29	85.71	0.00	0.00
38.	Ar_2	10.34	68.97	0.00	20.69
39.	Propen2	9.88	54.30	2.70	33.12
40.	DHB-Me	35.94	42.85	11.38	9.83
41.	DHB-Et	35.02	43.39	11.19	10.40
42.	HBeCHN(H)-Be(H)CHN(H)	38.73	39.91	21.42	-0.06
43.	FBeCHN(H)-Be(F)CHN(H)	41.49	37.07	23.47	-2.03

Table S11 (c): SAPT energy (kcal/mol) calculations at SAPT2+3(CCD)dmp2 using 6-311++G** basis set are carried out with PSI4 for the non-covalent systems.

S. No.	Non-covalent	Electrostatic	Exchange	Polarization	Dispersion
1.	H_2O-H_2O	-8.75	6.70	-2.09	-1.32
2.	NH_3 - NH_3	-5.69	5.19	-1.40	-1.25
3.	NH_3 - NH_4^+	-39.54	37.48	-23.08	-4.74
4.	H_2O- NH_4^+	-26.42	17.55	-10.40	-2.63
5.	H_2O-Li^+	-35.97	11.15	-10.85	-0.32
6.	NH_3-Li^+	-43.07	15.53	-12.71	-0.35
7.	C_2H_2-HCN	-3.34	2.90	-1.02	-1.06
8.	C_2H_2-HNC	-5.38	5.67	-2.24	-1.66
9.	NH_3-C_2H_4	-2.03	2.35	-0.40	-1.15
10.	CH_4-Bz	-1.13	2.88	-0.33	-2.50
11.	NH_3-Bz	-2.11	3.28	-0.57	-2.56
12.	H_2O-CNBz*	-5.42	3.90	-0.92	-2.87
13.	Cl^--FBz*	-20.54	16.48	-5.45	-5.28
14.	Li^+-Bz	-18.94	11.94	-31.72	-0.73
15.	Bz-Bz*	-4.11	12.37	-1.11	-9.76
16.	Pyridine-Bz*	-5.08	12.71	-1.17	-9.87
17.	Li^+-C_2H_6	-3.58	7.25	-18.80	-0.40
18.	Li^+-CH_4	-4.45	5.73	-13.03	-0.27
19.	CH_3NH_2-I_2	-	-	-	-
20.	$(CH_3)_3N$-I_2	-	-	-	-
21.	C_2H_2-ClCN	-2.58	2.73	-0.53	-1.12
22.	H_3N-ClCN	-7.01	5.41	-1.34	-1.24
23.	LiH-$ClCF_3$	-5.40	4.90	-1.33	-1.04
24.	C_2H_4-CH_3CN	-1.20	1.54	-0.19	-1.12
25.	LiF-CH_3F	-5.79	2.74	-1.09	-0.81
26.	H_2O-CH_3OH	-1.60	1.50	-0.29	-0.74
27.	FH_2P- NH_2F	-14.02	16.74	-4.07	-3.17
28.	FH_2P- NH_2Me	-24.63	30.56	-7.49	-5.34
29.	F(Me)S-NH_3	-11.46	11.94	-2.94	-2.73
30.	OH(Me)S-NH_3	-5.33	4.87	-0.99	-1.79
31.	$CN(H_3)Si$- $CN(H_3)Si$	-7.79	8.20	-2.17	-2.27
32.	$NC(H_3)Si$- $NC(H_3)Si$	-6.24	4.95	-1.52	-1.91
33.	C_2H_4-LiF	-10.56	6.89	-4.89	-0.62
34.	H_2O-LiF	-21.02	7.37	-4.29	-0.48
35.	NH_3-LiF	-26.67	11.19	-5.20	-0.60
36.	He_2	-0.003	0.004	0.001	-0.005
37.	Ne_2	-0.012	0.057	0.000	-0.016
38.	Ar_2	-0.035	0.120	-0.004	-0.074
39.	Propen2	-0.77	2.41	-0.20	-2.78
40.	DHB-Me	-19.87	16.97	-5.90	-6.26
41.	DHB-Et	-19.47	17.08	-5.83	-6.77
42.	HBeCHN(H)-Be(H)CHN(H)	-62.85	58.68	-26.39	-9.55
43.	FBeCHN(H)-Be(F)CHN(H)	-60.33	53.00	-27.93	-8.27

*Manyany-body treatments of dispersion on coupled-cluster doubles (CCD) method and δMP2 corrections using dmp2 are not done.
SAPT2+3(CCD)dmp2 energetics for CH_3NH_2-I_2 and $(CH_3)_3N$-I_2 is not obtained with PSI4 package using DGDZVP basis set for iodine.

Table S12: The variation of electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), H(**r**), and [-G(**r**)/V(**r**)] as obtained at a bond critical point for the covalent bonds, obtained at MP2, B3LYP, and M05-2X using 6-311++G** basis set. These all values are given in a.u.

S. No.	Covalent	ρ			$\nabla^2\rho$			H(r)			G(r)/v(r)		
		MP2	**B3LYP**	**M05-2X**	**MP2**	**B3LYP**	**M05-2X**	**MP2**	**B3LYP**	**M05-2X**	**MP2**	**B3LYP**	**M05-2X**
1.	H_2	0.2636	0.2648	0.2663	-1.0742	-1.0846	-1.1020	-0.2743	-0.2711	-0.2755	0.0205	0.0000	0.0000
2.	N_2	0.6372	0.6433	0.6484	-2.1834	-2.2471	-2.3203	-1.1030	-1.0963	-1.1161	0.3356	0.3278	0.3244
3.	O_2	0.5096	0.5141	0.5165	-0.5499	-0.6409	-0.6914	-0.6181	-0.6006	-0.6132	0.4374	0.4230	0.4180
4.	Cl_2	0.1424	0.1426	0.1437	-0.0035	0.0060	-0.0069	-0.0648	-0.0603	-0.0624	0.4966	0.5061	0.4930
5.	HF	0.3704	0.3757	0.3719	-2.8355	-2.8776	-2.8791	-0.8039	-0.8052	-0.8039	0.1057	0.0962	0.0947
6.	HCl	0.2487	0.2494	0.2503	-0.7106	-0.7032	-0.7289	-0.2381	-0.2310	-0.2353	0.2024	0.1928	0.1841
7.	FCl	0.1809	0.1846	0.1859	0.0634	0.0514	0.0126	-0.1155	-0.1131	-0.1223	0.5321	0.5269	0.5064
8.	BH_3	0.1807	0.1840	0.1856	-0.2530	-0.3432	-0.3408	-0.1950	-0.1968	-0.2014	0.4032	0.3606	0.3659
9.	NH_3	0.3335	0.3361	0.3357	-1.5289	-1.4832	-1.5089	-0.4510	-0.4320	-0.4374	0.1323	0.1241	0.1209
10.	CH_4	0.2719	0.2724	0.2730	-0.9106	-0.9003	-0.9176	-0.2765	-0.2687	-0.2723	0.1502	0.1397	0.1360
11.	H_2O	0.3646	0.3695	0.3674	-2.5173	-2.5234	-2.5377	-0.7133	-0.7074	-0.7092	0.1053	0.0977	0.0953
12.	PH_3	0.1619	0.1639	0.1643	0.0623	-0.0295	-0.0095	-0.1564	-0.1587	-0.1601	0.5237	0.4881	0.4963
13.	H_2S	0.2181	0.2184	0.2194	-0.6744	-0.6565	-0.6711	-0.2324	-0.2194	-0.2214	0.2154	0.2013	0.1950
14.	BCl_3	0.1529	0.1549	0.1552	0.0036	-0.0496	-0.0434	-0.1470	-0.1464	-0.1472	0.5015	0.4779	0.4809
15.	NCl_3	0.1872	0.1886	0.1896	-0.0904	-0.0859	-0.1098	-0.1179	-0.1121	-0.1149	0.4470	0.4470	0.4322
16.	OCl_2	0.1816	0.1850	0.1858	0.0116	0.0009	-0.0275	-0.1109	-0.1084	-0.1133	0.5064	0.5005	0.4843
17.	PCl_3	0.1292	0.1298	0.1295	-0.1980	-0.1784	-0.1867	-0.1067	-0.0975	-0.1014	0.3491	0.3518	0.3505
18.	SCl_2	0.1395	0.1397	0.1404	-0.0641	-0.0532	-0.0663	-0.0729	-0.0691	-0.0711	0.4382	0.4468	0.4340
19.	CCl_4	0.1953	0.1947	0.1958	-0.2452	-0.2326	-0.2506	-0.1338	-0.1253	-0.1279	0.3515	0.3490	0.3379
20.	C_2H_6	0.2393	0.2383	0.2369	-0.5557	-0.5339	-0.5294	-0.2001	-0.1881	-0.1869	0.2341	0.2250	0.2260
21.	C_2H_4	0.3346	0.3371	0.3371	-0.9757	-0.9859	-0.9963	-0.3862	-0.3795	-0.3811	0.2692	0.2596	0.2573
22.	C_2H_2	0.3896	0.3979	0.4016	-1.0922	-1.1510	-1.2129	-0.5478	-0.5553	-0.5672	0.3340	0.3252	0.3176
23.	CH_3OH	0.2509	0.2532	0.2511	-0.4171	-0.4701	-0.4219	-0.3434	-0.3308	-0.3328	0.4105	0.3920	0.4058
24.	CH_3SH	0.1794	0.1786	0.1784	-0.2963	-0.2787	-0.2814	-0.1254	-0.1171	-0.1173	0.2905	0.2883	0.2858

Table S13: The variation of electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), H(**r**), and [-G(**r**)/V(**r**)] as obtained at a bond critical point for the ionic and coordinate bonds, obtained at MP2, B3LYP and M05-2X using 6-311++G** basis set. These all values are given in a.u.

S. No.	Ionic	ρ			$\nabla^2\rho$			H(r)			G(r)/v(r)		
		MP2	**B3LYP**	**M05-2X**	**MP2**	**B3LYP**	**M05-2X**	**MP2**	**B3LYP**	**M05-2X**	**MP2**	**B3LYP**	**M05-2X**
25.	NaCl	0.0325	0.0332	0.0336	0.1903	0.1815	0.1832	0.0047	0.0043	0.0040	1.1242	1.1172	1.1048
26.	LiH	0.0392	0.0393	0.0384	0.1665	0.1594	0.0000	-0.0001	-0.0002	0.0004	0.9981	0.9939	1.0108
27.	NaH	0.0314	0.0317	0.0313	0.1314	0.1229	0.1616	0.0014	0.0015	0.0015	1.0481	1.0524	1.0528
28.	KH	0.0295	0.0299	0.0294	0.0803	0.0752	0.2209	-0.0010	-0.0008	-0.0008	0.9562	0.9588	0.9621
29.	CaS	0.0634	0.0672	0.0679	0.2036	0.2032	0.1116	-0.0107	-0.0112	-0.0123	0.8516	0.8472	0.8350
30.	AlN	0.1093	0.1012	0.0985	0.8412	0.7940	0.2004	-0.0176	-0.0111	-0.0106	0.9284	0.9498	0.9515
31.	$MgCl_2$	0.0522	0.0534	0.0534	0.3089	0.2936	0.2954	0.0020	0.0010	0.0008	1.0269	1.0137	1.0110
32.	MgH_2	0.0521	0.0531	0.0522	0.2346	0.2178	0.1229	-0.0026	-0.0033	-0.0027	0.9599	0.9462	0.9556
33.	CaH_2	0.0454	0.0470	0.0457	0.1207	0.1083	0.0754	-0.0058	-0.0061	-0.0056	0.8619	0.8443	0.8565
	Coordinate												
34.	NH_3-BH_3	0.0987	0.1010	0.0991	0.4777	0.4278	0.4608	-0.0550	-0.0584	-0.0550	0.7602	0.7390	0.7558
35.	NH_3-BF_3	0.1090	0.1132	0.1107	0.2750	0.1911	0.2275	-0.0778	-0.0841	-0.0796	0.6533	0.6106	0.6316
36.	PH_3-BH_3	0.1025	0.1036	0.1017	0.1212	0.0659	0.0978	-0.0819	-0.0818	-0.0791	0.5781	0.5457	0.5669
37.	PH_3-AlH_3	0.0327	0.0343	0.0339	0.0910	0.0783	0.0815	-0.0063	-0.0074	-0.0072	0.8219	0.7844	0.7934
38.	H_2S-BH_3	0.0765	0.0779	0.0760	0.1829	0.1325	0.1683	-0.0526	-0.0534	-0.0509	0.6515	0.6183	0.6463
39.	H_2S-AlH_3	0.0286	0.0303	0.0300	0.0871	0.0762	0.0795	-0.0043	-0.0055	-0.0052	0.8581	0.8179	0.8272
40.	CO-BH_3	0.1288	0.1328	0.1293	0.5631	0.4952	0.5305	-0.0889	-0.0951	-0.0896	0.7210	0.6971	0.7126
41.	$(CH_3)NH_2$-BH_3	0.1057	0.1081	0.1061	0.4801	0.4285	0.4623	-0.0630	-0.0664	-0.0627	0.7439	0.7233	0.7397
42.	HF-BH_3	0.0186	0.0193	0.0190	0.0626	0.0602	0.0634	-0.0012	-0.0013	-0.0012	0.9340	0.9280	0.9337

Table S14: The variation of electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), H(**r**), and [-G(**r**)/V(**r**)] as obtained at a critical point for the non-covalent bonds, obtained at MP2, B3LYP and M05-2X using 6-311++G** basis set. These all values are given in a.u.

S. No.	Non-covalent	ρ			$\nabla^2\rho$			H(r)			G(r)/v(r)		
		MP2	B3LYP	M05-2X	MP2	B3LYP	M05-2X	MP2	B3LYP	M052X	MP2	B3LYP	M05-2X
1.	H_2O-H_2O	0.0231	0.0236	0.0228	0.0911	0.0898	0.0937	0.0023	0.0025	0.0028	1.1285	1.1449	1.1590
2.	NH_3-NH_3	0.0158	0.0160	0.0157	0.0489	0.0478	0.0500	0.0015	0.0017	0.0018	1.1674	1.2003	1.2050
3.	NH_3-NH_4^+	0.0420	0.0780	0.0774	0.0915	0.0619	0.0584	-0.0060	-0.0295	-0.0302	0.8280	0.6038	0.5974
4.	H_2O-NH_4^+	0.0484	0.0497	0.0487	0.1454	0.1428	0.1470	-0.0064	-0.0061	-0.0060	0.8700	0.8726	0.8767
5.	H_2O-Li^+	0.0328	0.0336	0.0336	0.2652	0.2598	0.2644	0.0124	0.0121	0.0122	1.2999	1.2954	1.2923
6.	NH_3-Li^+	0.0321	0.0329	0.0328	0.2001	0.1934	0.1968	0.0071	0.0066	0.0067	1.1998	1.1874	1.1862
7.	C_2H_2-HCN	0.0080	0.0082	0.0081	0.0230	0.0223	0.0222	0.0012	0.0013	0.0013	1.3809	1.4418	1.4324
8.	C_2H_2-HNC	0.0133	0.0138	0.0135	0.0415	0.0405	0.0420	0.0024	0.0024	0.0025	1.4162	1.4579	1.4674
9.	NH_3-C_2H_4	0.0064	0.0065	0.0065	0.0192	0.0186	0.0189	0.0009	0.0009	0.0009	1.2862	1.3287	1.2965
10.	CH_4-Bz	0.0047	0.0046	0.0048	0.0190	0.0186	0.0187	0.0007	0.0007	0.0006	1.2074	1.2322	1.1913
11.	NH_3-Bz	0.0049	0.0048	0.0050	0.0193	0.0190	0.0190	0.0007	0.0008	0.0007	1.2113	1.2444	1.2057
12.	H_2O-CNBz	0.0051	0.0049	0.0053	0.0237	0.0232	0.0241	0.0010	0.0011	0.0010	1.2624	1.3001	1.2575
13.	Cl^--FBz	0.0068	0.0065	0.0070	0.0279	0.0279	0.0282	0.0013	0.0014	0.0012	1.2806	1.3223	1.2712
14.	Li^+-Bz	0.0131	0.0132	0.0138	0.0711	0.0697	0.0718	0.0019	0.0020	0.0017	1.1351	1.1493	1.1177
15.	Bz-Bz	0.0040	0.0038	0.0075	0.0145	0.0143	0.0198	0.0005	0.0006	0.0008	1.1922	1.2258	1.2276
16.	Pyridine-Bz	0.0043	0.0041	0.0044	0.0158	0.0156	0.0164	0.0006	0.0006	0.0006	1.1957	1.2307	1.1976
17.	Li^+-C_2H_6	0.0188	0.0195	0.0198	0.1239	0.1186	0.1216	0.0050	0.0046	0.0045	1.2358	1.2215	1.2124
18.	Li^+-CH_4	0.0181	0.0189	0.0190	0.1151	0.1103	0.1131	0.0047	0.0043	0.0043	1.2440	1.2251	1.2211
19.	CH_3NH_2-I_2	0.0402	0.0406	0.0403	0.0915	0.0912	0.0908	-0.0037	-0.0031	-0.0036	0.8784	0.8943	0.8805
20.	$(CH_3)_3N$-I_2	0.0492	0.0490	0.0492	0.0979	0.1004	0.0972	-0.0071	-0.0060	-0.0070	0.8168	0.8391	0.8172
21.	C_2H_2-ClCN	0.0060	0.0062	0.0063	0.0220	0.0216	0.0219	0.0013	0.0012	0.0012	1.4216	1.4293	1.3968
22.	H_3N-ClCN	0.0127	0.0129	0.0130	0.0456	0.0442	0.0451	0.0014	0.0014	0.0013	1.1590	1.1770	1.1529
23.	LiH-$ClCF_3$	0.0083	0.0084	0.0086	0.0255	0.0239	0.0234	0.0009	0.0009	0.0008	1.2123	1.2265	1.1844
24.	C_2H_4-CH_3CN	0.0035	0.0036	0.0037	0.0110	0.0108	0.0112	0.0006	0.0006	0.0006	1.3785	1.3959	1.3720
25.	LiF-CH_3F	0.0087	0.0088	0.0089	0.0452	0.0441	0.0454	0.0017	0.0017	0.0018	1.2220	1.2313	1.2247
26.	H_2O-CH_3OH	0.0060	0.0061	0.0062	0.0295	0.0290	0.0298	0.0014	0.0014	0.0014	1.3102	1.3219	1.3102
27.	FH_2P-NH_2F	0.0238	0.0245	0.0240	0.0620	0.0606	0.0628	-0.0003	0.0000	-0.0001	0.9835	0.9991	0.9921
28.	FH_2P-NH_2Me	0.0319	0.0329	0.0326	0.0691	0.0676	0.0690	-0.0024	-0.0021	-0.0025	0.8896	0.9015	0.8884
29.	F(Me)S-NH_3	0.0181	0.0185	0.0184	0.0536	0.0520	0.0535	0.0007	0.0009	0.0007	1.0558	1.0802	1.0607
30.	OH(Me)S-NH_3	0.0086	0.0087	0.0088	0.0281	0.0274	0.0281	0.0008	0.0009	0.0008	1.1437	1.1648	1.1446
31.	$CN(H_3)Si$-$CN(H_3)Si$	0.0114	0.0118	0.0117	0.0305	0.0301	0.0308	0.0007	0.0008	0.0007	1.1046	1.1302	1.1064
32.	$NC(H_3)Si$-$NC(H_3)Si$	0.0096	0.0099	0.0099	0.0290	0.0290	0.0296	0.0008	0.0009	0.0008	1.1350	1.1628	1.1400
33.	C_2H_4-LiF	0.0135	0.0140	0.0143	0.0575	0.0547	0.0567	0.0021	0.0020	0.0019	1.2111	1.1999	1.1860

34.	H_2O-LiF	0.0250	0.0257	0.0256	0.1902	0.1861	0.1900	0.0090	0.0087	0.0089	1.3054	1.3005	1.3009
35.	H_3N-LiF	0.0253	0.0259	0.0259	0.1544	0.1491	0.1521	0.0060	0.0056	0.0057	1.2239	1.2150	1.2148
36.	He_2	0.0003	0.0004	0.0004	0.0022	0.0023	0.0023	0.0002	0.0002	0.0002	1.7650	1.7636	1.7593
37.	Ne_2	0.0017	0.0019	0.0017	0.0144	0.0143	0.0144	0.0010	0.0010	0.0010	1.6648	1.6568	1.6793
38.	Ar_2	0.0015	0.0016	0.0016	0.0058	0.0058	0.0059	0.0004	0.0004	0.0004	1.6533	1.6377	1.6184
39.	$Propane_2$	0.0040	0.0038	0.0039	0.0139	0.0122	0.0122	0.0006	0.0005	0.0005	1.2726	1.2743	1.2373
40.	DHB-Me	0.0169	0.0172	0.0169	0.0492	0.0472	0.0488	0.0013	0.0014	0.0015	1.1311	1.1602	1.1601
41.	DHB-Et	0.0172	0.0169	0.0166	0.0491	0.0464	0.0479	0.0013	0.0015	0.0015	1.1299	1.1673	1.1728
42.	HBeCHN(H)-Be(H)CHN(H)	0.0593	0.0613	0.0606	0.3860	0.3644	0.3722	-0.0007	-0.0030	-0.0021	0.9928	0.9691	0.9782
43.	FBeCHN(H)-Be(F)CHN(H)	0.0583	0.0603	0.0594	0.3610	0.3377	0.3472	-0.0020	-0.0045	-0.0032	0.9790	0.9521	0.9661

Table S15: The variation of the absolute value of kinetic energy density G(**r**) and potential energy density V(**r**) at a critical point for the covalent, ionic, and coordinate bonds, obtained at MP2/6-311++G** level of theory. These all values are given in a.u.

S. No.	Covalent	G(r)	V(r)
1.	H_2	0.0057	-0.2801
2.	N_2	0.5571	-1.6601
3.	O_2	0.4806	-1.0988
4.	Cl_2	0.0639	-0.1287
5.	HF	0.0950	-0.8989
6.	HCl	0.0604	-0.2985
7.	FCl	0.1313	-0.2468
8.	BH_3	0.1317	-0.3267
9.	NH_3	0.0688	-0.5198
10.	CH_4	0.0489	-0.3254
11.	H_2O	0.0839	-0.7972
12.	PH_3	0.1719	-0.3283
13.	H_2S	0.0638	-0.2962
14.	BCl_3	0.1479	-0.2949
15.	NCl_3	0.0953	-0.2133
16.	OCl_2	0.1138	-0.2248
17.	PCl_3	0.0572	-0.1640
18.	SCl_2	0.0568	-0.1297
19.	CCl_4	0.0725	-0.2064
20.	C_2H_6	0.0611	-0.2612
21.	C_2H_4	0.1423	-0.5285
22.	C_2H_2	0.2747	-0.8225
23.	CH_3OH	0.2391	-0.5825
24.	CH_3SH	0.0514	-0.1768
	Ionic		
25.	NaCl	0.0428	-0.0381
26.	LiH	0.0417	-0.0418
27.	NaH	0.0314	-0.0300
25.	KH	0.0210	-0.0220
29.	CaS	0.0616	-0.0724
30.	AlN	0.2279	-0.2455
31.	$MgCl_2$	0.0753	-0.0733
32.	MgH_2	0.0612	-0.0638
33.	CaH_2	0.0359	-0.0417
	Coordinate		
34.	NH_3BH_3	0.1745	-0.2295
35.	NH_3BF_3	0.1465	-0.2243
36.	PH_3BH_3	0.1122	-0.1940
37.	PH_3AlH_3	0.0290	-0.0353
38.	H_2SBH_3	0.0983	-0.1509
39.	H_2SAlH_3	0.0261	-0.0304
40.	$CO\text{-}BH_3$	0.2296	-0.3185
41.	$(CH_3)NH_2BH_3$	0.2296	-0.3185
42.	$HFBH_3$	0.1830	-0.2461

Table S16: The variation of kinetic energy density G(**r**) and potential energy density V(**r**) at a critical point for the non-covalent, obtained at MP2/6-311++G** level of theory. These all values are given in a.u.

S. No.	Non-covalent	G(r)	V(r)	S. No.	Non-covalent	G(r)	V(r)
1.	H_2O-H_2O	0.0205	0.0181	23.	LiH-$ClCF_3$	0.0054	-0.0045
2.	NH_3-NH_3	0.0107	0.0092	24.	C_2H_4-CH_3CN	0.0022	-0.0016
3.	$NH_3NH_4^+$	0.0289	0.0349	25.	LiF-CH_3F	0.0096	-0.0078
4.	$H_2ONH_4^+$	0.0427	0.0491	26.	H_2O-CH_3OH	0.0060	-0.0046
5.	H_2O-Li^+	0.0539	0.0414	27.	FH_2P-NH_2F	0.0158	-0.0160
6.	NH_3-Li^+	0.0429	0.0357	28.	FH_2P-NH_2Me	0.0197	-0.0222
7.	C_2H_2HCN	0.0045	0.0033	29.	F(Me)S-NH_3	0.0127	-0.0121
8.	C_2H_2HNC	0.0080	0.0057	30.	OH(Me)S-NH_3	0.0062	-0.0054
9.	NH_3-C_2H_4	0.0039	0.0031	31.	$CN(H_3)Si$-$CN(H_3)Si$	0.0070	-0.0063
10.	CH_4-Bz	0.0041	0.0034	32.	$NC(H_3)Si$-$NC(H_3)Si$	0.0065	-0.0057
11.	NH_3-Bz	0.0041	0.0034	33.	C_2H_4-LiF	0.0122	-0.0101
12.	H_2O-CNBz	0.0049	0.0039	34.	H_2O-LiF	0.0385	-0.0295
13.	Cl^--FBz	0.0057	0.0045	35.	H_3N-LiF	0.0326	-0.0267
14.	Li^+-Bz	0.0159	0.0140	36.	He_2	0.0004	-0.0002
15.	Bz-Bz	0.0031	0.0026	37.	Ne_2	0.0026	-0.0015
16.	Pyridine-Bz	0.0034	0.0028	38.	Ar_2	0.0010	-0.0006
17.	$Li^+C_2H_6$	0.0260	0.0210	39.	$Propane_2$	0.0029	-0.0023
18.	Li^+-CH_4	0.0241	0.0193	40.	DHB-Me	0.0110	-0.0097
19.	CH_3NH_2-I_2	0.0266	0.0302	41.	DHB-Et	0.0110	-0.0098
20.	$(CH_3)_3N$-I_2	0.0316	0.0386	42.	HBeCHN(H)-Be(H)CHN(H)	0.0972	-0.0979
21.	C_2H_2-ClCN	0.0042	0.0030	43.	FBeCHN(H)-Be(F)CHN(H)	0.0922	-0.0942
22.	H_3N-ClCN	0.0100	0.0087				

Table S17. The SAPT interaction energy decomposes intoelectrostatics (elst), exchange (exch), induction (ind), and dispersion (disp)components. The subscript "resp" denotes that the orbital response of the perturbed system is taken into account. The superscripts refer to the orders of the interaction and Møller-Plesset fluctuation potential operators.

SAPT0	$E_{SAPT0} = E_{elst}^{(10)} + E_{exch}^{(10)} + E_{ind,resp}^{(20)} + E_{exch-ind,resp}^{(20)} + E_{disp}^{(20)} + E_{exch-disp}^{(20)}$
SAPT2	$E_{SAPT2} = E_{SAPT0} + E_{elst,resp}^{(12)} + E_{exch}^{(11)} + E_{exch}^{(12)} + {}^{t}E_{ind}^{(22)} + {}^{t}E_{exch-ind}^{(22)}$
SAPT2+	$E_{SAPT2+} = E_{SAPT2} + E_{disp}^{(21)} + E_{disp}^{(22)}$
SAPT2+(3)	$E_{SAPT2+(3)} = E_{SAPT2+} + E_{elst,resp}^{(13)} + E_{disp}^{(30)}$
SAPT2+3	$E_{SAPT2+3} = E_{SAPT2+(3)} + E_{exch-disp}^{(30)} + E_{ind-disp}^{(30)} + E_{exch-ind-disp}^{(30)}$

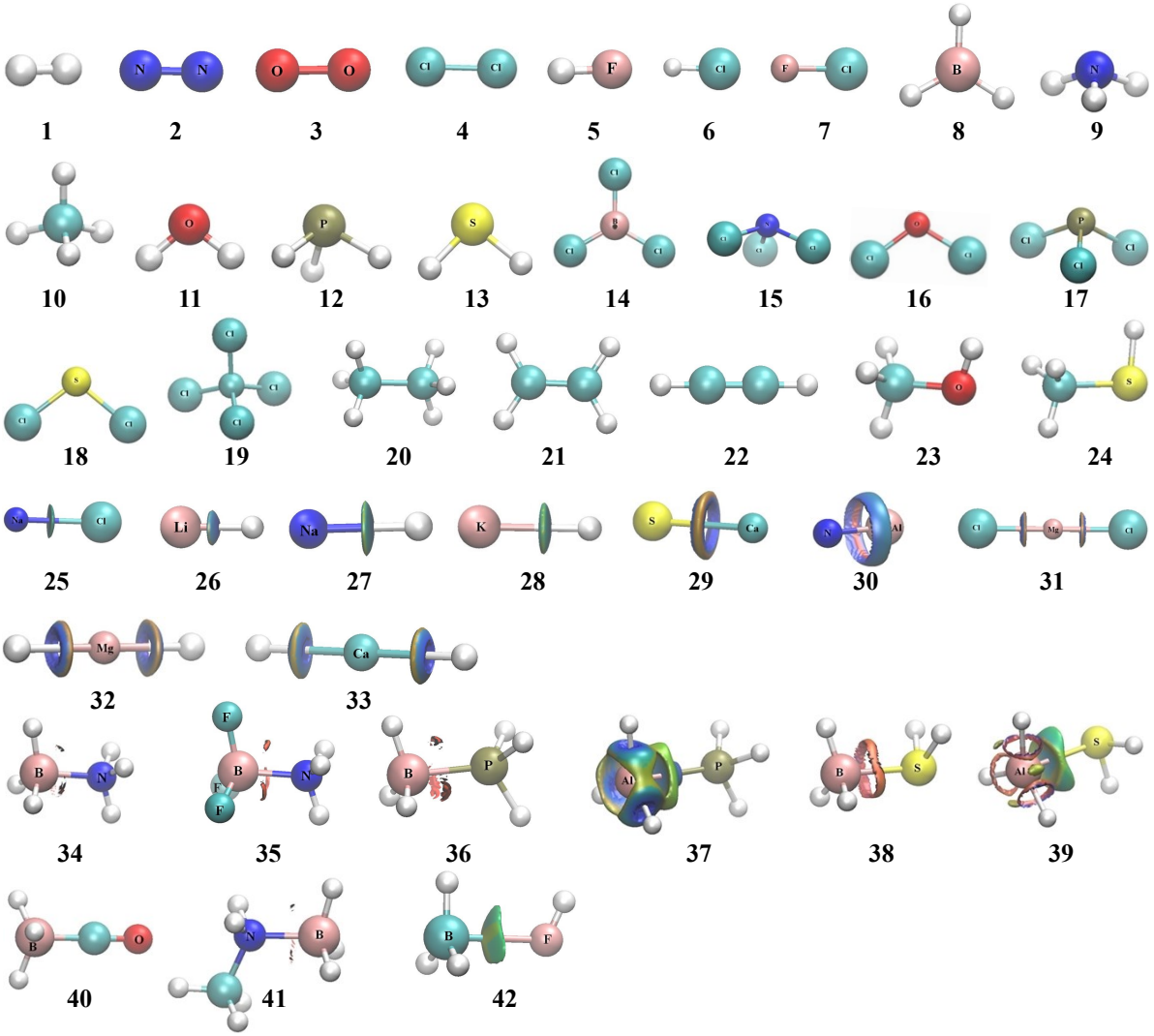

Figure S1 (a): NCI surfaces with s=0.5 a.u. of the covalent (1-24), ionic (25-33), and coordinate (34-42) bonded systems.

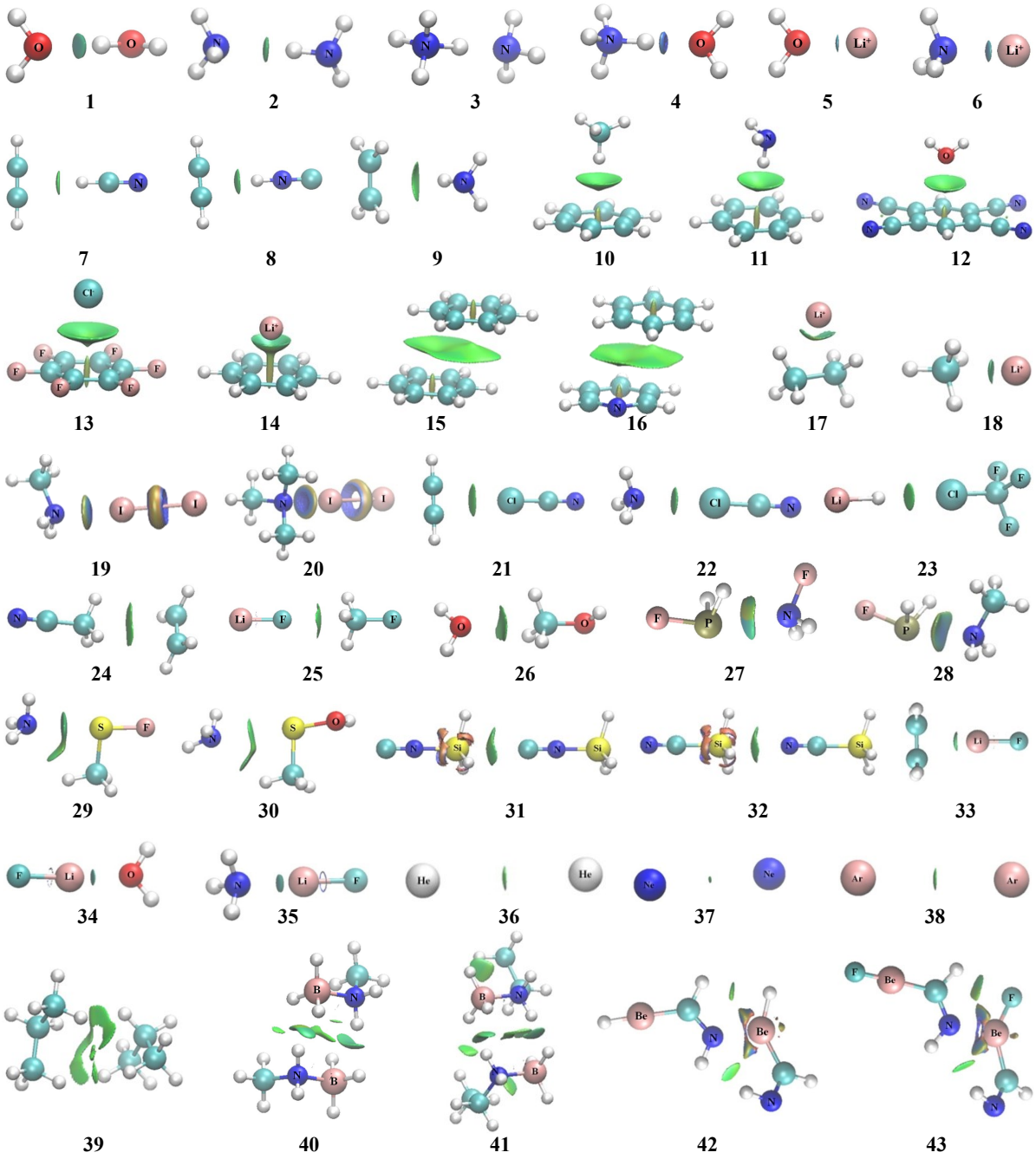

Figure S1 (b): NCI surfaces with s=0.5 a.u. of the non-covalent bonded systems, namely HB (1-2), CHB (3-4), ML (5-6), XHP (7-11), LP (12), AP (13), CP (14), PP (15-16), CA (17-18), XB (19-22), HXB (23), CB (24-26), PB (27-28), CGB (29-30), TB (31-32), LB (33-35), VDW (36-38), HHB (39), DHB (40-41), and BB (42-43).

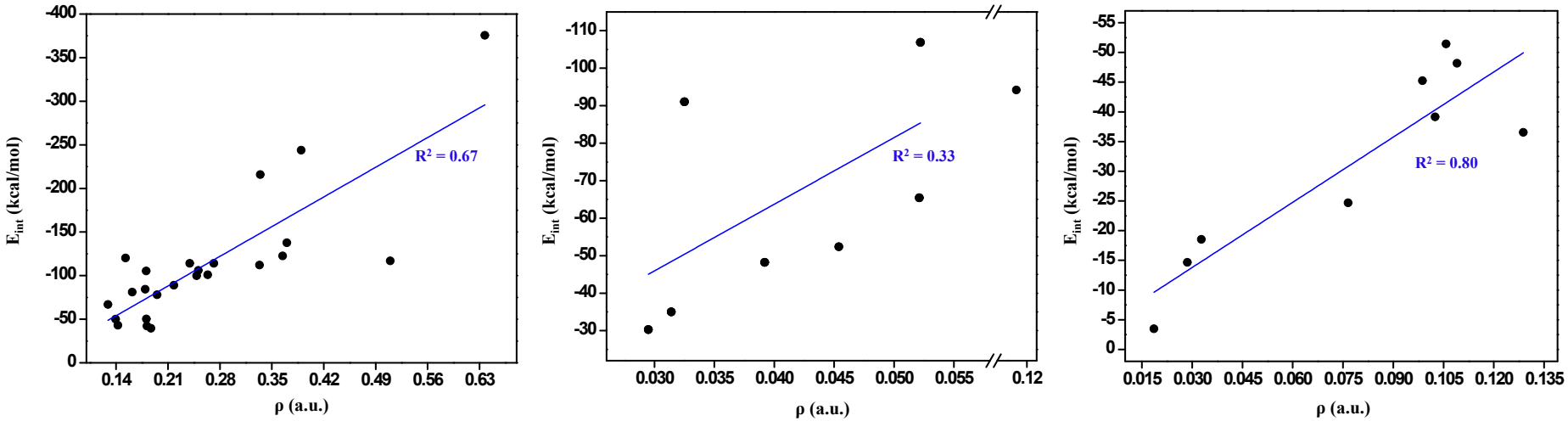

Figure S2: Linear fitting of interaction energy with electron density at a critical point for (a) covalent, (b) ionic, and (c) coordinate bonds. Values are calculated at MP2/6-311++G** level of theory.