Supplementary Information for:

Sigma-Hole Carbon-Bonding Interactions in Carbon-

Carbon Double Bonds: An Unnoticed Contact

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Table S1. Molecular graph and geometry of the complexes calculated at RI-MP2/aug-cc-pVTZ computational level.

E	f-f
4	C 0.0000000 0.0000000 -1.0831872
	C 0.0000000 0.0000000 0.2321315
	H 0.9048100 0.0000000 0.8156050
	H -0.9048100 0.0000000 0.8156050
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	H 0.9011282 0.0000000 0.8869730
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	Cl -1.4488144 0.0000000 -1.9987621
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a	
	f-br
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	C 0.0000000 0.0000000 0.5237620
	H 0.8982230 0.0000000 1.1226416
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	S -1.4576417 0.0000000 -1.8292454
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	cl-f C 0.0000000 0.0000000 -1.1652080 C 0.0000000 0.0000000 0.1514962 H 0.9180329 0.0000000 0.7129058 H -0.9180329 0.0000000 0.7129058 F -1.0803391 0.0000000 -1.9490642 F 1.0803391 0.0000000 -1.9490642 Cl 0.0000000 0.0000000 3.4860287

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cl-br C 0.000000 0.000000 -1.0944124 C 0.000000 0.000000 0.2341601 H -0.9132729 0.0000000 0.8120352 H 0.9132729 0.0000000 0.8120352 Cl 0.0000000 0.8120352 Cl 0.0000000 0.0000000 Br -1.5909238 0.0000000 -2.1210563 Br 1.5909238 0.0000000 -2.1210563
cl-i C 0.0000000 0.0000000 -1.0721464 C 0.0000000 0.0000000 0.2591999 H -0.9106891 0.0000000 0.8437692 H 0.9106891 0.0000000 0.8437692 Cl 0.0000000 0.0000000 3.4805971 I 1.7705835 0.0000000 -2.1775945 I -1.7705835 0.0000000 -2.1775945
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	C 0.0000000 0.0000000 -0.8664311
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S	H 0.9084337 0.0000000 1.0563080
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Д	Cl 0.0000000 0.0000000 3.7741004
	S -1.4557505 0.0000000 -1.8877624
	H -2.3098005 0.0000000 -0.8572034
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•	Cl 0.0000000 0.0000000 4.0820820
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	N 0.0000000 0.0000000 2.2327852
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	N 0.0000000 0.0000000 3.6933695
	C 0.0000000 0.0000000 4.8744984
	Li 0.0000000 0.0000000 6.7892079
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	l 🖬	I 1.7717332 0.0000000 -3.4059162

8	li-cn
	C 0.0000000 0.0000000 -1.6861298
	C 0.0000000 0.0000000 -0.3432970
	H = 0.9212280 = 0.0000000 = 0.2183980
<u>ب</u>	
	N 0.0000000 0.0000000 0.2185980
	N 0.0000000 0.0000000 2.7683041
	C 0.0000000 0.0000000 3.9486541
	Li 0.0000000 0.0000000 5.8691310
H	C 1.2203399 0.0000000 -2.4400046
9	N 2.2177075 0.0000000 -3.0567247
<i>P</i>	C -1.2203399 0.0000000 -2.4400046
	N -2.2177075 0.0000000 -3.0567247
V	
Q IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	li-nc
	C 0.0000000 0.0000000 -1.6746499
	C 0.0000000 0.0000000 -0.3398141
• н	H 0.9255447 0.0000000 0.2114951
	H -0.9255447 0.0000000 0.2114951
	N 0.000000 0.000000 2.7768225
j⊆ → _Q· · · · · · · · · · · · · · · · · · ·	C 0.0000000 0.0000000 3.9573916
	Li 0.000000 0.000000 5.8790795
	N 1 1563633 0 0000000 -2.4294882
N U	$\begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $
	C 2.1451747 0.0000000 -5.0814210
	N -1.1563633 0.0000000 -2.4294882
C	C -2.1451747 0.0000000 -3.0814216
	li-oh
<u>,</u> ₽	C 0.0000000 0.0000000 -1.9498970
	C 0.0000000 0.0000000 -0.6123924
б н	H 0.9197346 0.0000000 -0.0514717
	H -0.9197346 0.0000000 -0.0514717
	N 0.000000 0.000000 2.7548844
©€	C = 0.0000000 = 0.0000000 = 2.7540044
Q U	0 -1.0899469 0.0000000 -2.7554416
	H -1.8654014 0.0000000 -2.1830464
b	O 1.0899469 0.0000000 -2.7554416
	H 1.8654014 0.0000000 -2.1830464
в	li-sh
	C 0.0000000 0.0000000 -1.9305071
S	C 0.0000000 0.0000000 -0.5918421
	H 0.9187271 0.0000000 -0.0241279
	H -0.9187271 0.0000000 -0.0241279
	N 0.000000 0.000000 2.6825628
©€	C 0.0000000 0.0000000 3.8635356
	Li 0.000000 0.000000 5.7796477
	S -1.4495597 0.0000000 -2.9505731
/ 8	H -2.3117282 0.0000000 -1.9269975
s	S 1 4495597 0 0000000 -2 9505731
	H = 2.3117282 = 0.0000000 = 1.9269975
	11 2.511/202 0.0000000 1.52055/5
U	li ch2
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	н 0.0000000 -0.9191094 0.0615395
Ů••©→−©→−©·····••₩→−©−→−Ü	N U.UUUUUUU U.UUUUUUU 2.8045995
	C 0.0000000 0.0000000 3.9855610
Ъ	C 0.0000000 0.0000000 -1.8160032
	C 0.0000000 0.0000000 -3.1269962
	H 0.9284512 0.0000000 -3.6821858

	H -0.9284512 0.0000000 -3.6821858
	Li 0.0000000 0.0000000 5.9015537
	n-h
	C 0.0000000 0.0000000 -2.4319711
6 6	C 0.000000 0.000000 -1.0983474
	H 0.9187738 0.0000000 -0.5295637
	H -0.9187738 0.0000000 -0.5295637
©−−−−© −−−−₩	N 0.0000000 0.0000000 2.3932365
	C = 0.0000000 = 0.0000000 = 2.5552505
	H = 0.0000000 = 0.0000000 = 4.6256871
0 0	H 0.9231761 0.0000000 -2.9949199
	H = 0.9231761 = 0.0000000 = 2.9949199
	n-me
	C = 0.000000 = 0.000000 = 1.0260040
	C = 0.0000000 = 0.0000000 = 1.0200049
<u>_</u>	
B◆-€	H 0.0000000 -0.9217278 0.8776763
<u>بر</u> ۲	N 0.0000000 0.0000000 3.8200672
©©	H 0.0000000 0.0000000 6.0526798
	C 0.0000000 -1.2699171 -1.8242311
	H 0.0000000 -2.1468903 -1.1792181
H	H -0.8//2594 -1.3160254 -2.4/3569/
0. a	H 0.8772594 -1.3160254 -2.4735697
N	C 0.0000000 1.2699171 -1.8242311
8	H 0.8772594 1.3160254 -2.4735697
	H -0.8772594 1.3160254 -2.4735697
	H 0.0000000 2.1468903 -1.1792181
н н	n-cch
	C 0.0000000 0.0000000 -1.1110529
	C 0.0000000 0.0000000 0.2376077
	H 0.9275108 0.0000000 0.7902849
	H -0.9275108 0.0000000 0.7902849
6	N 0.0000000 0.0000000 3.6083798
	C 0.0000000 0.0000000 4.7753581
	H 0.0000000 0.0000000 5.8408476
	C -1.2180953 0.0000000 -1.8622727
	C -2.2440841 0.0000000 -2.5181250
	H -3.1420247 0.0000000 -3.0854573
	C 1.2180953 0.0000000 -1.8622727
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,©	H 3.1420247 0.0000000 -3.0854573
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	n-f
	C 0.0000000 0.0000000 -2.3333823
<u>ч</u>	C 0.0000000 0.0000000 -1.0128049
	H 0.9331540 0.0000000 -0.4798527
	H -0.9331540 0.0000000 -0.4798527
	F -1.0789619 0.0000000 -3.0976676
	F 1.0789619 0.0000000 -3.0976676
	N 0.000000 0.000000 2.3673073
E	C 0.0000000 0.0000000 3.5342383
	Н 0.0000000 0.0000000 4.5996824

	n-cl
Q	C 0.0000000 0.0000000 -2.2916822
	C 0.000000 0.000000 -0.9610586
©6	H -0.9302665 0.0000000 -0.4165306
	N 0.0000000 0.0000000 2.3809224
	C 0.0000000 0.0000000 3.5478263
/ H	H 0.0000000 0.0000000 4.6133229
	Cl -1.4481384 0.0000000 -3.2281348
v	Cl 1.4481384 0.0000000 -3.2281348
	n-br
	C = 0.000000 = 0.000000 = 2.2748730
	C = 0.0000000 = 0.0000000 = 0.9427836
	H 0.9290552 0.0000000 -0.3937789
ю — • ю́·····• • ····• • М — • ю́— • н	H -0.9290552 0.0000000 -0.3937789
	N 0.0000000 0.0000000 2.3904529
	C 0.0000000 0.0000000 3.5573549
/ 1	H 0.0000000 0.0000000 4.6228626
	Br 1.5913569 0.0000000 -3.2827280
•	Br -1.5913569 0.0000000 -3.2827280
	n-i
$ $ \rangle	
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	H 0.9266168 0.0000000 -0.3625846
	H -0.9266168 0.0000000 -0.3625846
QQ	N 0.0000000 0.0000000 2.3939335
	C 0.0000000 0.0000000 3.5608491
	H 0.0000000 0.0000000 4.6263696
/ 0	I -1.7722014 0.0000000 -3.3422970
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	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539
	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 0.0392539
	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 0.0392539 N -1.1795615 0.0000000 -2.6826059
	I 1.7722014 0.0000000 -3.3422970 n-no
	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 2.6826059 O -2.2310666 0.0000000 -2.0546550 N 1.1795615 0.0000000 -2.6826059
	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 0.0392539 N -1.1795615 0.0000000 -2.6826059 O -2.2310666 0.0000000 -2.6826059 O 2.2310666 0.0000000 -2.0546550
	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 -2.6826059 O -2.2310666 0.0000000 -2.0546550 N 1.1795615 0.0000000 -2.0546550 N 0.1795615 0.0000000 -2.0546550 N 0.0000000 0.0000000 2.7813553
	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 -2.6826059 O -2.2310666 0.0000000 -2.0546550 N 1.1795615 0.0000000 -2.0546550 N 1.1795615 0.0000000 -2.0546550 N 0.0000000 0.0000000 2.7813553 C 0.0000000 0.0000000 3.9479484
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	I 1.7722014 0.0000000 -3.3422970 n-no C 0.0000000 0.0000000 -1.8419510 C 0.0000000 0.0000000 -0.5049868 H 0.9324733 0.0000000 0.0392539 H -0.9324733 0.0000000 0.0392539 N -1.1795615 0.0000000 -2.6826059 O -2.2310666 0.0000000 -2.0546550 N 1.1795615 0.0000000 -2.0546550 N 1.1795615 0.0000000 2.7813553 C 0.0000000 0.0000000 3.9479484 H 0.0000000 0.0000000 5.0136482
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0	n-nc
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	C = 0.0000000 = 0.0000000 = 0.2959775
	H = 0.9309656 = 0.0000000 = 0.2355775
単	H = 0.9309656 = 0.0000000 = 0.2464332
	N 0,000000 0,0000000 2,9543625
	C = 0.0000000 = 0.0000000 = 2.9343023
	H 0.0000000 0.0000000 5.1868330
a b	N 1.150/992 0.0000000 -2.382/383
P	C 2.1483282 0.0000000 -3.0312215
	N -1.156/992 0.0000000 -2.382/383
	C -2.1483282 0.0000000 -3.0312215
	n-oh
l 📕	C 0.0000000 0.0000000 -1.8963949
	C 0.000000 0.000000 -0.5572947
4 6	H 0.9237767 0.0000000 -0.0031389
	H = 0.9237767 = 0.0000000 = 0.0031389
	N 0.000000 0.000000 2.9079812
∭ ∭ ∭ ∭ ∭ ∭ ∭ ∭ ∭ ∭	C = 0.0000000 = 0.0000000 = 2.5075012
	H = 0.0000000 = 0.0000000 = 1.0751542
	0 -1.0879990 -0.0000000 -2.6994976
0 0	H = 1.8673310 = 0.0000000 = 2.0004970
	0 1 0879990 0 0000000 -2 6994976
h	H = 1.8673310 = 0.0000000 = 2.0004570
	n ch
н	
	C = 0.0000000 = 0.0000000 = 1.8737807
S	
	H = 0.9230899 = 0.0000000 = 0.0207144
	H 0.9230899 0.0000000 -0.0207144
	1000000000000000000000000000000000000
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	H 0.0000000 0.0000000 -5.0769967
	S 1.4476575 0.0000000 2.8991752
/ 6	H 2.3127649 0.0000000 1.8780354
S	5 -1.44/65/5 0.0000000 2.8991/52
	H -2.3127649 0.0000000 1.8780354
Ъ	
	n-ch2
	C 0.0000000 0.0000000 -0.4491076
8	H 0.0000000 0.9238196 0.1124371
, r	H 0.0000000 -0.9238196 0.1124371
	N 0.000000 0.000000 2.9650069
│	C 0.0000000 0.0000000 4.1320764
	H 0.0000000 0.0000000 5.1975275
7	C 0.0000000 0.0000000 -1.7580060
U U	C 0.0000000 0.0000000 -3.0679584
	H 0.9288254 0.0000000 -3.6222066
	H -0.9288254 0.0000000 -3.6222066

H F ⁻ 0.004 0.003 H LiCN 0.001 0 Cl ⁻ 0.003 0.002 HCN 0.001 0).001).000
CI ⁻ 0.003 0.002 HCN 0.001 0	0.000
	000
Me F ⁻ 0.001 0.003 Me LiCN 0.000 0	0.000
Cl [−] 0.000 0.002 HCN 0.000 0	0.000
C=CH F ⁻ 0.001 0.001 C=CH LiCN -0.001 0	0.001
Cl [−] 0.000 0.000 HCN 0.000 0	0.000
F F ⁻ -0.006 0.020 F LiCN -0.001 0	0.005
Cl ⁻ -0.004 0.015 HCN 0.000 0	0.002
Cl F ⁻ -0.005 0.019 Cl LiCN -0.001 0	0.005
Cl ⁻ -0.004 0.014 HCN 0.000 0).003
Br F ⁻ -0.006 0.016 Br LiCN -0.002 0	0.004
Cl ⁻ -0.004 0.011 HCN -0.001 0).002
I F ⁻ -0.006 0.012 I LiCN -0.002 0	0.003
Cl ⁻ -0.005 0.008 HCN -0.001 0	0.001
NO F ⁻ 0.010 -0.016 NO LiCN -	-
Cl ⁻ 0.007 -0.013 HCN 0.001 -0	0.003
CN F ⁻ 0.003 0.001 CN LiCN 0.000 0	0.000
Cl ⁻ 0.001 0.001 HCN 0.000 0	0.000
NC F ⁻ 0.000 0.009 NC LiCN 0.000 0	0.003
Cl [−] 0.000 0.007 HCN 0.000 0	0.002
OH F ⁻ -0.009 0.020 OH LiCN -0.002 0	0.005
Cl ⁻ -0.007 0.015 HCN -0.001 0	0.002
SH F ⁻ -0.005 0.013 SH LiCN -0.001 0	0.004
Cl ⁻ -0.004 0.009 HCN 0.000 0	0.002
=CH ₂ F ⁻ -0.003 0.008 =CH ₂ LiCN 0.000 0).002
Cl ⁻ -0.002 0.005 HCN 0.000 0	0.001

Table S2. C=C and C–X distances variations upon complexation (Δd_{cc} and Δd_{cx} , respectively). Distances in Å.

α	E _b	d			
180	-12.86	2.738			
175	-12.83	2.737			
170	-12.75	2.734			
165	-12.61	2.729			
160	-12.43	2.723			
155	-12.19	2.715			
150	-11.91	2.705			
145	-11.57	2.695			
140	-11.18	2.683			
135	-10.75	2.672			
130	-10.27	2.662			
125	-9.74	2.654			
120	-9.16	2.651			
115	-8.55	2.740			
110	-7.90	2.666			
105	-7.25	2.687			
100	-6.62	2.717			
95	-6.06	2.755			
90	-5.60	2.796			

Table S3. Binding energy along the out-of-plane relaxed scan of α . E_{b} in kcal·mol⁻¹ and α in degrees.

β	E_b	<i>d</i> _{H…F-}
180	-12.86	2.337
175	-13.01	2.186
170	-13.48	2.032
165	-14.22	1.886
160	-15.13	1.764
155	-15.54	1.676
150	-16.93	1.618
145	-17.65	1.580
140	-18.20	1.556
135	-18.56	1.540
130	-18.73	1.532
125	-18.70	1.529
120	-18.48	1.531

Table S4. Binding energy along the in-plane relaxed scan of β . E_b in kcal·mol⁻¹ and β in degrees.

Table S5. Binding energies of a set of representative carbon bond and hydrogen bond complexes (E_{b-CB} and E_{b-HB} , respectively).

Х	Y	E _{b-CB}	E _{b-HB}
Н	LiCN	-1.63	-2.22
	HCN	-0.63	-0.86
F	F⁻	-12.86	-18.74
	Cl⁻	-8.51	-9.66
	LiCN	-3.23	-
	HCN	-1.36	-2.20
CN	F ⁻	-27.82	-34.66
	Cl⁻	-19.81	-20.43

X	Y	$H_{\text{BCP}}\text{x10}^{3}$	X	Y	$H_{\text{BCP}} \textbf{x10}^{3}$
Н	F ⁻	1.64	Н	LiCN	1.27
	Cl⁻	1.28 ^ª		HCN	1.09
Me	F ⁻	1.63	Me	LiCN	1.21
	Cl⁻	1.25ª		HCN	1.05
C≡CH	F^{-}	2.09	C≡CH	LiCN	1.57
	Cl⁻	1.48ª		HCN	1.33
F	F^{-}	1.95	F	LiCN	1.52
	Cl⁻	1.47		HCN	1.30
Cl	F^{-}	2.12	Cl	LiCN	1.64
	Cl⁻	1.52 ^ª		HCN	1.40
Br	F^{-}	2.18	Br	LiCN	1.67
	Cl⁻	1.52ª		HCN	1.42
I	F^{-}	2.24	I	LiCN	1.71
	Cl⁻	1.52ª		HCN	1.47
NO	F^{-}	2.41	NO	LiCN	-
	Cl⁻	1.53		HCN	1.53
CN	F^{-}	2.51 ^ª	CN	LiCN	1.91
	Cl⁻	1.52ª		HCN	1.63
NC	F^{-}	2.42	NC	LiCN	1.89
	Cl⁻	1.53ª		HCN	1.61
ОН	F^{-}	1.75	ОН	LiCN	1.31
	Cl⁻	1.36ª		HCN	1.12
SH	F^{-}	2.01	SH	LiCN	1.53
	Cl⁻	1.46 ^ª		HCN	1.30
$=CH_2$	F^{-}	1.97	$=CH_2$	LiCN	1.46
	Cl⁻	1.43ª		HCN	1.25

Table S6. Total electron density energy (H_{BCP}), in au, for the intermolecular bond critical points in all complexes.

Table S7. Second-order perturbation stabilization energies for the donor-acceptor Lp(Y) $\rightarrow \sigma^*(C1-C2)$, Lp(Y) $\rightarrow \pi^*(C1=C2)$, and Lp(Y) $\rightarrow \sigma^*(C2-H)$ (σ^* , π^* , and $\sigma^*(H)$, respectively, in kcal·mol⁻¹) and electron charge transfer from the Lewis base to the Lewis acid (Δq in au) calculated from the NBO atomic charges in **li-x** and **n-x** complexes.

X	Y	σ*	π^*	σ*(H)	Δq
Н	LiCN	0.34	-	-	-0.0008
	HCN	0.22	-	-	-0.0006
Me	LiCN	0.20	-	-	-0.0003
	HCN	0.12	-	-	-0.0002
C≡CH	LiCN	0.41	-	-	-0.0011
	HCN	0.22	-	-	-0.0008
F	LiCN	0.33	-	-	-0.0004
	HCN	0.16	-	-	-0.0003
Cl	LiCN	0.28	-	-	-0.0007
	HCN	0.14	-	-	-0.0006
Br	LiCN	0.28	-	-	-0.0008
	HCN	0.15	-	-	-0.0006
I	LiCN	0.34	-	-	-0.0011
	HCN	0.19	-	-	-0.0007
NO	LiCN	-	-	-	-
	HCN	0.25	-	-	-0.0007
CN	LiCN	0.66	-	-	-0.0020
	HCN	0.35	-	-	-0.0013
NC	LiCN	0.62	-	-	-0.0016
	HCN	0.32	-	-	-0.0011
ОН	LiCN	0.25	-	-	-0.0003
	HCN	0.13	-	-	-0.0002
SH	LiCN	0.24	-	-	-0.0004
	HCN	0.13	-	-	-0.0004
=CH ₂	LiCN	0.38	-	-	-0.0008
	HCN	0.22	-	-	-0.0005

Table S8. DF-DFT-SAPT total energy (E_{SAPT}) and its exchange, electrostatic, induction, and dispersion energy contributions (E_{exch} , E_{el} , E_i , and E_d , respectively) of all complexes. Energies in kcal·mol⁻¹.

X	Y	$E_{\rm ex}$	E _{el}	Ei	E_{d}	E _{SAPT}	X	Y	E_{ex}	$E_{\rm el}$	Ei	E_{d}	E _{SAPT}
Н	F ⁻	9.8	-6.7	-5.9	-2.7	-5.6	н	LiCN	1.7	-1.1	-0.6	-1.2	-1.2
	Cl⁻	5.6	-3.8	-3.1	-2.3	-3.6		HCN	1.0	-0.6	-0.2	-0.9	-0.6
Me	F^-	9.5	-3.5	-6.8	-2.8	-3.7	Me	LiCN	1.6	-0.2	-0.6	-1.2	-0.5
	Cl⁻	5.4	-1.4	-3.6	-2.4	-2.1		HCN	1.0	-0.1	-0.2	-0.9	-0.3
C≡CH	F ⁻	15.6	-13.8	-9.9	-3.7	-11.9	C≡CH	LiCN	2.6	-2.7	-0.9	-1.6	-2.6
	Cl⁻	8.9	-8.4	-5.4	-3.2	-8.1		HCN	1.4	-1.3	-0.3	-1.1	-1.3
F	F ⁻	13.3	-14.6	-6.8	-3.3	-11.4	F	LiCN	2.4	-2.9	-0.7	-1.4	-2.6
	CI	7.6	-9.2	-3.5	-2.7	-7.8		HCN	1.3	-1.3	-0.2	-1.0	-1.2
Cl	F ⁻	16.2	-16.8	-9.2	-3.8	-13.6	Cl	LiCN	2.8	-3.4	-0.9	-1.6	-3.1
	CI	9.3	-10.6	-4.9	-3.2	-9.4		HCN	1.5	-1.6	-0.3	-1.2	-1.5
Br	F ⁻	17.2	-17.4	-10.1	-4.0	-14.3	Br	LiCN	2.9	-3.5	-1.0	-1.7	-3.2
	CI	9.8	-10.9	-5.5	-3.4	-9.9		HCN	1.6	-1.6	-0.3	-1.2	-1.5
I	F [−]	18.4	-17.4	-11.4	-4.2	-14.6	1	LiCN	3.1	-3.5	-1.1	-1.8	-3.2
	CI	10.5	-10.8	-6.2	-3.6	-10.0		HCN	1.7	-1.6	-0.3	-1.3	-1.5
NO	F ⁻	21.2	-29.3	-10.6	-4.4	-23.1	NO	LiCN	-	-	-	-	-
	CI 	12.4	-19.5	-5.8	-3.7	-16.6		HCN	1.9	-2.9	-0.4	-1.2	-2.6
CN	F	22.5	-32.6	-11.4	-4.6	-26.2	CN	LiCN	4.0	-7.6	-1.3	-1.9	-6.7
	CI 	13.5	-22.6	-6.5	-3.9	-19.5		HCN	2.1	-3.4	-0.4	-1.3	-3.1
NC	F CI⁻	21.6	-28.0	-11.1	-4.5	-21.9	NC	LICN	3.9	-6.3	-1.2	-1.9	-5.4 2 F
		12.9	-19.1	-0.1	-3.8	-10.1			2.0	-2.8	-0.4	-1.5	-2.5
ОН	F CI⁻	10.9	-8.9	-6./	-3.0	-7.6	ОН	LICN	1.8	-1.2	-0.6	-1.3	-1.3
<u></u>	CI 	6.3	-5.5	-3.5	-3.0	-5.4		HCN	1.0	-0.5	-0.2	-1.0	-0.6
SH	F CI⁻	14.6 ° Г	-12.5	-9.4	-3./	-11.0	SH	LICN	2.5	-2.3	-0.9	-1.6	-2.3
.	CI 	ð.5	-8.0	-5.1	-3.2	-7.8	<i></i>	HUN	1.4	-1.0	-0.2	-1.1	-1.0
$=CH_2$	F	13.1	-10.2	-8.1	-3.3	-8.5	=CH ₂	LICN	2.2	-1.8	-0.7	-1.4	-1.8
	CI	1.3	-5.8	-4.Z	-2.8	-5.5		HUN	1.2	-0.9	-0.2	-1.0	-0.9



Figure S1. Exponential relationship between C···Y equilibrium distance and the electron density (top) and laplacian (bottom) at the BCP (ρ and $\nabla^2 \rho$, respectively, in a.u.) for the complexes.



Figure S2. Electron density (ρ , top) and Laplacian ($\nabla^2 \rho$, bottom) at the intermolecular BCP versus the binding energy.



Figure S3. AIM Electronic charge shift (ΔQ) from the Lewis base to the Lewis acid versus NBO electronic charge shift (Δq) from the Lewis base to the Lewis in **f-x** and **cl-x** complexes.



Figure S4. AIM Electronic charge shift (ΔQ) from the Lewis base to the Lewis acid versus the binding energy (E_b) in **li-x** and **n-x** complexes.



Figure S5. SAPT electrostatic, induction, and dispersion energy contributions (E_{el} , E_i , and E_d , respectively) of **cl-x** (top) and **li-x** (bottom) complexes. Energies in kcal·mol⁻¹.



Figure S6. Representation of the SAPT total energy (E_{SAPT}) versus the binding energy (E_b) for all complexes. Energies in kcal·mol⁻¹.



Figure S7. Representation of the SAPT electrostatic contribution (E_{el}) versus the binding energy (E_b) for all complexes. Energies in kcal·mol⁻¹.



Figure S8. Representation of the sum of E_{el} and E_i ($E_{el}+E_i$) versus the second-order perturbation stabilization energies for the donor-acceptor Lp(Y) $\rightarrow \sigma^*$ (C1–C2) and Lp(Y) $\rightarrow \pi^*$ (C1=C2) ($E^{(2)}$) for all complexes. Energies in kcal·mol⁻¹.



Figure S9. Histogram of the β angle distribution in neutral carbon-bonding complexes retrieved from the CSD search.



Figure S10. Histogram of the β angle distribution in neutral carbon-bonding complexes retrieved from the CSD search.



Figure S11. Geometry of a fragment of the X-ray structure with reference code EBOJOU retrieved from the CSD and its molecular graph, calculated at BP86/def2-TZVP computational level. Bond, ring and cage critical points are denoted with green, red and blue spheres, respectively.



Figure S12. Geometry of a fragment of the X-ray structure with reference code IGAMAG retrieved from the CSD and its molecular graph, calculated at BP86/def2-TZVP computational level. Bond and ring critical points are denoted with green and red spheres, respectively.



Figure S13. Geometry of a fragment of the X-ray structure with reference code POWLOD retrieved from the CSD and its molecular graph, calculated at BP86/def2-TZVP computational level. Bond and ring critical points are denoted with green and red spheres, respectively.



Figure S14. Geometry of a fragment of the X-ray structure with reference code LIQGOH retrieved from the CSD and its molecular graph, calculated at BP86/def2-TZVP computational level. Bond and ring critical points are denoted with green and red spheres, respectively.