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

Cooperativity between H-Bonds and Tetrel Bonds.

Transformation of a Noncovalent C···N Tetrel Bond to a Covalent Bond

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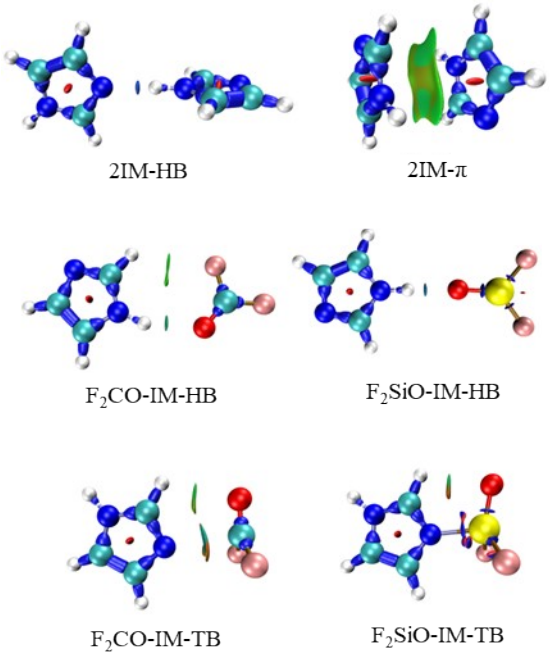

Fig. S1 NCI diagram of binary complexes. Blue, red, and green regions denote strong attractive, strong repulsion, and weak attractive interactions, respectively

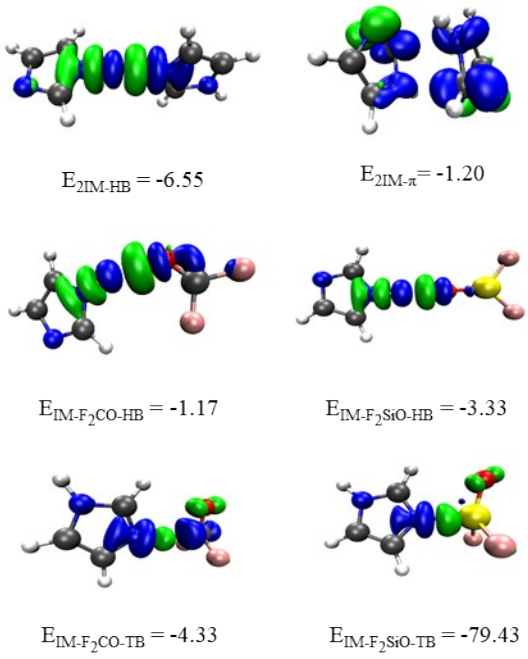

Fig. S2 NOCV density contour map and orbital energy (E, kJ/mol) of binary complexes. Blue is giving electrons, while green is taking electrons.

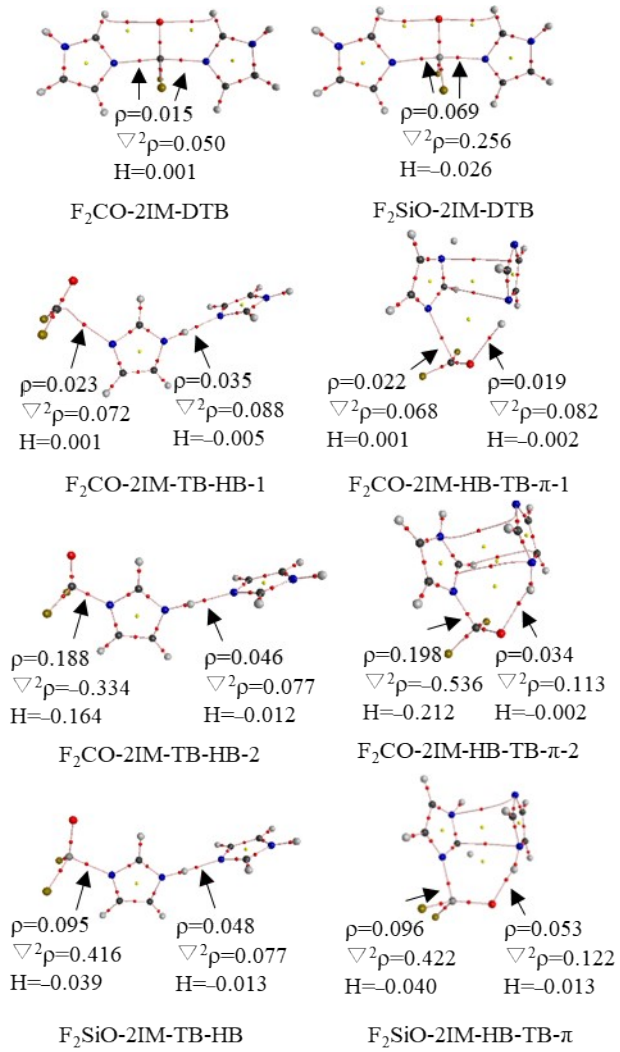

Fig.S3 AIM diagrams of the ternary complexes. Yellow and red dots indicate the locations of ring and bond critical points, respectively. all in a.u.

Table S1 The binding distances of tetrel bond (R_{TB}) and hydrogen bond (R_{HB}) in the ternary complexes as well as their difference (ΔR) with respect to the binary analogues, all in Å

	R_{TB}	ΔR_{TB}	R_{HB}	ΔR_{HB}
F_2CO-2IM-DTB	2.731	0.166		
F_2SiO-2IM-DTB	1.997	0.124		
F_2CO-2IM-TB-HB-1	2.501	-0.064	1.868	-0.024
F_2CO-2IM-TB-HB-2	1.616	-0.949	1.773	-0.119
F_2SiO-2IM-TB-HB	1.859	-0.014	1.754	-0.138
F_2CO-2IM-HB-TB-π-1	2.518	-0.047	2.012	-0.086
F_2CO-2IM-HB-TB-π-2	1.605	-0.960	1.826	-0.272
F_2SiO-2IM-HB-TB-π	1.857	-0.016	1.641	-0.228

COORDINATES OF MONOMERS AND COMPLEXES

F_2CO

C	0.00000000	0.14348000	0.00000000
O	-0.00007100	1.32118700	0.00000000
F	-1.06171400	-0.63508800	0.00000000
F	1.06177700	-0.63495300	0.00000000

F_2SiO

Si	0.00000000	0.13283600	0.00000000
O	-0.00037900	1.65618700	0.00000000
F	-1.24395800	-0.83962100	0.00000000
F	1.24429500	-0.83917900	0.00000000

IM

C	0.55701900	1.01516800	-0.00006800
C	1.14865000	-0.22833300	-0.00005100
C	-0.96282200	-0.58583300	0.00007800
N	-0.79166700	0.76591000	0.00003800
H	-1.52342400	1.45634500	0.00013200
H	0.95850500	2.01264100	-0.00013500
H	2.20040200	-0.45713400	-0.00010400
H	-1.93627200	-1.04591200	0.00014800
N	0.19791100	-1.21904500	-0.00001000

2IM-π

C	-1.27096600	0.92792900	0.76359500
C	-2.37990700	-0.22520100	-0.66157300
C	-1.77819900	-1.13569200	0.18098400
N	-1.08192600	-0.37919100	1.08501500
H	-0.43858200	-0.72966200	1.77792400
H	-0.81761600	1.72960600	1.32078700
H	-3.03014000	-0.42712800	-1.49594000
H	-1.78460300	-2.21061500	0.21631000
C	1.27048800	-0.92755000	-0.76387800
C	2.38038100	0.22454000	0.66138900
C	1.77856700	1.13562900	-0.18045100
N	1.08166900	0.37978400	-1.08455600
H	0.43801700	0.73077700	-1.77692100
H	0.81663600	-1.72880600	-1.32126100
H	3.03105000	0.42585900	1.49556400
H	1.78528200	2.21056800	-0.21524700
N	2.05858000	-1.06018800	0.29319900
N	-2.05864000	1.05980500	-0.29388800

2IM-HB

C	-2.13283500	-0.86454100	0.55069300
C	-2.29029800	0.96106300	-0.57670700
C	-3.57987700	0.54159400	-0.34655100
N	-3.45634700	-0.62015600	0.37145500
H	-4.21252200	-1.19362600	0.70720500
H	-1.76065100	-1.72145500	1.08575800
H	-1.96130100	1.83642100	-1.10923200
H	-4.53567400	0.95076000	-0.61970100
C	2.30912900	-0.58621100	-0.90927400
C	3.62822100	0.30436600	0.51867900
C	2.34833600	0.63575700	0.91340300
N	1.51950600	0.05851300	-0.01068600
H	0.49414400	0.09678600	-0.02092700
H	1.90409400	-1.12684900	-1.74829600
H	4.55716400	0.57468200	0.99173900
H	1.97106900	1.21186600	1.73995800
N	3.59835400	-0.45950600	-0.62088300
N	-1.39756700	0.08104200	-0.01530800

F_2CO-IM-HB

C	1.57750900	0.87246200	-0.00025600
C	3.45287200	-0.15837500	0.00044400
C	2.48193400	-1.13641100	0.00022800
N	1.29114800	-0.45837900	-0.00011000
H	0.36503000	-0.85834200	-0.00029400
H	0.81015000	1.62817400	-0.00057400
H	4.52133100	-0.29012400	0.00077700
H	2.53166500	-2.21064000	0.00034200
N	2.88331900	1.09054300	0.00012900
F	-2.17606700	1.16379800	-0.00030200
F	-3.79653600	-0.20943800	0.00037200
O	-1.72728900	-1.01125500	-0.00033600
C	-2.49193600	-0.10991100	-0.00013900

F_2SiO-IM-HB

C	2.63247500	1.07680600	-0.00075900
C	3.97713100	-0.58668200	0.00039700
C	2.70557400	-1.12002100	0.00077500
N	1.86081600	-0.04235900	0.00003600
H	0.84630600	-0.07083000	0.00007500
H	2.21112100	2.06781800	-0.00145000
H	4.91517800	-1.11524600	0.00075800
H	2.34298500	-2.13254800	0.00148300

N	3.92556600	0.78475500	-0.00054400
F	-3.43579300	1.28481800	0.00096300
F	-3.55669800	-1.21240400	-0.00095100
O	-1.02225000	-0.08498500	-0.00000300
Si	-2.54292300	-0.00988800	0.00000900

F_2CO-IM-TB

C	-1.17063000	0.93110100	0.00005600
C	-1.59253200	-1.17525200	0.00005300
C	-2.81518700	-0.54308400	-0.00009500
N	-2.52337700	0.79701900	-0.00000700
H	-3.19045600	1.55040400	-0.00005100
H	-0.66943300	1.88428200	0.00009400
H	-1.39420400	-2.23305100	0.00010400
H	-3.82464500	-0.91303200	-0.00022500
N	-0.57706600	-0.25160700	0.00010700
F	2.08813200	-0.60894400	-1.06341700
F	2.08813400	-0.60881400	1.06345400
O	1.86614200	1.33174900	-0.00010300
C	1.95606600	0.15379200	-0.00003400

F_2SiO-IM-TB

C	-1.27457100	1.04526900	-0.00010900
C	-1.34342600	-1.14575800	-0.00019000
C	-2.63945300	-0.70165700	-0.00000200
N	-2.56467000	0.67044100	-0.00008200
H	-3.34584600	1.30665700	-0.00008500
H	-0.87682700	2.04673000	-0.00012700
H	-0.95349400	-2.14735700	-0.00028300
H	-3.57530600	-1.22916100	0.00005500
N	-0.51859100	-0.04851100	-0.00001000
F	1.67716100	-0.81914100	-1.24653000
F	1.67707700	-0.81932900	1.24655900
O	1.60729300	1.65794000	0.00019900
Si	1.34518000	0.14037100	0.00007500

F_2CO-2IM-DTB

C	0.00000000	3.06745800	0.97047500
C	0.00000000	3.91619200	-1.00029300
C	0.00000000	4.98287100	-0.12964000
N	0.00000000	4.41991700	1.12121100
H	0.00000000	4.91682200	1.99600900
H	0.00000000	2.37969300	1.79901700
H	0.00000000	3.94158800	-2.07634700

H	0.00000000	6.04718800	-0.28231400
C	0.00000000	-3.06745800	0.97047500
C	0.00000000	-3.91619200	-1.00029300
C	0.00000000	-4.98287100	-0.12964000
N	0.00000000	-4.41991700	1.12121100
H	0.00000000	-4.91682200	1.99600900
H	0.00000000	-2.37969300	1.79901700
H	0.00000000	-3.94158800	-2.07634700
H	0.00000000	-6.04718800	-0.28231400
N	0.00000000	-2.73043800	-0.30880500
N	0.00000000	2.73043800	-0.30880500
F	-1.06329800	0.00000000	-1.01615700
F	1.06329800	0.00000000	-1.01615700
O	0.00000000	0.00000000	0.93310200
C	0.00000000	0.00000000	-0.25115000

F_2SiO-2IM-DTB

C	0.00000000	2.72250800	1.06316400
C	0.00000000	2.85010700	-1.11069900
C	0.00000000	4.13966900	-0.64105900
N	0.00000000	4.03127500	0.72864000
H	0.00000000	4.79469000	1.38393200
H	0.00000000	2.29347700	2.05093500
H	0.00000000	2.48832300	-2.12283600
H	0.00000000	5.08882400	-1.14498900
C	0.00000000	-2.72250800	1.06316400
C	0.00000000	-2.85010700	-1.11069900
C	0.00000000	-4.13966900	-0.64105900
N	0.00000000	-4.03127500	0.72864000
H	0.00000000	-4.79469000	1.38393200
H	0.00000000	-2.29347700	2.05093500
H	0.00000000	-2.48832300	-2.12283600
H	0.00000000	-5.08882400	-1.14498900
N	0.00000000	-1.99269300	-0.04160800
N	0.00000000	1.99269300	-0.04160800
F	-1.29662700	0.00000000	-0.90444500
F	1.29662700	0.00000000	-0.90444500
O	0.00000000	0.00000000	1.66030400
Si	0.00000000	0.00000000	0.09344200

F_2CO-2IM-TB-HB-1

C	-0.74124100	0.03385300	0.04664000
C	-1.56533000	2.00695800	-0.13328000
C	-0.19406200	2.15363100	-0.12117400

N	0.31119700	0.88680100	-0.00580500
H	1.30418500	0.62136000	0.02834000
H	-0.63263300	-1.03391600	0.13928000
H	-2.31657100	2.77444700	-0.21047900
H	0.43998800	3.02045500	-0.18222400
N	-1.89859800	0.68054500	-0.02834500
F	-4.28483700	-0.45317500	-1.05853000
F	-4.32341100	-0.30674700	1.06469400
O	-3.11619800	-1.92616200	0.13130100
C	-3.78751500	-0.95683100	0.05242900
C	5.15016500	-0.57923600	0.68311200
C	3.95385500	-0.04450600	1.10073000
C	3.74475000	-0.40290800	-1.01102200
N	4.99507100	-0.79910800	-0.66143600
H	5.68504100	-1.18850100	-1.28258600
H	6.06089500	-0.81392500	1.20369700
H	3.67371400	0.26356300	2.09303300
H	3.36609000	-0.47082100	-2.01652700
N	3.08652900	0.06178500	0.04086800

F_2CO-2IM-TB-HB-2

C	3.66354700	-0.34271900	-1.01368700
C	3.76960300	0.14943600	1.08233300
C	5.02152400	-0.29376700	0.72730700
N	4.93047200	-0.59993600	-0.60579300
H	5.67294700	-0.95807700	-1.18428900
H	3.32540600	-0.50126200	-2.02332600
H	3.43018800	0.48268200	2.04759100
H	5.93214000	-0.41448400	1.28548200
C	-0.76062300	-0.32667800	0.05157900
C	-1.81711500	1.58166600	-0.17344200
C	-0.46795800	1.84323700	-0.19732700
N	0.16859100	0.63726800	-0.05512700
H	1.19638100	0.47495100	-0.03773000
H	-0.59802200	-1.38266700	0.17501300
H	-2.66810400	2.23292500	-0.25251000
H	0.07204900	2.76684500	-0.30155300
N	-1.96065200	0.23288800	-0.01877300
N	2.93246100	0.11608900	-0.00683100
F	-3.95239800	-0.23709100	-1.07698900
F	-3.96663000	0.00306400	1.09191800
O	-3.03768200	-1.85951100	0.20664300
C	-3.29004100	-0.68163200	0.07481900

F_2SiO-2IM-TB-HB

C	3.84938800	-0.52486500	-0.95102100
C	4.12893600	0.30522300	1.01933900
C	5.31205700	-0.31213000	0.68985200
N	5.11122700	-0.83069100	-0.56299800
H	5.78093200	-1.35473100	-1.10264100
H	3.43562300	-0.82061300	-1.89984200
H	3.88119500	0.82874100	1.92618300
H	6.24138100	-0.42462200	1.21806300
C	-0.43487000	-0.14639100	0.06199200
C	-1.46783600	1.75818600	-0.25026000
C	-0.11836700	2.00588400	-0.27416700
N	0.50289900	0.79945700	-0.07632900
H	1.53058800	0.61764100	-0.04526300
H	-0.28188900	-1.19911700	0.22981500
H	-2.30242200	2.42577300	-0.36561100
H	0.43119400	2.91891000	-0.41317900
N	-1.64257600	0.41336800	-0.04055800
N	3.22603400	0.16850800	-0.00739300
F	-3.92043100	-0.14984200	-1.24433800
F	-3.95088300	0.19353900	1.22326700
O	-2.69251100	-2.09454400	0.29927700
Si	-3.16668800	-0.64277400	0.09174600

F_2CO-2IM-HB-TB-π-1

C	0.10431100	0.97946500	-1.14708500
C	-0.64465500	2.12959700	0.50563500
C	0.66820000	2.51064600	0.33323800
N	1.11969700	1.77466200	-0.72864300
H	2.08085300	1.69749300	-1.02589300
H	0.21012100	0.28035300	-1.95853500
H	-1.35057100	2.48943700	1.23482600
H	1.29564700	3.21128400	0.85448200
C	2.05561600	-0.36754000	1.16054900
C	2.91021300	-1.19462100	-0.62187700
C	1.67805100	-1.79740400	-0.46880500
N	1.15457200	-1.25962700	0.67503700
H	0.21556400	-1.41076200	1.02293900
H	1.87375500	0.20763900	2.05247500
H	3.63966700	-1.36830400	-1.39520600
H	1.15316500	-2.53755400	-1.04689800
N	3.13940400	-0.30138500	0.39663300
N	-0.98840800	1.17511300	-0.42017100
C	-2.42303200	-0.80937400	0.16746000

O	-1.78329800	-1.18863600	1.09114400
F	-3.48493600	-0.05033600	0.23809800
F	-2.28405300	-1.22593700	-1.07165500

F_2CO-2IM-HB-TB-π-2

C	-0.05590200	0.76837500	-1.04317100
C	-1.16294200	1.70202500	0.60934000
C	-0.17110500	2.57354700	0.23387300
N	0.49472900	1.96848500	-0.79834000
H	1.36295500	2.28023000	-1.20776700
H	0.29672900	0.04583300	-1.75563400
H	-1.91228100	1.77107800	1.37709700
H	0.10323900	3.54222200	0.60897700
C	1.89243900	0.00028700	1.12301900
C	2.94218000	-0.71598900	-0.60018900
C	1.94057200	-1.63327300	-0.34190900
N	1.29241100	-1.16374000	0.76625900
H	0.37327400	-1.47531600	1.10533700
H	1.56234100	0.58059400	1.96901100
H	3.68767900	-0.75076100	-1.37733300
H	1.64634300	-2.54559200	-0.83091900
N	2.90520200	0.30710800	0.31609600
N	-1.06965200	0.60540100	-0.20109800
F	-1.56471500	-1.44146300	-1.10885400
F	-3.13682300	-0.38758900	-0.00467500
O	-1.44518000	-1.31073200	1.13615100
C	-1.81921200	-0.78192800	0.09626600

F_2SiO-2IM-HB-TB-π

C	-0.29905200	0.88385300	0.69706900
C	1.29675300	1.99994900	-0.31316300
C	0.25232800	2.86503700	-0.11635400
N	-0.71951900	2.14170400	0.52508800
H	-1.67424700	2.42402000	0.70046800
H	-0.88760700	0.09783900	1.14580200
H	2.25208700	2.15307700	-0.78064800
H	0.12885800	3.89983800	-0.37688900
C	-2.14062300	-0.22921500	-1.14706500
C	-3.34817500	-0.45015400	0.60620000
C	-2.48272900	-1.53077900	0.57765600
N	-1.73504500	-1.38077200	-0.55630200
H	-0.79072300	-1.81344100	-0.70391000
H	-1.69505400	0.13720100	-2.05790700
H	-4.11842300	-0.23516600	1.32873000

H	-2.34847900	-2.36739400	1.24146400
N	-3.12739200	0.36697600	-0.47484700
N	0.93488100	0.77290400	0.19935700
F	2.54340000	-0.98057600	1.41045800
F	2.98875100	-0.30450100	-0.97653000
O	0.83188300	-1.93248900	-0.48731200
Si	1.82483500	-0.84344300	-0.01307800