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

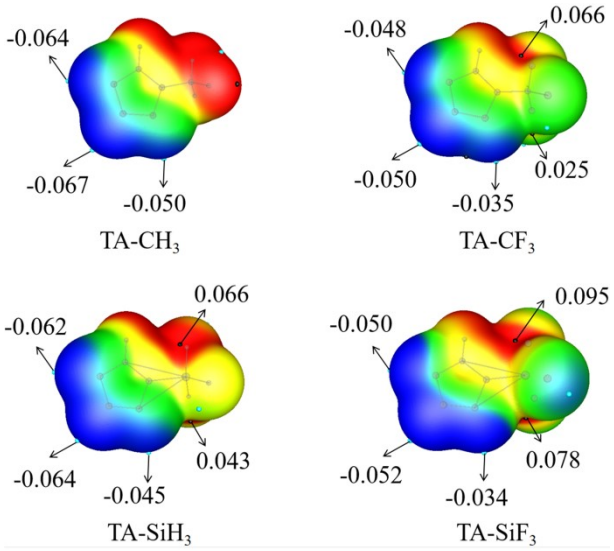

Fig. S1. MEP maps of other positions of TA-TtR_3. Color ranges are: red, greater than 0.02; yellow, between 0.02 and 0; green, between -0.02 and 0; blue, less than -0.02. All are in a.u.

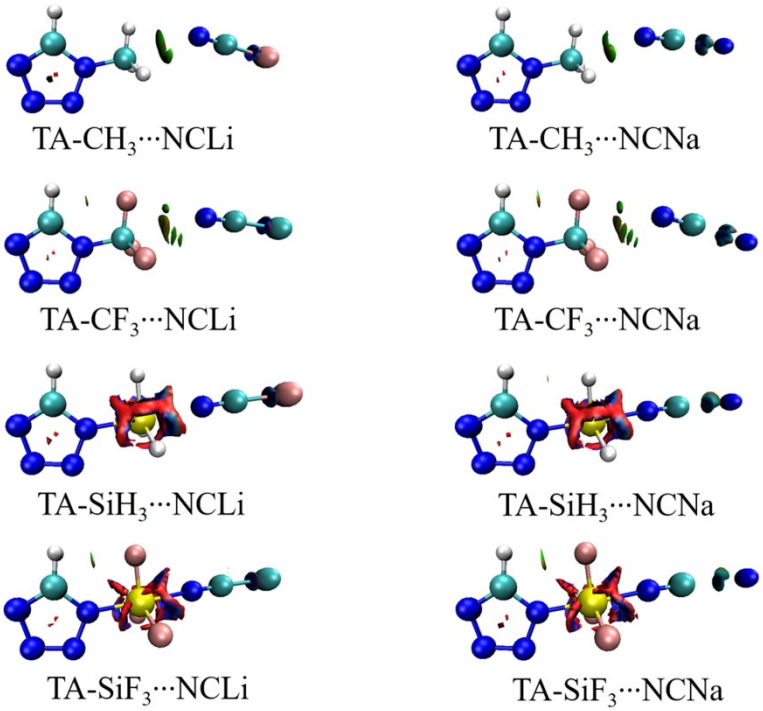

Fig. S2 NCI diagram of binary complex. Blue, green, and red areas represent strong attraction, weak attraction, and strong repulsion interactions, respectively

Table S1 Charge transfer (CT, e) and second-order perturbation energies ($E^{(2)}$, kcal/mol) in the binary complexes

	CT	type	$E_1^{(2)}$	type	$E_2^{(2)}$
TA-CH_3···NCLi	0.0032	$LP_N \rightarrow \sigma^*_{N-C}$	1.48	$LP_N \rightarrow \sigma^*_{C-H}$	0.17
TA-CH_3···NCNa	0.0037	$LP_N \rightarrow \sigma^*_{N-C}$	1.69	$LP_N \rightarrow \sigma^*_{C-H}$	0.19
TA-CF_3···NCLi	0.0026	$LP_N \rightarrow \sigma^*_{N-C}$	0.15	a	a
TA-CF_3···NCNa	0.0030	$LP_N \rightarrow \sigma^*_{N-C}$	0.16	a	a
TA-SiH_3···NCLi	0.1229	$LP_N \rightarrow \sigma^*_{N-Si}$	38.74	$LP_N \rightarrow \sigma^*_{Si-H}$	32.33[b]
TA-SiH_3···NCNa	0.1486	$LP_N \rightarrow \sigma^*_{N-Si}$	47.15	$LP_N \rightarrow \sigma^*_{Si-H}$	39.63[b]
TA-SiF_3···NCLi	0.1737	c	c	c	c
TA-SiF_3···NCNa	0.1884	c	c	c	c
TA-GeF_3···NCNa	0.1936	c	c	c	c

Note: (a) No presence due to the weak interaction, (b) Data are the sum of three $LP_N \rightarrow \sigma^*_{Si-H}$ orbital interactions, and (c) No obtained since NBO deems the Tt···N bond to be a single unit.

Table S2 Value of V_{max} on the σ-hole of the N-Tt bond for BX_3···TA-TtR_3 and its change (ΔV_{max}) relative to the monomer, all in a.u.

	V_{max}	ΔV_{max}
3-BH_3···TA-CH_3	0.067	0.017
4-BH_3···TA-CH_3	0.067	0.017
3-BF_3···TA-CH_3	0.073	0.023
4-BF_3···TA-CH_3	0.073	0.023
3-BH_3···TA-CF_3	0.072	0.018
4-BH_3···TA-CF_3	0.072	0.018
3-BF_3···TA-CF_3	0.077	0.023
4-BF_3···TA-CF_3	0.077	0.023
3-BH_3···TA-SiH_3	0.106	0.020
4-BH_3···TA-SiH_3	0.106	0.020
3-BF_3···TA-SiH_3	0.113	0.027
4-BF_3···TA-SiH_3	0.112	0.026
3-BH_3···TA-SiF_3	0.132	0.022
4-BH_3···TA-SiF_3	0.132	0.022
3-BF_3···TA-SiF_3	0.139	0.029
4-BF_3···TA-SiF_3	0.139	0.029

Table S3. Electron densities (ρ), Laplacians ($\nabla^2\rho$), and energy densities (H) at the Tt···N and N-Tt BCPs in the ternary systems, all in a.u.

	Tt···N			N-Tt		
	ρ	$\nabla^2\rho$	H	ρ	$\nabla^2\rho$	H
3-BH_3···TA-CH_3···NCNa	0.0114	0.0551	0.0026	0.2502	-0.2343	-0.3693
4-BH_3···TA-CH_3···NCNa	0.0101	0.0484	0.0025	0.2461	-0.2512	-0.3608
3-BF_3···TA-CH_3···NCNa	0.0118	0.0575	0.0027	0.2480	-0.2011	-0.3651
4-BF_3···TA-CH_3···NCNa	0.0104	0.0498	0.0025	0.2441	-0.2201	-0.3569
3-BH_3···TA-CF_3···NCNa	0.0325	0.1805	0.0035	0.2864	-1.1265	-0.3990
4-BH_3···TA-CF_3···NCNa	0.0060	0.0321	0.0016	0.2864	-1.1248	-0.3981
3-BF_3···TA-CF_3···NCNa	0.0063	0.0342	0.0017	0.2820	-1.1003	-0.3914
4-BF_3···TA-CF_3···NCNa	0.0064	0.0339	0.0017	0.2823	-1.1015	-0.3927
3-BH_3···TA-SiH_3···NCNa	0.0523	0.2433	-0.0102	0.0804	0.3801	-0.0261
4-BH_3···TA-SiH_3···NCNa	0.0523	0.2437	-0.0102	0.0804	0.3795	-0.0262
3-BF_3···TA-SiH_3···NCNa	0.0552	0.2639	-0.0110	0.0769	0.3612	-0.0240
4-BF_3···TA-SiH_3···NCNa	0.0550	0.2625	-0.0109	0.0773	0.3631	-0.0242
3-BH_3···TA-SiF_3···NCNa	0.0768	0.3898	-0.0226	0.0989	0.4472	-0.0422
4-BH_3···TA-SiF_3···NCNa	0.0803	0.4187	-0.0240	0.1032	0.4794	-0.0447
3-BF_3···TA-SiF_3···NCNa	0.0787	0.4002	-0.0236	0.0960	0.4337	-0.0399
4-BF_3···TA-SiF_3···NCNa	0.0785	0.3995	-0.0235	0.0963	0.4348	-0.0401

Table S4. Charge transfer (CT, e) in the triad and its change (ΔCT, e) relative to the dyad

	CT	ΔCT
3-BH_3···TA-CH_3···NCNa	0.0056	0.0019
4-BH_3···TA-CH_3···NCNa	0.0049	0.0012
3-BF_3···TA-CH_3···NCNa	0.0061	0.0024
4-BF_3···TA-CH_3···NCNa	0.0053	0.0016
3-BH_3···TA-CF_3···NCNa	0.0031	0.0001
4-BH_3···TA-CF_3···NCNa	0.0027	-0.0003
3-BF_3···TA-CF_3···NCNa	0.0029	-0.0001
4-BF_3···TA-CF_3···NCNa	0.0026	-0.0004
3-BH_3···TA-SiH_3···NCNa	0.1771	0.0285
4-BH_3···TA-SiH_3···NCNa	0.1769	0.0283
3-BF_3···TA-SiH_3···NCNa	0.1863	0.0377
4-BF_3···TA-SiH_3···NCNa	0.1853	0.0367
3-BH_3···TA-SiF_3···NCNa	0.2022	0.0138
4-BH_3···TA-SiF_3···NCNa	0.2056	0.0172
3-BF_3···TA-SiF_3···NCNa	0.2070	0.0186
4-BF_3···TA-SiF_3···NCNa	0.2064	0.0180

Table S5. Second-order perturbation energies ($E^{(2)}$, kcal/mol) in the ternary complexes

	type	$E_1^{(2)}$	type	$E_2^{(2)}$
3-BH_3···TA-CH_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	2.66	$LP_N \rightarrow \sigma^*_{C-H}$	0.37
4-BH_3···TA-CH_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	2.19	$LP_N \rightarrow \sigma^*_{C-H}$	0.24
3-BF_3···TA-CH_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	2.85	$LP_N \rightarrow \sigma^*_{C-H}$	0.37
4-BF_3···TA-CH_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	2.35	$LP_N \rightarrow \sigma^*_{C-H}$	0.26
3-BH_3···TA-CF_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	0.23	a	a
4-BH_3···TA-CF_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	0.25	a	a
3-BF_3···TA-CF_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	0.28	a	a
4-BF_3···TA-CF_3···NCNa	$LP_N \rightarrow \sigma^*_{N-C}$	0.29	a	a
3-BH_3···TA-SiH_3···NCNa	b	b	b	b
4-BH_3···TA-SiH_3···NCNa	b	b	b	b
3-BF_3···TA-SiH_3···NCNa	b	b	b	b
4-BF_3···TA-SiH_3···NCNa	b	b	b	b
3-BH_3···TA-SiF_3···NCNa	b	b	b	b
4-BH_3···TA-SiF_3···NCNa	b	b	b	b
3-BF_3···TA-SiF_3···NCNa	b	b	b	b
4-BF_3···TA-SiF_3···NCNa	b	b	b	b

Note: (a) No presence due to the weak interaction, (b) No obtained since NBO deems the Tt···N bond to be a single unit.

Table S6. Electrostatic (E^{ele}), exchange (E^{ex}), repulsion (E^{rep}), polarization (E^{pol}), and dispersion energies (E^{disp}) as well as the total interaction energy (E_{total}) in the binary complexes with Tt···N distance of 3 Å, all in kcal/mol

	E^{ele}	E^{ex}	E^{rep}	E^{pol}	E^{disp}	E_{total}
TA-CH_3···NCLi	-7.21	-5.38	8.96	-1.31	-1.80	-6.73
TA-CH_3···NCNa	-8.38	-6.43	10.74	-1.66	-1.85	-7.58
TA-CF_3···NCLi	-6.55	-8.67	15.51	-1.27	-2.46	-3.43
TA-CF_3···NCNa	-7.22	-9.13	16.34	-1.49	-2.51	-4.01
TA-SiH_3···NCLi	-11.03	-8.28	13.80	-3.18	-2.41	-11.10
TA-SiH_3···NCNa	-12.23	-8.59	14.26	-3.60	-2.30	-12.45
TA-SiF_3···NCLi	-12.54	-7.82	13.99	-2.83	-1.73	-10.95
TA-SiF_3···NCNa	-13.92	-8.05	14.38	-3.20	-1.57	-12.37
TA-GeF_3···NCNa	-15.66	-7.90	14.17	-4.02	-1.30	-14.71

Table S7. Electrostatic (E^{ele}), exchange (E^{ex}), repulsion (E^{rep}), polarization (E^{pol}), and dispersion energies (E^{disp}) as well as the total interaction energy (E_{total}) of TA-SiF_3···NCNa at different Si···N distances, all in kcal/mol

$R_{Si\cdots N}$/Å	E^{ele}	E^{ex}	E^{rep}	E^{pol}	E^{disp}	E_{total}
2.0	-81.43	-77.23	158.42	-49.86	-0.83	-50.93
2.2	-56.65	-50.50	99.87	-29.85	-1.97	-39.10
2.4	-39.43	-33.04	63.35	-16.91	-2.36	-28.39
2.6	-27.49	-21.31	39.80	-9.38	-2.25	-20.64
2.8	-19.35	-13.35	24.34	-5.33	-1.93	-15.61
3.0	-13.92	-8.05	14.38	-3.20	-1.57	-12.37

Table S8. The mean of the three angles N-Tt-R (α, deg) and length of N-Tt bond (R, Å) in the equilibrium complex (1) and complex with Tt···N distance of 3 Å (2)

	α_1	α_2	R_1	R_2
TA-SiH_3···NCLi	96.5	103.7	1.874	1.821
TA-SiH_3···NCNa	95.0	103.4	1.890	1.824
TA-SiF_3···NCLi	94.0	103.4	1.832	1.771
TA-SiF_3···NCNa	93.2	104.4	1.841	1.773
TA-GeF_3···NCNa	93.5	103.8	1.899	1.848

TA-CH_3

C	-0.27580000	1.07144400	-0.00089600
N	0.56820400	0.02536100	-0.00353900
N	-0.14767200	-1.10450400	-0.00206800
N	-1.41617500	-0.73377500	0.00203600
N	-1.51886400	0.61455100	0.00152600
H	0.03342900	2.10150900	-0.00232000
C	2.01817100	-0.01368900	0.00240500
H	2.38865900	1.00448000	-0.07143200
H	2.36361900	-0.46818800	0.92641900
H	2.36160900	-0.59575700	-0.84741100

TA-CF_3

C	1.15261700	1.08324200	-0.00008800
N	0.30334800	0.03160200	-0.00005700
N	1.00799100	-1.11144000	0.00015800
N	2.26833800	-0.74509600	-0.00012000
N	2.38215600	0.60821600	0.00018000
H	0.84894500	2.11377400	-0.00014000
C	-1.13492000	-0.00470600	-0.00002300
F	-1.57874700	1.24876700	-0.00048200
F	-1.58217200	-0.62774900	1.07627000
F	-1.58218900	-0.62856900	-1.07582400

TA-SiH_3

C	0.74113300	1.07657300	-0.00016400
N	-0.15075300	0.06078500	-0.00006000
N	0.55520100	-1.09579000	-0.00006600
N	1.82739700	-0.76191200	0.00020100
N	1.96809400	0.58548800	0.00009600
H	0.47397400	2.11859600	-0.00028200
H	-2.35518900	1.40855200	-0.00045500
H	-2.36884000	-0.70661600	-1.22057500
H	-2.36883700	-0.70579800	1.22105600
Si	-1.94482000	-0.00672600	0.00000300

TA-SiF_3

C	1.49759600	1.07876100	-0.00012700
N	0.60118600	0.06069300	-0.00007400
N	1.30522500	-1.10405100	-0.00014300
N	2.57078400	-0.77089300	0.00060200
N	2.71656500	0.57896800	-0.00021300
H	1.23142000	2.12092800	-0.00033700

Si	-1.14581100	-0.00378400	-0.00001200
F	-1.62431800	1.49833900	-0.00040600
F	-1.66181500	-0.74289700	1.28527400
F	-1.66186300	-0.74361200	-1.28486100

NCLi

C	0.00000000	0.00000000	-0.15449100
N	0.00000000	0.00000000	1.02674700
Li	0.00000000	0.00000000	-2.08676000

NCNa

C	0.00000000	0.00000000	-0.70013700
N	0.00000000	0.00000000	-1.88276100
Na	0.00000000	0.00000000	1.58001400

TA-CH_3-NCLi

C	1.92258000	1.02846400	0.00583200
N	1.01061600	0.04316400	-0.00202700
N	1.65139800	-1.13005100	-0.00455400
N	2.94354300	-0.84541900	0.00189600
N	3.13555200	0.49282500	0.00842500
H	1.67932800	2.07581800	0.00945700
C	-0.44280300	0.11428200	-0.00894000
H	-0.74590000	1.15478100	0.00813300
H	-0.82768500	-0.35790600	-0.90604000
H	-0.83663600	-0.38952500	0.86672600
C	-4.47399200	-0.01288900	0.00312000
N	-3.39481400	0.46599400	-0.01139500
Li	-6.24262900	-0.81596700	0.02507800

TA-CH_3-NCNa

C	-2.74022700	1.01024000	-0.00154800
N	-1.82705500	0.02629400	0.00282000
N	-2.46654700	-1.14748100	0.00128800
N	-3.75937500	-0.86441100	-0.00407400
N	-3.95297800	0.47356700	-0.00594100
H	-2.49775800	2.05774300	-0.00155200
C	-0.37304500	0.10235800	0.00970100
H	-0.07340100	1.14360200	0.00136900
H	0.01450600	-0.37545000	0.90233200
H	0.02368700	-0.39177200	-0.87011100
C	3.70598400	0.25509400	-0.00104000
N	2.55525000	0.52555900	-0.00031800

Na	5.92105700	-0.33954300	-0.00283200

TA-CF_3-NCLi

C	2.22301900	1.01614900	-0.00060500
N	1.32188600	0.01206700	-0.00009800
N	1.96518400	-1.16333200	-0.00006300
N	3.24571400	-0.86385100	-0.00009800
N	3.42969800	0.48043400	-0.00037200
H	1.97056600	2.06001300	-0.00084700
C	-0.12948000	0.06211100	0.00024800
F	-0.59064800	-0.53813300	-1.07837400
F	-0.47549800	1.34051700	-0.00012800
F	-0.59016200	-0.53739000	1.07948400
C	-4.48541600	-0.04373200	-0.00029300
N	-3.34956800	0.27943500	0.00084200
Li	-6.33431000	-0.62180200	-0.00186000

TA-CF_3-NCNa

C	2.87684500	0.89489700	0.00140200
N	1.88679200	-0.02107500	0.00016600
N	2.41821500	-1.25075400	-0.00038000
N	3.72143100	-1.07153600	-0.00005300
N	4.02905000	0.24984400	0.00092200
H	2.72184300	1.95761900	0.00218600
C	0.44478100	0.16453100	-0.00038000
F	0.22162700	1.46915500	0.00065800
F	-0.06805000	-0.39165900	1.07809600
F	-0.06706400	-0.38978900	-1.08027100
C	-3.84421400	0.28041900	-0.00074300
N	-2.72487000	0.66111900	-0.00125900
Na	-5.97084200	-0.55993200	0.00127500

TA-SiH_3-NCLi

C	1.98398000	1.05775600	-0.00047000
N	1.09451500	0.04739000	0.00022800
N	1.80297700	-1.09832900	-0.00003200
N	3.08465000	-0.76713300	-0.00124200
N	3.22212600	0.57772200	-0.00159500
H	1.71364000	2.09883300	-0.00035800
H	-0.92549400	1.48018300	0.00063900
H	-0.95817800	-0.71397300	-1.26051800
H	-0.95640100	-0.71180800	1.26538400
Si	-0.77939600	0.01399100	0.00170300

C	-4.16549900	0.00563400	-0.00098700
N	-2.98964300	0.03896500	0.00245000
Li	-6.12509800	-0.10658500	-0.00630500

TA-SiH_3-NCNa

C	-2.67520700	1.04338800	-0.00006100
N	-1.77429000	0.04433900	0.00002100
N	-2.46989100	-1.10817600	-0.00001700
N	-3.75678800	-0.79215100	-0.00009200
N	-3.90930800	0.55090200	-0.00013600
H	-2.41644500	2.08747100	-0.00006200
H	0.20220900	1.51127400	0.00005000
H	0.26357300	-0.69029500	1.26768400
H	0.26370300	-0.69048000	-1.26727500
Si	0.11604000	0.03854100	0.00014600
C	3.42656800	0.07156700	-0.00000700
N	2.24956700	0.09233900	0.00019200
Na	5.74356500	-0.08709500	-0.00016400

TA-SiF_3-NCLi

C	2.14549000	1.05754100	0.00011600
N	1.25837600	0.04319400	0.00001900
N	1.96678900	-1.10455300	-0.00008100
N	3.24351300	-0.76976600	0.00019800
N	3.38014900	0.57616000	-0.00026400
H	1.87059500	2.09621200	0.00012700
Si	-0.57344600	0.00692400	-0.00000800
F	-0.66657800	1.61299600	0.00022500
F	-0.69275100	-0.79098200	1.38053200
F	-0.69273900	-0.79062400	-1.38075600
C	-3.71613400	0.00801100	0.00014700
N	-2.54572400	0.03212600	0.00001000
Li	-5.69052700	-0.10303000	-0.00026000

TA-SiF_3-NCNa

C	-2.64899700	1.03282300	-0.00041000
N	-1.74632700	0.03327700	-0.00013400
N	-2.43659500	-1.12459200	0.00008700
N	-3.71954800	-0.81061400	-0.00060500
N	-3.87682100	0.53268100	-0.00035000
H	-2.39022900	2.07560800	-0.00046600
Si	0.09445200	0.02948000	0.00026900
F	0.13904700	1.64011800	-0.00050800
F	0.20492700	-0.76934000	-1.38338100

F	0.20439200	-0.76790400	1.38477900
C	3.20991200	0.07533600	0.00037900
N	2.03796900	0.08592600	0.00053900
Na	5.54148900	-0.09817400	-0.00071600

3-BH_3···TA-CH_3···NCNa

C	-1.98564500	1.36603400	-0.00174900
N	-1.24660100	0.25185300	0.00132400
N	-2.04815500	-0.80277200	0.00164300
N	-3.25920400	-0.29134600	-0.00128800
N	-3.26398700	1.03767900	-0.00343900
H	-1.58495000	2.36021300	-0.00267200
C	0.19673100	0.09573400	0.00452100
H	0.64945600	1.07717600	-0.00042500
H	0.50175500	-0.43814800	0.89375500
H	0.50428600	-0.44835700	-0.87762500
B	-4.58589900	-1.18440400	-0.00245000
H	-5.16469800	-0.86738400	-1.00698200
H	-4.18858500	-2.31597400	0.00061500
H	-5.16912900	-0.86346200	0.99825300
N	3.03937700	0.05998700	0.00848700
C	4.21108600	-0.02991800	0.00178100
Na	6.39075700	-0.26917800	-0.00609800

4-BH_3···TA-CH_3···NCNa

C	-2.15871500	-0.78471200	0.00012700
N	-1.25808700	0.20223700	0.00026800
N	-1.89670000	1.37812600	-0.00004200
N	-3.18560900	1.11561800	-0.00039600
N	-3.35590400	-0.21732900	-0.00028800
H	-1.95621100	-1.83935800	0.00032500
C	0.19997900	0.12595600	0.00089000
H	0.49642200	-0.91572400	-0.00068200
H	0.58663300	0.61514100	-0.88534200
H	0.58585000	0.61223100	0.88906100
B	-4.78216000	-0.97084100	-0.00076700
H	-4.47003300	-2.14157900	-0.00021300
H	-5.33782000	-0.62214800	1.00896000
H	-5.33673500	-0.62284700	-1.01134100
N	3.07194500	-0.29138100	0.00158500
C	4.25112100	-0.21152500	0.00052500
Na	6.54171500	-0.02915600	-0.00128000

3-BF_3···TA-CH_3···NCNa

C	-0.65694700	1.77531700	0.00007200
N	-0.00542000	0.60703500	-0.00009500
N	-0.88192200	-0.38319800	-0.00011500
N	-2.04430600	0.22283300	0.00007600
N	-1.95741800	1.54330700	0.00020300
H	-0.18249200	2.73626100	0.00012500
C	1.42357200	0.34155500	-0.00030300
H	1.94896200	1.28590100	0.00013100
H	1.68543500	-0.22000200	0.88530800
H	1.68532100	-0.21915500	-0.88648800
B	-3.52029900	-0.59273900	0.00004000
F	-4.12588500	-0.16823500	1.14731100
F	-3.16563000	-1.90907900	0.00041300
F	-4.12549800	-0.16879200	-1.14765100
C	5.38880200	-0.14402600	-0.00001400
N	4.23141600	0.05936500	-0.00017800
Na	7.53530700	-0.59880200	0.00020800

4-BF_3···TA-CH_3···NCNa

C	-0.94540200	-0.40718500	-0.00250500
N	-0.00238900	0.53595700	-0.00184000
N	-0.58543400	1.74283400	0.00137300
N	-1.88261400	1.54409500	0.00277300
N	-2.11006000	0.22334200	0.00030200
H	-0.79877600	-1.47131500	-0.00485600
C	1.45189500	0.39206700	-0.00443200
H	1.69846700	-0.66238300	-0.00236500
H	1.85695100	0.85993800	-0.89373400
H	1.86019400	0.86424300	0.88108900
B	-3.61983700	-0.50070300	0.00116300
F	-4.22940800	-0.08351300	-1.14762900
F	-3.27691800	-1.84272100	-0.00234700
F	-4.22557100	-0.08860100	1.15384100
N	4.28449000	-0.16707000	-0.00791100
C	5.46276400	-0.25752400	-0.00200500
Na	7.75690200	-0.40651900	0.00636600

3-BH_3···TA-CF_3···NCNa

C	-2.37876100	1.27690800	-0.00460700
N	-1.45986300	0.29107000	-0.00045700
N	-2.06135200	-0.89799900	0.00205600
N	-3.34335300	-0.59653300	-0.00078900

N	-3.57816000	0.72343700	-0.00485700
H	-2.15248700	2.32708300	-0.00723800
C	0.00455000	0.37431900	0.00161400
F	0.30154300	1.66091900	-0.00249800
F	0.46355800	-0.21943600	-1.07561500
F	0.46011300	-0.21173300	1.08449500
B	-4.50897900	-1.71116700	0.00049900
H	-5.12866300	-1.48361300	-1.00772200
H	-3.91764300	-2.75708100	0.00453800
H	-5.13208300	-1.47774700	1.00525700
N	3.11730200	0.61822200	0.00489600
C	4.18540000	0.11165200	0.00122400
Na	6.20542600	-0.96956500	-0.00455500

4-BH_3···TA-CF_3···NCNa

C	2.39351300	0.80084900	-0.00771300
N	1.46047600	-0.16258600	0.00613300
N	2.04550100	-1.36797000	-0.00713400
N	3.33539400	-1.14978900	-0.02894300
N	3.55919000	0.18139400	-0.02945700
H	2.22809000	1.86144900	-0.00209200
C	-0.00120200	-0.03896100	0.03084500
F	-0.26611900	1.25428500	0.03846000
F	-0.45424100	-0.62119200	1.11665900
F	-0.48988900	-0.61542200	-1.04287100
B	5.02176600	0.87274300	-0.05358100
H	4.75633300	2.05295200	-0.04575400
H	5.56972200	0.49007700	0.94630800
H	5.53363900	0.49544100	-1.07445300
N	-3.10253500	0.34214300	0.07212000
C	-4.27829600	0.23382000	0.01646500
Na	-6.55224100	-0.02720600	-0.08117700

3-BF_3···TA-CF_3···NCNa

C	1.17792400	1.82343300	-0.00518000
N	0.42964600	0.70274800	-0.00054500
N	1.21030800	-0.37379400	0.00256200
N	2.42316400	0.13158400	-0.00127800
N	2.45197900	1.46582900	-0.00527000
H	0.78751700	2.82418800	-0.00810100
C	-1.03552400	0.55102100	0.00188100
F	-1.52786700	1.77527900	-0.00335200
F	-1.38539500	-0.09773700	1.08602700

F	-1.38787300	-0.10803300	-1.07522800
B	3.86654300	-0.83899100	-0.00015300
F	4.48470600	-0.45637900	-1.15274500
F	4.48893000	-0.44746000	1.14713800
F	3.37531800	-2.10823100	0.00565600
N	-4.11908200	0.31621100	0.00546600
C	-5.18340400	-0.19807100	0.00136800
Na	-7.18879000	-1.30932200	-0.00487000

4-BF_3···TA-CF_3···NCNa

C	-1.37191900	0.48699900	0.00268600
N	-0.40025500	-0.43355900	0.00118400
N	-0.93058500	-1.66583200	-0.00394100
N	-2.22799000	-1.50628800	-0.00571900
N	-2.50472100	-0.18953300	-0.00166700
H	-1.25907200	1.55508800	0.00660500
C	1.05951400	-0.24426500	0.00476200
F	1.26220300	1.05912500	0.00761600
F	1.55209600	-0.80090600	-1.07553100
F	1.54757000	-0.80494200	1.08501800
B	-4.06361300	0.48926700	-0.00260300
F	-3.75415300	1.83434700	0.00274900
F	-4.63622200	0.04776900	-1.15619700
F	-4.64125800	0.03979700	1.14537900
N	4.11081900	0.28212200	0.01116000
C	5.29092500	0.34705300	0.00258000
Na	7.58209400	0.42498000	-0.01292500

3-BH_3···TA-SiH_3···NCNa

C	-2.11251500	1.37831900	-0.00051100
N	-1.27702100	0.32551000	0.00005600
N	-2.02589300	-0.78314700	0.00038400
N	-3.28106500	-0.36003200	-0.00026100
N	-3.37792700	0.97137100	-0.00086400
H	-1.79514300	2.40580000	-0.00079200
Si	0.64780700	0.19855300	0.00068400
H	0.77304800	1.66847000	-0.00018600
H	0.68953100	-0.53485000	1.27290800
H	0.69021600	-0.53645500	-1.27059700
B	-4.54619100	-1.34924000	-0.00029600
H	-5.15664600	-1.07776500	-1.00699700
H	-4.07205900	-2.45705200	0.00039000
H	-5.15741600	-1.07684600	1.00568800

N	2.70424000	0.11088000	0.00115100
C	3.87434200	-0.00953800	0.00055700
Na	6.17480200	-0.40814700	-0.00109500

4-BH_3···TA-SiH_3···NCNa

C	-2.18635400	-0.80051700	-0.00001500
N	-1.25647400	0.16009500	-0.00008700
N	-1.90055500	1.34269900	-0.00001300
N	-3.19653100	1.10493000	-0.00030000
N	-3.38274800	-0.22539100	-0.00013800
H	-2.01320100	-1.86042600	0.00007200
Si	0.67069900	0.07506700	0.00000500
H	0.63536400	-1.39925400	-0.00003400
H	0.79315400	0.80357700	-1.26998100
H	0.79301900	0.80349100	1.27005100
B	-4.81359600	-0.95746300	-0.00020300
H	-5.37379400	-0.60805100	-1.00957000
H	-4.52645100	-2.13640500	-0.00006000
H	-5.37398600	-0.60785300	1.00898900
N	2.72340100	-0.07316700	0.00009900
C	3.89837000	-0.12819400	0.00010900
Na	6.23294100	-0.16823700	0.00036300

3-BF_3···TA-SiH_3···NCNa

C	0.85262700	1.83359300	-0.00048800
N	0.12118000	0.70629100	0.00005300
N	0.96794700	-0.32635600	0.00039800
N	2.17223700	0.21795600	-0.00017300
N	2.15224300	1.54722300	-0.00055400
H	0.44091700	2.82677200	-0.00078900
Si	-1.79831700	0.38690400	0.00053400
H	-2.05491600	1.83938100	-0.00034100
H	-1.74507700	-0.34412000	-1.27218900
H	-1.74475800	-0.34246700	1.27419100
B	3.59491500	-0.66501700	-0.00008400
F	4.24039100	-0.28024600	1.14981600
F	3.19020700	-1.97537000	0.00043400
F	4.24004800	-0.28104700	-1.15044300
N	-3.81227100	0.08980300	0.00088500
C	-4.96239800	-0.15513900	0.00043600
Na	-7.20734900	-0.81421100	-0.00092000

4-BF_3···TA-SiH_3···NCNa

C	-1.07192900	0.45916500	-0.00027800
N	-0.08202000	-0.43540500	-0.00017700
N	-0.64296100	-1.66098600	0.00017600
N	-1.95023500	-1.51625500	0.00031700
N	-2.22174500	-0.20409600	0.00005800
H	-0.97719700	1.52895900	-0.00056000
Si	1.84897100	-0.21361100	-0.00043800
H	1.69328700	1.25259000	-0.00082000
H	2.00371300	-0.93428500	1.27019300
H	2.00350700	-0.93498200	-1.27067900
B	-3.73560700	0.45210100	0.00012700
F	-4.34532800	0.02159500	-1.15010900
F	-3.46736200	1.81558900	-0.00024500
F	-4.34497600	0.02215400	1.15076000
N	3.86556700	0.07705300	-0.00048900
C	5.03205500	0.22568700	-0.00008800
Na	7.35883100	0.46840200	0.00061000

3-BH_3···TA-SiF_3···NCNa

C	2.18589200	1.34763900	0.00003600
N	1.36303900	0.28265100	-0.00006000
N	2.11996700	-0.82202200	0.00010400
N	3.36629700	-0.38467800	0.00028000
N	3.45049400	0.94831900	-0.00001300
H	1.85432900	2.36936900	-0.00007400
Si	-0.49750600	0.14551500	0.00010200
F	-0.62149200	1.74954200	-0.00069900
F	-0.51451600	-0.65071100	1.38609300
F	-0.51461700	-0.65232800	-1.38495400
B	4.64359900	-1.36018700	0.00036200
H	5.24853200	-1.07712600	1.00654600
H	5.24829500	-1.07760300	-1.00610300
H	4.18133700	-2.47215400	0.00066800
N	-2.41285300	0.05873200	0.00018100
C	-3.57900500	-0.05627900	0.00006700
Na	-5.88906500	-0.48422400	-0.00111800

4-BH_3···TA-SiF_3···NCNa

C	2.25347800	0.81044400	-0.00015800
N	1.32232700	-0.14216000	-0.00013800
N	1.94856100	-1.32733400	-0.00002700
N	3.23430400	-1.10045700	-0.00046100
N	3.43359300	0.22184400	-0.00027500

H	2.08663600	1.86670500	-0.00012700
Si	-0.52094300	-0.05467100	0.00007300
F	-0.45698600	1.54976800	-0.00015600
F	-0.63280600	-0.84437300	1.38246000
F	-0.63315300	-0.84479500	-1.38204500
B	4.86520000	0.93076100	-0.00043800
H	5.41816100	0.57536900	1.00487100
H	4.59500200	2.10881500	-0.00030300
H	5.41784900	0.57553000	-1.00597600
N	-2.41249800	0.08890400	0.00028100
C	-3.57630000	0.14581600	0.00033700
Na	-5.79918400	0.21060300	0.00033100

3-BF_3···TA-SiF_3···NCNa

C	-1.09032000	1.77229900	0.00003700
N	-0.38872300	0.62405000	-0.00012100
N	-1.25671200	-0.39201900	0.00015300
N	-2.44329100	0.18179200	-0.00003200
N	-2.39227100	1.51080100	-0.00028500
H	-0.65095800	2.75233300	0.00001500
Si	1.45670400	0.28329900	-0.00002700
F	1.74434600	1.86506200	-0.00043600
F	1.37242700	-0.50553800	-1.38650000
F	1.37242200	-0.50467600	1.38693500
B	-3.89472100	-0.67047200	0.00014600
F	-4.52438300	-0.26522200	-1.14961100
F	-4.52369500	-0.26588600	1.15052600
F	-3.51791100	-1.98707900	-0.00033900
N	3.34145500	-0.01664100	0.00004800
C	4.48590600	-0.26819300	0.00004100
Na	6.72955600	-0.97969300	-0.00039500

4-BF_3···TA-SiF_3···NCNa

C	1.36550400	0.49289400	0.00005100
N	0.36609100	-0.39311200	0.00005400
N	0.90880200	-1.62907100	-0.00063800
N	2.21281000	-1.49709500	-0.00016500
N	2.50197800	-0.18730400	-0.00018400
H	1.27881300	1.56256000	0.00028100
Si	-1.49423300	-0.15720900	0.00034100
F	-1.28858400	1.43682500	0.00077600
F	-1.65589100	-0.94263700	1.38216600
F	-1.65616700	-0.94184500	-1.38190800

B	4.03184500	0.44859700	-0.00014200
F	3.78008500	1.81330300	0.00006700
F	4.62905800	0.00571900	-1.15077600
F	4.62913300	0.00538300	1.15032100
N	-3.37980200	0.14252800	0.00055700
C	-4.54033100	0.30468000	0.00025200
Na	-6.87978800	0.56069000	-0.00084900