

SUPPLEMENTARY MATERIAL

Physical Chemistry Chemical Physics

A theoretical study of the interactions of NF₃ with neutral ambidentate electron donor and acceptor molecules

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Total Energy (Hartree) and Dipole moment (μ) of dimers at MP2/6-311++g(d,p) Level

XY	Comp.	PG	MP2 Energy	Dipole
HF	A	C3V	-453.730468	2.06
HF	B	CS	-453.728948	2.80
HF	C	CS	-453.729120	2.28
HF	D	CS	-453.728292	2.22
HF	E	C3V	-453.727460	1.68
CIF	A	C3V	-912.676998	1.45
CIF	B	CS	-912.675599	2.21
CIF	C	CS	-912.675733	1.47
CIF	D	CS	-912.675948	1.88
CIF	E	C3V	-912.675625	1.10
HNC	A	C3V	-446.624389	2.76
HNC	B	CS	-446.623884	3.63
HNC	C	CS	-446.623870	3.10
HNC	D	CS	-446.623343	3.32
HNC	E	C3V	-446.621986	2.41
HCN	A	C3V	-446.652878	3.12
HCN	B	CS	-446.652785	4.03
HCN	C	CS	-446.652633	3.48
HCN	D	CS	-446.653178	3.68
HCN	E	C3V	-446.651917	2.94

Total Energy (Hartree) and Dipole moment (μ) of trimers at MP2/6-311++g(d,p) Level

XY	Comp.	PG	MP2 Energy	Dipole
HF	BD	CS	-554.010571	4.27
HF	CD	CS	-554.010835	3.10
HF	AE	CS	-554.011347	4.32
HF	CE	CS	-554.009996	3.56
CIF	BD	CS	-1471.904305	3.54
CIF	CD	CS	-1471.907160	3.33
CIF	AE	C3V	-1471.905475	2.96
CIF	CE	CS	-1471.904224	2.66
HNC	BD	CS	-539.801204	6.49
HNC	CD	CS	-539.801348	5.26
HNC	AE	C3V	-539.800310	7.13
HNC	CE	CS	-539.799853	4.93
HCN	BD	CS	-539.859550	7.17
HCN	CD	CS	-539.859539	5.67
HCN	AE	C3V	-539.858270	6.27

Variations in the properties of NF₃ and XY upon complexation and total complex volume obtained using the AIM methodology at the M05-2x/6-311++G(d,p) computational level

XY	Comp.	ΔE NF ₃ (kJ mol ⁻¹) ^a	Charge NF ₃ (e) ^b	Δ VOL NF ₃ (au) ^c	ΔE XY (kJ mol ⁻¹) ^a	Δ VOL XY (au) ^c
HF	A	-21.04	0.019	-8.45	11.35	-5.45
HF	B	-28.70	0.004	-2.63	21.36	-3.22
HF	C	-29.61	0.003	-3.17	22.31	-4.36
HF	D	-20.94	0.001	-6.70	13.80	-2.61
HF	E	-21.34	0.001	-1.31	17.99	-0.26
CIF	A	-31.45	0.017	-8.59	21.42	-4.50
CIF	B	-39.42	-0.004	-1.06	32.82	-2.21
CIF	C	-43.59	-0.003	-1.87	37.74	-3.16
CIF	D	-39.66	0.003	-3.74	33.35	-1.36
CIF	E	-41.61	0.003	-3.45	36.70	-2.22
HNC	A	-221.89	0.010	-5.63	216.30	0.15
HNC	B	-226.77	0.002	-1.85	221.13	-1.48
HNC	C	-227.84	0.001	-2.42	222.35	-2.16
HNC	D	-225.43	-0.011	1.44	219.49	-3.61
HNC	E	-225.28	-0.008	3.42	222.80	0.67
HCN	A	-241.23	0.004	-2.43	238.10	0.16
HCN	B	-243.46	-0.001	-0.65	239.13	-0.35
HCN	C	-245.47	-0.001	-0.67	241.30	-0.31

HCN	D	-234.42	-0.007	-0.66	227.03	-3.04
HCN	E	-236.65	-0.006	0.88	233.27	-0.29

^a Negative values mean a stabilization of the corresponding subunit in the complex

^b Positive values mean charge transfer from NF₃ to XY in the complex

^c Negative values mean a contraction of the volume of the corresponding subunit in the complex

DEF (NEDA analysis) values of calculated dimers at the M02x/6-311++G(d,p) computational level

XY	Comp.	DEF NF₃	DEF XY
HF	A	32.43	19.37
HF	B	17.11	12.13
HF	C	18.12	13.35
HF	D	23.64	15.02
HF	E	18.49	10.00
CIF	A	72.80	27.66
CIF	B	34.73	19.92
CIF	C	34.98	20.79
CIF	D	16.65	14.18
CIF	E	16.86	10.71
HNC	A	37.99	4.10
HNC	B	26.57	4.73
HNC	C	28.28	5.36
HNC	D	16.44	10.00
HNC	E	10.71	6.69
HCN	A	26.57	2.80
HCN	B	19.87	5.27
HCN	C	18.74	5.23
HCN	D	25.86	13.93
HCN	E	20.63	6.95

DEF (NEDA analysis) values of calculated trimers at the M02x/6-311++G(d,p) computational level

XY	Comp.	DEF NF₃	DEF X₁Y₁	DEF X₂Y₂
HF	BD	46.65	17.70	13.81
HF	CD	45.10	15.36	15.02
HF	AE	62.63	15.31	21.42
HF	CE	45.98	15.48	15.56
CIF	BD	55.61	13.56	22.80
CIF	CD	55.19	13.01	23.85
CIF	AE	93.72	10.42	29.87
CIF	CE	56.07	12.09	24.02
HNC	BD	50.38	12.26	5.77
HNC	CD	52.17	12.38	6.36
HNC	AE	57.99	10.59	4.81
HNC	CE	43.64	9.37	6.07
HCN	BD	53.51	17.70	6.65
HCN	CD	52.76	17.66	6.69
HCN	AE	52.55	8.74	3.26

Interaction Energies (kJ mol⁻¹) and cooperative effect energy (kJ mol⁻¹) of the calculated trimers

XY	Comp.	M052x/6-311++g(d,p)		MP2/6-311++g(d,p)		MP2/aug-cc-pvtz	
		E _{int}	Coop-Effect ^a	E _{int}	Coop-Effect ^a	E _{int}	Coop-Effect ^a
HF	BD	-16.42	-1.21	-13.59	-1.11	-12.48	-0.99
HF	CD	-15.95	-0.55	-14.28	-1.25	-12.70	-0.97
HF	AE	-16.11	-1.17	-15.63	-0.89	-14.82	-1.22
HF	CE	-13.59	-0.36	-12.08	-0.42	-10.53	-0.52
CIF	BD	-14.04	-0.32	-12.68	-0.45	-11.84	-0.24
CIF	CD	-13.00	-0.02	-*	-*	-*	-*
CIF	AE	-16.92	-1.49	-15.75	-0.47	-14.31	-0.48
CIF	CE	-12.07	-0.21	-12.47	-0.32	-9.40	-0.19
HNC	BD	-15.38	-1.53	-17.04	-1.68	-17.55	-1.69
HNC	CD	-15.09	-1.27	-17.42	-1.75	-17.29	-1.56
HNC	AE	-12.05	-0.89	-14.70	-1.12	-15.62	-1.38
HNC	CE	-11.91	0.09	-13.50	-0.20	-13.46	-0.45
HCN	BD	-14.37	-1.22	-14.42	-1.10	-15.11	-0.99
HCN	CD	-13.72	-1.08	-14.39	-1.10	-*	-*
HCN	AE	-9.51	-0.75	-11.05	-0.60	-11.60	-0.90

^a Negative values mean greater stability of the trimer compared to the sum of energies of the isolated dimers

* These geometries spontaneously evolve to other ones

Interaction distances (Å) calculated for the trimers computed in this study

XY	Comp.	M052x/6-311++g(d,p)		MP2/6-311++g(d,p)		MP2/aug-cc-pvtz	
		d ₁	d ₂	d ₁	d ₂	d ₁	d ₂
HF	BD	2.805	2.015	2.942	2.080	2.917	2.045
HF	CD	2.850	1.979	2.966	2.017	2.926	1.997
HF	AE	2.897	2.021	3.04	2.022	3.088	1.992
HF	CE	2.883	1.971	3.021	2.009	3.073	1.991
CIF	BD	2.868	2.793	2.978	2.923	2.986	2.859
CIF	CD	2.891	2.762	-*	-*	-*	-*
CIF	AE	2.930	2.727	2.952	2.803	3.052	2.68
CIF	CE	2.886	2.759	2.917	2.860	3.069	2.814
HNC	BD	3.296	2.110	3.333	2.107	3.226	2.092
HNC	CD	3.284	2.083	3.309	2.063	3.198	2.039
HNC	AE	3.426	2.217	3.547	2.153	3.506	2.118
HNC	CE	3.418	2.094	3.481	2.06	3.443	2.038
HCN	BD	3.092	2.324	3.165	2.351	3.058	2.379
HCN	CD	3.082	2.283	3.143	2.300	-	-
HCN	AE	3.236	2.478	3.353	2.435	3.279	2.375

* These geometries spontaneously evolve to other ones

Geometrical comparative analysis of the interactions distances (Å) calculated for the trimers and the corresponding dimers

XY	Comp.	Δd_1^a			Δd_2^a		
		M052x/ 6-311++g(d,p)	MP2/ 6-311++g(d,p)	MP2/aug- cc-pvtz	M052x/6- 311++g(d,p)	MP2/ 6-311++g(d,p)	MP2/aug- cc-pvtz
HF	BD	-0.044	-0.084	-0.075	-0.073	-0.051	-0.036
HF	CD	0.001	-0.060	-0.066	-0.050	-0.040	-0.036
HF	AE	-0.129	-0.067	-0.087	-0.036	-0.031	-0.028
HF	CE	-0.143	-0.086	-0.102	-0.058	-0.048	-0.042
CIF	BD	0.032	0.062	-0.044	-0.041	-0.049	-0.007
CIF	CD	0.055	—*	—*	-0.037	—*	—*
CIF	AE	0.017	-0.016	-0.020	-0.020	-0.030	-0.014
CIF	CE	-0.027	-0.051	-0.003	-0.040	-0.047	-0.021
HNC	BD	-0.064	-0.121	-0.100	-0.054	-0.063	-0.051
HNC	CD	-0.076	-0.145	-0.128	-0.048	-0.055	-0.050
HNC	AE	-0.155	-0.151	-0.187	-0.043	-0.052	-0.048
HNC	CE	-0.163	-0.217	-0.250	-0.037	-0.058	-0.051
HCN	BD	-0.062	-0.083	-0.081	-0.044	-0.050	-0.005
HCN	CD	-0.072	-0.105	—	-0.070	-0.053	—
HCN	AE	-0.049	-0.093	-0.089	-0.054	-0.051	-0.054

^a Negative values mean shortening of the distance in the trimer compared to isolated dimer.

* These geometries spontaneously evolve to other ones

Cartesian coordinates of the optimized structures at MP2/6-311++g(d,p) Level.

OPTIMIZED GEOMETRY OF DIMERS

HF:NF3 DIMER A

0,1
N,0.,0.,-0.0086525337
F,1.2295525966,0.,-0.5957159492
F,-0.6147762983,-1.064823784,-0.5957159492
F,-0.6147762983,1.064823784,-0.5957159492
H,0.,0.,2.0441122344
F,0.,0.,2.9644742123

HF:NF3 DIMER B

0,1
N,-1.0263716939,0.7280886578,0.
F,-1.1561234542,-0.1155792984,1.0628710359
F,-1.1561234542,-0.1155792984,-1.0628710359
F,0.3363452155,0.9797471793,0.
H,1.884913257,-0.4836413707,0.
F,2.5374511298,-1.1287458696,0.

HF:NF3 DIMER C

0,1
N,-0.3893188493,-1.2109685169,0.
F,-0.0973147323,-2.0093082861,1.0617240374
F,-0.0973147323,-2.0093082861,-1.0617240374
F,0.6893452347,-0.3332626947,0.
H,0.2345355147,1.6728718478,0.
F,-0.0384942056,2.5492238259,0.

HF:NF3 DIMER D

0,1
N,0.2418344692,1.415052202,0.
F,-0.5551375994,1.0933383378,-1.0644841919
F,-0.5551375994,1.0933383378,1.0644841919
F,0.1757680949,2.7885352704,0.
H,0.158695618,-2.3904323858,0.
F,0.6045741626,-1.589175705,0.

HF:NF3 DIMER E

0,1
N,0.,0.,0.2329942125
F,1.2312271049,0.,0.8306395705
F,-0.6156135525,-1.0662739507,0.8306395705
F,-0.6156135525,1.0662739507,0.8306395705
F,0.,0.,3.6831190759
H,0.,0.,4.600063685

CIF:NF3 DIMER A

0,1
N,0.,0.,0.0002836637
F,1.229960333,0.,-0.5917857575
F,-0.6149801665,-1.065176894,-0.5917857575
F,-0.6149801665,1.065176894,-0.5917857575
Cl,0.,0.,2.8335262083
F,0.,0.,4.5108547283

CIF:NF3 DIMER B

0,1
N,-0.0006649087,-0.9260679004,0.
F,-0.7703598855,-0.5514816138,-1.0638390557
F,-0.7703598855,-0.5514816138,1.0638390557
F,0.9789065494,0.0438813614,0.
Cl,0.155394938,2.8992138076,0.
F,-0.4049507005,4.4775785307,0.

CIF:NF3 DIMER C

0,1
N,0.622712,1.5128,0.
F,0.622712,2.367033,1.063675
F,0.622712,2.367033,-1.063675
F,-0.680284,1.055747,0.
Cl,-0.487052,-1.845303,0.
F,-0.129485,-3.480863,0.

CIF:NF3 DIMER D

0,1
N,0.233361025,1.3924089451,0.0000000017
F,-0.5737727357,1.0979394195,-1.0644787389
F,-0.573772738,1.0979394131,1.0644787388
F,0.2191150967,2.7655258466,0.0000000058
F,0.5305627989,-1.5089022781,-0.0000000066
Cl,0.1934005948,-3.1483386687,-0.0000000118

CIF:NF3 DIMER E

0,1
N,0.,0.,0.0399976669
F,1.2302953773,0.,0.6395044282
F,-0.6151476886,-1.0654670509,0.6395044282
F,-0.6151476886,1.0654670509,0.6395044282
F,0.,0.,3.3401382555
Cl,0.,0.,5.0139522809

HNC:NF3 DIMER A

O,1
N,-0.4527296509,0.,0.
F,0.1364357712,1.230012086,-0.0000000005
F,0.1364357712,-0.6150060434,-1.0652217132
F,0.1364357712,-0.6150060426,1.0652217137
C,-4.8432234482,0.,0.
N,-3.661903524,0.,0.
H,-2.6579300356,0.,0.

HNC:NF3 DIMER B

O,1
N,-1.6356733094,0.760758897,0.
F,-1.6685186622,-0.0922732845,1.0630188968
F,-1.6685186622,-0.0922732845,-1.0630188968
F,-0.3091797358,1.1636598991,0.
H,1.5103977573,-0.0181560231,0.
N,2.372851246,-0.5276072861,0.
C,3.3901499761,-1.1281389778,0.

HNC:NF3 DIMER C

O,1
N,-1.2407036234,-0.4044793008,0.
F,-2.0264388913,-0.0810137328,-1.0619673703
F,-2.0264388913,-0.0810137328,1.0619673703
F,-0.3201803851,0.6380478266,0.
H,1.7628035253,0.255574605,0.
N,2.7364743583,0.0189282303,0.
C,3.8841840637,-0.2609259124,0.

HNC:NF3 DIMER D

O,1
N,0.245256262,1.7660023658,0.0000000017
F,-0.5823624573,1.5415978324,-1.064171572
F,-0.5823624596,1.5415978276,1.0641715727
F,0.3392160991,3.1418391351,0.0000000049
H,0.2596354469,-3.8696328828,-0.0000000108
C,0.2134419185,-1.6881835529,-0.000000006
N,0.2385740963,-2.8690161256,-0.0000000086

HNC:NF3 DIMER E

O,1
N,0.,0.,-0.0055138922
F,1.2311579504,0.,0.5914811305
F,-0.6155789752,-1.0662140611,0.5914811305
F,-0.6155789752,1.0662140611,0.5914811305
C,0.,0.,4.078419837
N,0.,0.,5.2599097332
H,0.,0.,6.2606623578

HCN:NF3 DIMER A

O,1
N,-0.3172577747,0.,0.
F,0.2768938488,1.2300964029,-0.0000000005
F,0.2768938488,-0.6150482019,-1.0652947338
F,0.2768938488,-0.615048201,1.0652947343
N,-5.0439992369,0.,0.
C,-3.8724475671,0.,0.
H,-2.8034562997,0.,0.

HCN:NF3 DIMER B

O,1
N,-0.2875022848,-0.069728907,0.
F,-1.0830475701,0.2469079811,-1.0639447224
F,-1.0830475701,0.2469079811,1.0639447224
F,0.6168935571,0.9719528094,0.
H,0.2788773496,3.34854581,0.
C,0.1783810678,4.4120888781,0.
N,0.0685244506,5.5783954464,0.

HCN:NF3 DIMER C

O,1
N,-0.41319707,-1.3993746075,0.
F,-0.0816554565,-2.1853040283,1.0632571126
F,-0.0816554565,-2.1853040283,-1.0632571126
F,0.6120499,-0.4711739612,0.
H,0.2559646851,1.8548255422,0.
C,0.0497576521,2.9030583804,0.
N,-0.1769790441,4.052334116,0.

HCN:NF3 DIMER D

O,1
N,0.2913306156,1.6671629143,0.0000000018
F,-0.5005096209,1.3362788835,-1.0641872849
F,-0.5005096231,1.3362788787,1.0641872854
F,0.2049896832,3.0427787464,0.0000000049
N,0.4945529024,-1.5748932689,-0.0000000053
C,0.2031956949,-2.7093044904,-0.0000000082
H,-0.061980129,-3.7439981049,-0.0000000108

HCN:NF3 DIMER E

O,1
N,0.,0.,-0.0321285402
F,1.2313675287,0.,0.5647731336
F,-0.6156837643,-1.0663955612,0.5647731336
F,-0.6156837643,1.0663955612,0.5647731336
N,0.,0.,3.7827581951
C,0.,0.,4.9541362663
H,0.,0.,6.0222280571

OPTIMIZED GEOMETRY OF TRIMERS

HF:NF₃:HF TRIMER BD

0,1
N,-0.5262763088,0.7996072217,0.
F,0.3244167478,0.7510634386,1.0615994156
F,0.3244167478,0.7510634386,-1.0615994156
F,-0.8988661658,2.1430046049,0.
F,0.0463503548,-2.0863801146,0.
H,0.5724846831,-2.8376878127,0.
H,0.4415660057,3.7331436167,0.
F,1.0237720792,4.443139991,0.

HF:NF₃:HF TRIMER CD

0,1
N,0.5270614889,-0.1963262758,0.
F,1.1592925477,-0.7603405291,1.0601572147
F,1.1592925477,-0.7603405291,-1.0601572147
F,1.0745486669,1.0923872108,0.
F,-0.6762010303,-2.9077948205,0.
H,-1.5147935628,-3.2796267406,0.
H,-0.3110817215,2.5585654702,0.
F,-0.9954279348,3.1712572127,0.

HF:NF₃:HF TRIMER AE

0,1
N,-0.0313553784,-0.0543091087,0.1412327341
F,1.1718984385,-0.1015194189,-0.4939874217
F,-0.669958559,-1.1604022664,-0.3298383138
F,-0.6738676174,0.9641341073,-0.4939874217
H,0.0564238923,0.0977290484,2.156034089
F,0.0928833596,0.1608786983,3.0745414504
F,-0.1729598723,-0.2995752872,-3.2133544446
H,-0.2060572439,-0.3569016166,-4.1278577215

HF:NF₃:HF TRIMER CE

0,1
N,-0.9925727157,0.0546832584,0.
F,-1.0674469205,-0.7898852878,1.0624080336
F,0.3548896597,0.3969288123,0.
F,-1.0674469205,-0.7898852878,-1.0624080336
F,1.2207425812,-2.4977731461,0.
H,1.9234049519,-3.0872469463,0.
H,0.8830618549,2.334854547,0.
F,1.0544805313,3.2372045316,0.

CIF:NF3:CIF TRIMER BD

0,1
N,-0.8360985972,0.6206860604,0.
F,0.0190273172,0.6268857021,1.0630692271
F,0.0190273172,0.6268857021,-1.0630692271
F,-1.3005643438,1.9236808052,0.
F,0.3105267852,-2.1282225019,0.
Cl,0.9097254304,-3.6906196082,0.
Cl,0.5060081666,4.221872081,0.
F,1.5661424997,5.5186736272,0.

CIF:NF3:CIF TRIMER CD

0,1
N,1.3043075969,-0.0296539414,0.
F,1.6145313568,-0.8284562645,1.0653399894
F,1.6145313568,-0.8284562645,-1.0653399894
F,2.3431916677,0.8679821057,0.
F,-1.9322241305,-3.0368244795,0.
Cl,-1.8267774214,-1.3638125753,0.
Cl,-0.8352019558,2.6838389097,0.
F,-1.9127485484,1.4005472031,0.

CIF:NF3:CIF TRIMER AE

0,1
N,-0.3658741248,0.,0.
F,0.2240687336,1.2303387086,-0.0000000005
F,0.2240687336,-0.6151693547,-1.0655045766
F,0.2240687336,-0.6151693538,1.0655045771
F,2.90713367,0.,0.
Cl,4.5809435799,0.,0.
F,-4.8471707211,0.,0.
Cl,-3.1689289986,0.,0.

CIF:NF3:CIF TRIMER CE

0,1
N,-1.3391390244,0.5991688364,0.
F,-1.7013908555,-0.173488836,1.0637164889
F,0.034697226,0.4625577116,0.
F,-1.7013908555,-0.173488836,-1.0637164889
F,-0.1485390037,-2.4483734755,0.
Cl,0.7085923101,-3.8859957153,0.
Cl,1.2567485652,3.0486834439,0.
F,1.7904607122,4.6362624129,0.

HNC:NF3:HNC TRIMER BD

0,1
N,-0.4733532333,0.899342386,0.
F,0.3760932467,0.851335257,1.0614618286
F,0.3760932467,0.851335257,-1.0614618286
F,-0.8406656203,2.2489465692,0.
H,0.4964463904,-4.5274687106,0.
C,0.1828152333,-2.3683496868,0.
N,0.3526720458,-3.5366977848,0.
H,0.4025809434,3.9496291663,0.
N,0.9316282848,4.8014132136,0.
C,1.5535686484,5.8054869847,0.

HNC:NF3:HNC TRIMER CD

0,1
N,0.1370188128,-0.6088196197,0.
F,0.6730826423,-1.2649818967,-1.0600230145
F,0.6730826423,-1.2649818967,1.0600230145
F,-1.1757889542,-1.1057568476,0.
H,4.7903683442,2.2759420455,0.
C,3.0518014072,0.9576772075,0.
N,3.9931251204,1.6702051629,0.
H,-2.6930353026,0.2918235066,0.
N,-3.4236827788,0.9792512951,0.
C,-4.2818760671,1.7906713086,0.

HNC:NF3:HNC TRIMER AE

0,1
N,-0.4871791701,0.,0.
F,0.0960702672,1.231161142,-0.0000000005
F,0.0960702672,-0.6155805715,-1.0662168249
F,0.0960702672,-0.6155805706,1.0662168254
C,3.4221121406,0.,0.
N,4.6030777991,0.,0.
H,5.6041226449,0.,0.
C,-4.8272389939,0.,0.
N,-3.6459988283,0.,0.
H,-2.6404210207,0.,0.

HNC:NF3:HNC TRIMER CE

0,1
N,-1.5386954569,0.274811937,0.
F,-1.7060862877,-0.555725099,1.0629567777
F,-0.1630426042,0.4694083694,0.
F,-1.7060862877,-0.555725099,-1.0629567777
C,0.9428393389,-2.8310180829,0.
N,1.6711860989,-3.7607951172,0.
H,0.7536775519,2.3136813861,0.
N,1.1850678266,3.219202154,0.
C,1.6940444024,4.2851095058,0.
H,2.2893904317,-4.5482040505,0.

HCN:NF3:HCN TRIMER BD

0,1
N,-0.611479074,0.800620443,0.
F,0.2419322566,0.774585318,1.0624165398
F,0.2419322566,0.774585318,-1.0624165398
F,-1.0159279425,2.1309706439,0.
H,0.6539661669,-4.4526798254,0.
N,0.1778861828,-2.2646288379,0.
C,0.4270029077,-3.4088310179,0.
H,0.4548743163,3.9654814588,0.
C,1.0615804431,4.8451315463,0.
N,1.726167308,5.8097021578,0.

HCN:NF3:HCN TRIMER CD

0,1
N,0.2396715444,0.6853262553,0.
F,0.8389670555,1.2882633528,1.0614922229
F,0.8389670555,1.2882633528,-1.0614922229
F,-1.0133863456,1.2976369264,0.
H,4.6153980256,-2.4177472105,0.
N,2.9240661925,-0.9500685417,0.
C,3.8084920804,-1.7175855317,0.
H,-2.7001100366,-0.2656387196,0.
C,-3.467943925,-1.0092228645,0.
N,-4.3090803372,-1.8245549765,0.

HCN:NF3:HCN TRIMER AE

0,1
N,-0.3364668515,0.,0.
F,0.2523055762,1.2313068337,-0.0000000005
F,0.2523055762,-0.6156534173,-1.0663429976
F,0.2523055762,-0.6156534164,1.0663429981
N,3.3707613289,0.,0.
C,4.5420658534,0.,0.
H,5.6103375262,0.,0.
N,-5.0132780573,0.,0.
C,-3.8416893966,0.,0.
H,-2.7719617645,0.,0.