

Supporting Information

Molecular Electrostatics for Probing Lone Pair- π Interactions

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Table S1. MESP topography features of neutral molecules.

System	CP	No. of CPs	Distance of CP from lone pair atom (Å)	Location of CP	$V_{\min}$ (kcal/mol)	Largest eigenvalue, LE (a.u.)
H ₂ O	(3,+3)	2	1.24	One above and one below the plane of the molecule forming a tetrahedral structure.	-54.0	0.1304
N ₂	(3,+3)	2	1.54	Along the internuclear axis close to N atom.	-11.4	0.0320
CO ₂	(3,+3)	2	1.48	Along the internuclear axis close to O atom.	-14.3	0.0350
H ₂ CO	(3,+3)	2	1.29	Two on each side of the C2 axis close to the O atom.	-39.2	0.0960
H ₂ S	(3,+3)	2	1.78	One above and one below the plane of the molecule.	-25.8	0.0491
HCN	(3,+3)	1	1.37	Along the internuclear axis near the N atom.	-43.2	0.0858
NCCH ₃	(3,+3)	1	1.34	Along the internuclear axis near the N atom.	-53.0	0.1429
HF	Degenerate ring	-	1.30	Degenerate ring 1.30 Å away from the F end	-29.0	0.0769
HCl	Degenerate ring	-	1.90	Degenerate ring 1.90 Å away from the Cl end	-12.3	0.0219
CH ₃ OH	(3,+3)	2	1.24	Two CPs equidistant from the O atom forming 117.5° with the OH bond.	-52.2	0.1310
PH ₃	(3,+3)	1	1.88	Along the C3 axis near the P atom	-23.8	0.0403
O(CH ₃) ₂	(3,+3)	1	1.24	One above and one below the plane of the molecule near the O atom.	-48.3	0.1260
N(CH ₃) ₃	(3,+3)	1	1.26	Along the C3 axis close to the N atom.	-58.9	0.1491
NH ₂ COH	(3,+3)	4	1.25	Two CPs in the plane of the molecule near the O atom, two CPs above and below the plane at 1.60 Å from the N atom.	-55.6	0.1223
Pyrimidine	(3,+3)	2	1.29	One CP corresponding to each N atom lying in the plane of the molecule.	-53.2	0.1309
Pyridine	(3,+3)	1	1.28	One CP in the molecular plane at close to the N atom.	-61.2	0.1411
Furan	(3,+3)	5	1.31	One CP on the C2 axis near the O atom, one CP each above and below each C=C bond.	-28.4	0.0832
Imidazole	(3,+3)	3	1.28	One CP on the C2 near the N atom, one CP each above and below the C=C bond.	-68.4	0.1433

Pyrazine	(3,+3)	2	1.29	On the C2 axis at 1.29 Å from each N atom	-51.1	0.1291
N ₃ H	(3,+3)	2	1.41	One CP for each terminal N atom at 1.41 Å and 1.50 Å respectively.	-30.3	0.0725

Table S2. MESP topography features of radicals and anions.

System	CP	No .of CPs	Distance of CP from lone pair atom (Å)	Location of CP	$V_{\min}$ (kcal/mol)	Largest eigenvalue, LE (a.u.)
HO•	(3,+3)	2	1.29	One above and one below the plane of the molecule near the O atom.	-37.0	0.0975
CH ₃ O•	(3,+3)	2	1.28	One above and one below the C2 axis near the O atom.	-41.3	0.1056
CH ₃ OO•	(3,+3)	3	1.28	Two CPs in the molecular plane at 1.28 Å from the radical O and one CP on the adjacent O atom.	-44.2	0.1029
HCO•	(3,+3)	2	1.40	One CP in the molecular plane at 1.40 Å from the O atom and one CP on the adjacent C atom.	-24.2	0.0541
CH ₃ CO•	(3,+3)	2	1.35	One CP in the molecular plane at 1.35 Å from the O atom and one CP on the C atom.	-33.8	0.0711
CH ₃ NH•	(3,+3)	1	1.29	One CP above the C-N plane at 1.35 Å from the N atom and 123.6° with the NH bond.	-63.5	0.1387
HOO•	(3,+3)	3	1.29	Two CPs in the plane of the molecule near the radical O atom and one CP 1.40 Å from the adjacent O atom.	-38.9	0.0186
F ⁻	Degenerate surface	-	1.08	Degenerate surface at 1.08 Å from F atom.	-240.3	0.3205
CH ₃ CO ₂ ⁻	(3,+3)	4	1.15	Two CPs each on both sides of each O atom.	-188.8	0.2099
HCO ₂ ⁻	(3,+3)	4	1.16	Two CPs each on both sides of each O atom.	-186.9	0.2045
NO ₃ ⁻	(3,+3)	6	1.20	Two CPs each on both sides of each O atom.	-167.7	0.1769

Cl ⁻	Degenerate surface	-	1.57	Degenerate surface at 1.57 Å from Cl atom.	-171.0	0.1298
Br ⁻	Degenerate surface	-	1.74	Degenerate surface at 1.74 Å from Br atom.	-155.7	0.1019
H ₂ PO ₄ ⁻	(3,+3)	4	1.19	One CP corresponding to each O atom.	-168.4	0.1606

Table S3. SCF energies of all optimized HFB:lone pair complexes in au.

Complex	SCF Energy
HFB:H ₂ O	-904.207559
HFB:N ₂	-937.307643
HFB:CO ₂	-1016.395200
HFB:H ₂ CO	-942.287732
HFB:H ₂ S	-1227.161618
HFB:HCN	-921.203887
HFB:NCCH ₃	-960.541625
HFB:HF	-928.227782
HFB:HCl	-1288.571848
HFB:OHMe	-943.507338
HFB:PH ₃	-1170.911997
HFB:OMe ₂	-982.814291
HFB:NMe ₃	-1002.261930
HFB:NH ₂ COH	-997.693544
HFB:Pyrimidine	-1092.121292
HFB:Pyridine	-1076.079283
HFB:Furan	-1057.817256
HFB:Imidazole	-1054.016931
HFB:Pyrazine	-1092.114643
HFB:N ₃ H	-992.589713
HFB:HO [•]	-903.516527
HFB:CH ₃ O [•]	-942.838331
HFB:CH ₃ OO [•]	-1018.013248
HFB:HCO [•]	-941.635621
HFB:CH ₃ CO [•]	-980.970072
HFB:CH ₃ NH [•]	-922.973959
HFB:HOO [•]	-978.699582
HFB:F ⁻	-927.656741
HFB:CH ₃ CO ₂ ⁻	-1056.351810
HFB:HCO ₂ ⁻	-1017.028337
HFB:NO ₃ ⁻	-1108.206977
HFB:Cl ⁻	-1288.057345
HFB:Br ⁻	-3401.873332
HFB:H ₂ PO ₄ ⁻	-1471.471182

Table S4. SCF energies of optimized complexes of 1,2,4,5-tetracyanobenzene (TCB), 1,3,5-trinitrobenzene (TNB), 2,4,6-trifluoro-1,3,5-triazine (CNF) with lone pair molecules in au.

System	CNF	TNB	TCB
H ₂ O	-654.6532	-922.3519	-677.7286
N ₂	-687.7504	-955.4503	-710.8265
CO ₂	-766.8386	-1034.5382	-789.9147
H ₂ S	-977.6048	-1245.3061	-1000.6827
N(CH ₃) ₃	-752.7069	-1020.4085	-775.7837
O(CH ₃) ₂	-733.2587	-1000.9589	-756.3342
Imidazole	-804.4626	-1072.1670	-827.5402
Pyridine	-826.5246	-1094.2276	-849.6013
Furan	-808.2628	-1075.9675	-831.3332
HCO•	-692.0792	-959.7809	-715.1587
CH ₃ O•	-693.2805	-960.9824	-716.3605
H ₂ PO ₄ ⁻	-1221.9153	-1489.6352	-1245.0124
NO ₃ ⁻	-858.6560	-1126.3718	-881.7480
Cl ⁻	-1038.5032	-1306.2275	-1061.6018
Br ⁻	-3152.3180	-3420.0424	-3175.4166
HCO ₂ ⁻	-767.4786	-1035.1989	-790.5744

Table S5. AIM parameters of HFB:lone pair complexes

Lone pair species	No of RCPs	No of CCPs	$\rho(r)$ at CCP (e/Å ³)	$\nabla^2(\rho(r))$ at CCP (e/Å ⁵)
H ₂ O	3	1	0.005	-0.006
N ₂	7	1	0.005	-0.006
CO ₂	2	1	0.003	-0.003
H ₂ CO	3	1	0.004	-0.005
H ₂ S	1	0		
HCN	2	1	0.005	-0.006
NCCH ₃	2	1	0.005	-0.006
HF	2	1	0.003	-0.004
HCl	2	1	0.004	-0.004
OHMe	3	1	0.005	-0.006
PH ₃	7	1	0.005	-0.005
OMe ₂	2	1	0.005	-0.006
NMe ₃	5	1	0.007	-0.008
NH ₂ COH	2	1	0.005	-0.006

Pyrimidine	4	1	0.005	-0.006
Pyridine	4	1	0.005	-0.006
Furan	4	1	0.005	-0.006
Imidazole	3	1	0.005	-0.006
Pyrazine	4	1	0.005	-0.006
N ₃ H	3	1	0.005	-0.006
OH [•]	1	0		
CH ₃ O [•]	1	0		
CH ₃ OO [•]	3	0		
HCO [•]	2	1	0.004	-0.005
CH ₃ CO [•]	5	1	0.004	-0.005
CH ₃ NH [•]	2	1	0.005	-0.006
HOO [•]	3	1	0.005	-0.006
F ⁻	2	1	0.008	-0.011
CH ₃ CO ₂ ⁻	3	1	0.006	-0.008
HCO ₂ ⁻	3	1	0.006	-0.007
NO ₃ ⁻	3	1	0.006	-0.008
Cl ⁻	5	1	0.006	-0.006
Br ⁻	2	1	0.005	-0.005
H ₂ PO ₄ ⁻	4	1	0.005	-0.006

Table S6. Eigen values associated with (3, +3) CPs of lone pair bearing molecules.

Lone pair species	Eigen values		
	EVal-1	EVal-2	EVal-3
H ₂ O	0.0064	0.0327	0.1304
N ₂	0.0066	0.0066	0.0320
CO ₂	0.0004	0.0004	0.0350
H ₂ CO	0.0124	0.0960	0.0151
H ₂ S	0.0491	0.0143	0.0095
HCN	0.0118	0.0118	0.0858
NCCH ₃	0.1429	0.0181	0.0181
HF	0.0769	0.0000	0.0121
HCl	0.0219	0.0000	0.0075
OHMe	0.0354	0.1310	0.0059
PH ₃	0.0098	0.0098	0.0403
OMe ₂	0.0364	0.1260	0.0028
NMe ₃	0.0435	0.0435	0.1491
NH ₂ COH	0.1223	0.0143	0.0110
Pyrimidine	0.0380	0.1309	0.0212
Pyridine	0.0221	0.1411	0.0398
Furan	0.0259	0.0832	0.0042
Imidazole	0.0094	0.0039	0.0238

Pyrazine	0.0380	0.1291	0.0227
N ₃ H	0.0223	0.0725	0.0017
OH [•]	0.0975	0.0250	0.0176
CH ₃ O [•]	0.0173	0.1056	0.0222
CH ₃ OO [•]	0.1029	0.0307	0.0179
HCO [•]	0.0210	0.0045	0.0063
CH ₃ CO [•]	0.0711	0.0064	0.0079
CH ₃ NH [•]	0.0327	0.1387	0.0224
HOO [•]	0.0950	0.0303	0.0186
F ⁻	0.3205	0.0000	0.0000
CH ₃ CO ₂ ⁻	0.2099	0.0241	0.0157
HCO ₂ ⁻	0.0230	0.2045	0.0155
NO ₃ ⁻	0.1769	0.0330	0.0148
Cl ⁻	0.1298	0.0000	0.0000
Br ⁻	0.1019	0.0000	0.0000
H ₂ PO ₄ ⁻	0.0090	0.1606	0.0278

Table S7. Interaction energies (E_{int}), distance parameters (R_{hfb} and R_{c}) and θ , θ' and $\Delta\theta$ values for lone pair- π complexes of 1,2,4,5-tetracyanobenzene (TCB), 2,4,6-trifluoro-1,3,5-triazine (CNF) and 1,3,5-trinitrobenzene (TNB).

Host	System	E_{int} (kcal/mol)	R_{hfb} (Å)	R_{c} (Å)	θ	θ'	$\Delta\theta$
2,4,6-trifluoro-1,3,5-triazine (CNF)	H ₂ O	-5.0	2.92	3.24	119.8	128.1	8.3
	N ₂	-1.5	3.01	3.32	180	179.5	-0.5
	CO ₂	-2.2	3.12	3.42	180	178.9	-1.1
	H ₂ S	-3.1	4.32	3.68	102.5	98.1	-4.4
	N(CH ₃) ₃	-7.6	3.00	3.28	107.9	133.5	25.6
	O(CH ₃) ₂	-6.3	2.92	3.19	121.3	110.5	-10.8
	Imidazole	-7.1	2.92	3.21	127.8	128.3	0.5
	Pyridine	-6.6	2.97	3.28	121.6	121.2	-0.4
	Furan	-4.6	3.17	3.29	126.6	94.6	-32.0
	HCO [•]	-2.8	3.83	3.11	141.3	141.5	0.2
	CH ₃ O [•]	-3.7	3.75	3.04	124.2	109.5	-14.7
	H ₂ PO ₄ ⁻	-16.7	2.84	3.00	124.2	96.4	-27.8
	NO ₃ ⁻	-18.6	2.77	3.06	107.1	87.6	-19.5
	Cl ⁻	-16.8	3.36	2.88	-		
	Br ⁻	-14.5	3.54	3.07	-		
	HCO ₂ ⁻	-22.3	2.73	3.00	111.2	106.0	-5.2
1,3,5-trinitrobenzene (TNB)	H ₂ O	-4.2	2.98	3.21	119.8	137.3	17.5
	N ₂	-1.2	3.12	3.41	180	178.5	-1.5
	CO ₂	-1.9	3.08	3.37	180	179.8	-0.2
	H ₂ S	-3.4	4.20	3.59	102.5	97.1	-5.4
	N(CH ₃) ₃	-8.1	2.98	3.28	107.9	107.6	-0.3

	O(CH ₃) ₂	-6.1	2.93	3.22	121.3	108.9	-12.4
	Imidazole	-8.7	3.21	3.48	127.8	91.5	-36.3
	Pyridine	-7.3	3.18	3.43	121.6	92.2	-29.4
	Furan	-6.9	3.25	3.26	126.6	94.6	-32.0
	HCO [•]	-3.6	3.37	3.34	141.3	96.7	-44.6
	CH ₃ O [•]	-5.0	3.17	2.67	124.2	135.9	11.7
	H ₂ PO ₄ ⁻	-27.9	2.81	2.93	124.2	95.5	-28.7
	NO ₃ ⁻	-27.9	3.14	2.50	107.1	103.4	-3.7
	Cl ⁻	-31.5	3.21	2.51	-		
	Br ⁻	-29.4	3.41	2.72	-		
	HCO ₂ ⁻	-34.7	2.75	3.04	111.2	98.7	-12.5
1,2,4,5-tetracyanobenzene (TCB)	H ₂ O	-4.7	2.92	3.24	119.8	128.1	8.3
	N ₂	-1.4	3.01	3.32	180	179.5	-0.5
	CO ₂	-2.2	3.12	3.42	180	178.9	-1.1
	H ₂ S	-4.2	4.32	3.68	102.5	98.1	-4.4
	N(CH ₃) ₃	-8.1	3.00	3.28	107.9	133.5	25.6
	O(CH ₃) ₂	-6.1	2.92	3.19	121.3	110.5	-10.8
	Imidazole	-7.9	2.92	3.21	127.8	128.3	0.5
	Pyridine	-6.9	2.97	3.28	121.6	121.2	-0.4
	Furan	-1.1	3.17	3.29	126.6	94.6	-32.0
	HCO [•]	-5.1	3.83	3.11	141.3	141.5	0.2
	CH ₃ O [•]	-6.9	3.75	3.04	124.2	109.5	-14.7
	H ₂ PO ₄ ⁻	-29.5	2.84	3.00	124.2	96.4	-27.8
	NO ₃ ⁻	-28.2	2.77	3.06	107.1	87.6	-19.5
	Cl ⁻	-30.7	3.36	2.88	-		
	Br ⁻	-28.6	3.54	3.07	-		
	HCO ₂ ⁻	-34.7	2.73	3.00	111.2	106.0	-5.2

Table S8. Cartesian coordinates of all optimized HFB:lone pair complexes.

HFB:H₂O				HFB:N₂			
6	1.270997000	0.564357000	-0.311910000	6	0.241869000	1.365835000	-0.480072000
6	0.148914000	1.380226000	-0.317923000	6	-1.063086000	0.892151000	-0.480357000
6	1.126380000	-0.815712000	-0.312237000	6	1.305288000	0.472825000	-0.478137000
6	-1.118224000	0.815433000	-0.323269000	6	-1.304298000	-0.475090000	-0.478083000
6	-0.140677000	-1.380554000	-0.318741000	6	1.064055000	-0.894424000	-0.475698000
6	-1.262854000	-0.564683000	-0.323664000	6	-0.240880000	-1.368116000	-0.476306000
9	2.486217000	1.105559000	-0.291731000	9	0.474060000	2.673707000	-0.475718000
9	2.202669000	-1.597044000	-0.291691000	9	2.553287000	0.927756000	-0.471497000
9	-0.279745000	-2.702479000	-0.303804000	9	2.081735000	-1.748549000	-0.467526000
9	-2.478597000	-1.105971000	-0.313274000	9	-0.473105000	-2.675951000	-0.467743000
9	-2.194985000	1.596923000	-0.312194000	9	-2.552299000	-0.930008000	-0.472145000
9	0.287671000	2.702165000	-0.302096000	9	-2.080767000	1.746304000	-0.476280000
8	-0.026668000	0.000220000	2.659988000	7	-0.001312000	0.004361000	2.498332000

1	-0.825742000	0.004887000	3.192573000	7	-0.004958000	0.010151000	3.600254000
1	0.682782000	0.006579000	3.307093000				
HFB:CO2				H2CO			
6	0.616643000	-1.001968000	1.063747000	6	1.323252000	0.259542000	-0.632306000
6	0.522930000	0.331193000	1.439519000	6	0.435595000	1.322526000	-0.544964000
6	0.934214000	-1.333199000	-0.246734000	6	0.844979000	-1.043095000	-0.640060000
6	0.745657000	1.333602000	0.505265000	6	-0.929058000	1.083075000	-0.467224000
6	1.158311000	-0.330692000	-1.181306000	6	-0.520049000	-1.282604000	-0.561273000
6	1.064007000	1.002869000	-0.805308000	6	-1.407471000	-0.219373000	-0.476197000
9	0.389808000	-1.960870000	1.955067000	9	2.631928000	0.488136000	-0.691727000
9	1.017049000	-2.609053000	-0.608627000	9	1.695524000	-2.062870000	-0.710755000
9	1.459191000	-0.647603000	-2.436178000	9	-0.976265000	-2.531540000	-0.556515000
9	1.272983000	1.961979000	-1.700859000	9	-2.713942000	-0.449088000	-0.388471000
9	0.644303000	2.609263000	0.862666000	9	-1.777596000	2.102345000	-0.371194000
9	0.204566000	0.647862000	2.689983000	9	0.893091000	2.570792000	-0.524224000
6	-3.416544000	-0.001192000	-0.523414000	6	0.317613000	-0.137112000	3.587826000
8	-4.542970000	-0.026029000	-0.797230000	1	-0.514261000	-0.223595000	4.320731000
8	-2.287332000	0.023796000	-0.248906000	1	1.338916000	-0.109294000	4.026984000
				8	0.126440000	-0.078105000	2.405431000
HFB:H2S				HFB:HCN			
6	-0.685893000	0.125649000	-1.069992000	6	1.130124000	-0.475926000	-0.749261000
6	-0.184058000	-1.134378000	-0.778380000	6	0.897969000	0.891104000	-0.697072000
6	0.005660000	1.259623000	-0.669832000	6	0.088071000	-1.365501000	-0.529433000
6	1.015267000	-1.261843000	-0.091464000	6	-0.375811000	1.369056000	-0.423728000
6	1.205590000	1.134258000	0.017249000	6	-1.185904000	-0.887732000	-0.255693000
6	1.711151000	-0.127005000	0.305358000	6	-1.417616000	0.479399000	-0.202791000
9	-1.858541000	0.246536000	-1.687674000	9	2.354334000	-0.932685000	-0.997748000
9	-0.498266000	2.464878000	-0.917725000	9	0.313034000	-2.675624000	-0.568774000
9	1.867589000	2.219344000	0.402237000	9	-2.181960000	-1.739657000	-0.034605000
9	2.860462000	-0.247996000	0.959097000	9	-2.636418000	0.936338000	0.067962000
9	1.493216000	-2.467560000	0.193823000	9	-0.595893000	2.679060000	-0.364501000
9	-0.872925000	-2.217374000	-1.124825000	9	1.899347000	1.743270000	-0.897389000
16	-2.467659000	-0.012063000	1.939464000	6	1.161609000	-0.001849000	3.456942000
1	-2.810097000	1.070980000	1.221940000	7	0.592807000	-0.023623000	2.453617000
1	-3.037483000	-0.836232000	1.044614000	1	1.687710000	0.017755000	4.386386000
HFB:NCCH3				HFB:HF			
6	-0.669492000	0.004031000	1.455518000	6	0.789821000	-1.141264000	-0.323815000
6	-0.769010000	-1.199199000	0.772436000	6	1.384888000	0.112922000	-0.320916000
6	-0.769016000	1.203483000	0.765848000	6	-0.593854000	-1.253208000	-0.326289000
6	-0.966904000	-1.202959000	-0.600626000	6	0.596259000	1.255379000	-0.320219000
6	-0.966965000	1.199849000	-0.607208000	6	-1.382346000	-0.110789000	-0.326054000
6	-1.065917000	-0.003441000	-1.290553000	6	-0.787397000	1.143311000	-0.322984000
9	-0.463074000	0.007789000	2.769913000	9	1.544990000	-2.234933000	-0.311419000
9	-0.659040000	2.357415000	1.418784000	9	-1.163814000	-2.454145000	-0.316770000
9	-1.048567000	2.350175000	-1.270350000	9	-2.707331000	-0.217507000	-0.316721000
9	-1.243602000	-0.007169000	-2.608883000	9	-1.543023000	2.236867000	-0.310620000

9	-1.048239000	-2.356886000	-1.257508000	9	1.165778000	2.456333000	-0.305927000
9	-0.658841000	-2.349504000	1.431703000	9	2.709532000	0.219562000	-0.306727000
6	3.241335000	-0.001681000	-0.321611000	9	0.001300000	-0.005239000	2.754406000
7	2.084454000	-0.003098000	-0.274601000	1	-0.111116000	-0.046553000	3.665664000
6	4.684012000	0.000354000	-0.380747000				
1	5.044616000	0.920981000	-0.842375000				
1	5.106221000	-0.072524000	0.622802000				
1	5.042002000	-0.845769000	-0.969499000				
HFB:HCl				HFB:OHMe			
6	1.430264000	-0.027914000	-0.479559000	6	-0.589528000	-1.341550000	-0.393493000
6	0.759350000	1.187414000	-0.526621000	6	0.644885000	-0.891142000	-0.838573000
6	0.715735000	-1.218291000	-0.520121000	6	-1.560973000	-0.428193000	-0.009818000
6	-0.626237000	1.211951000	-0.611850000	6	0.908558000	0.469719000	-0.898013000
6	-0.669821000	-1.193123000	-0.605219000	6	-1.298086000	0.933147000	-0.070048000
6	-1.340230000	0.021858000	-0.650812000	6	-0.062467000	1.383114000	-0.513417000
9	2.755696000	-0.051925000	-0.393098000	9	-0.833131000	-2.644729000	-0.316552000
9	1.356832000	-2.379989000	-0.468085000	9	-2.740674000	-0.855901000	0.428627000
9	-1.355082000	-2.331020000	-0.627512000	9	-2.229388000	1.807296000	0.301293000
9	-2.668120000	0.045905000	-0.713333000	9	0.194602000	2.687907000	-0.560266000
9	-1.269783000	2.373665000	-0.640659000	9	2.101815000	0.898252000	-1.303137000
9	1.442236000	2.325401000	-0.481078000	9	1.588227000	-1.764211000	-1.181643000
17	-0.154101000	0.016134000	2.767711000	8	0.884205000	-0.311777000	2.264489000
1	-1.350661000	-0.003991000	3.227885000	1	0.561422000	0.098289000	3.070169000
				6	2.250371000	0.028684000	2.113722000
				1	2.393566000	1.094446000	1.889198000
				1	2.847567000	-0.228893000	2.996103000
				1	2.634203000	-0.549813000	1.271548000
HFB:PH₃				HFB:H₂PO₄⁻			
6	0.636215000	-1.247663000	-0.583509000	6	-0.876049000	1.239915000	0.873963000
6	1.409584000	-0.095226000	-0.559043000	6	-0.540619000	0.065539000	1.531480000
6	-0.747744000	-1.153805000	-0.629811000	6	-1.537681000	1.178723000	-0.342594000
6	0.798820000	1.150922000	-0.582827000	6	-0.864745000	-1.162473000	0.975519000
6	-1.358471000	0.092309000	-0.654359000	6	-1.858153000	-0.048125000	-0.900558000
6	-0.585119000	1.244821000	-0.628774000	6	-1.525274000	-1.218837000	-0.241090000
9	1.220419000	-2.440613000	-0.546229000	9	-0.597845000	2.417033000	1.422609000
9	-1.488641000	-2.256985000	-0.638185000	9	-1.860071000	2.305350000	-0.984102000
9	-2.683967000	0.182067000	-0.687174000	9	-2.473699000	-0.101401000	-2.083928000
9	-1.170753000	2.437814000	-0.636415000	9	-1.816339000	-2.400248000	-0.789739000
9	1.538459000	2.254074000	-0.544207000	9	-0.542556000	-2.289034000	1.611240000
9	2.733977000	-0.184647000	-0.496938000	9	0.096412000	0.116921000	2.702756000
15	-0.114455000	0.007016000	2.859550000	15	2.071450000	0.088906000	-0.614405000
1	0.523573000	0.961256000	3.689146000	8	2.266241000	-1.096109000	0.550963000
1	-1.359023000	0.143975000	3.521610000	8	1.983400000	1.401271000	0.097765000
1	0.287135000	-1.084021000	3.668263000	8	3.546279000	0.049987000	-1.381353000
				8	1.043030000	-0.452782000	-1.559014000
				1	2.687168000	-0.679831000	1.308525000
				1	3.491487000	-0.638745000	-2.049168000
HFB:OMe₂				HFB:NMe₃			
6	-1.068827000	1.224696000	-0.156083000	6	1.133799000	0.499891000	-1.120288000
6	-1.673480000	0.035105000	0.225318000	6	1.011945000	-0.876161000	-0.995692000
6	0.087765000	1.202414000	-0.922676000	6	1.032832000	1.309560000	0.001245000

6	-1.118706000	-1.177324000	-0.159915000	6	0.796875000	-1.442449000	0.252059000
6	0.643578000	-0.010245000	-1.305701000	6	0.815913000	0.743935000	1.248934000
6	0.037990000	-1.199992000	-0.926638000	6	0.695325000	-0.632237000	1.373136000
9	-1.584900000	2.387463000	0.229590000	9	1.309360000	1.046809000	-2.320016000
9	0.678183000	2.343565000	-1.267743000	9	1.105088000	2.632230000	-0.126731000
9	1.772933000	-0.032500000	-2.009601000	9	0.685577000	1.523166000	2.319302000
9	0.581734000	-2.363481000	-1.273917000	9	0.441675000	-1.173134000	2.562286000
9	-1.680482000	-2.319734000	0.223340000	9	0.648254000	-2.759019000	0.369610000
9	-2.773583000	0.057355000	0.968482000	9	1.063415000	-1.649482000	-2.077861000
8	1.163483000	-0.020308000	1.892926000	7	-1.985459000	0.142982000	-0.275115000
6	1.993148000	1.113598000	1.819872000	6	-2.514979000	0.969427000	0.791599000
1	2.558826000	1.140214000	0.874839000	1	-2.048309000	1.959167000	0.762941000
1	1.353043000	1.995952000	1.874529000	1	-3.610160000	1.110559000	0.730539000
1	2.712839000	1.144408000	2.650360000	1	-2.290729000	0.515156000	1.761834000
6	1.904597000	-1.212837000	1.805855000	6	-2.207544000	0.753000000	-1.571416000
1	2.472663000	-1.267805000	0.863448000	1	-1.754739000	0.138075000	-2.355679000
1	2.614667000	-1.312153000	2.639323000	1	-3.278909000	0.877053000	-1.816369000
1	1.198743000	-2.044655000	1.842537000	1	-1.740529000	1.742570000	-1.603110000
				6	-2.535774000	-1.197218000	-0.224201000
				1	-2.084019000	-1.816140000	-1.005874000
				1	-2.312541000	-1.655801000	0.744234000
				1	-3.632531000	-1.223137000	-0.364265000
HFB:NH₂COH				HFB:Pyrimidine			
6	0.096706000	-0.265882000	1.470868000	6	-1.433447000	-1.195567000	-0.694320000
6	0.262909000	1.054312000	1.081684000	6	-1.430522000	0.006239000	-1.387975000
6	0.639944000	-1.288023000	0.707079000	6	-1.431536000	-1.197113000	0.693395000
6	0.971888000	1.353945000	-0.071968000	6	-1.419523000	1.206227000	-0.691540000
6	1.349231000	-0.989283000	-0.447153000	6	-1.426692000	0.003153000	1.389695000
6	1.514926000	0.331833000	-0.836994000	6	-1.417613000	1.204683000	0.695900000
9	-0.609912000	-0.553647000	2.561672000	9	-1.416675000	-2.347479000	-1.358971000
9	0.465131000	-2.556122000	1.070908000	9	-1.412831000	-2.350493000	1.355431000
9	1.860786000	-1.970277000	-1.186081000	9	-1.409462000	0.001954000	2.718910000
9	2.186688000	0.617518000	-1.949305000	9	-1.382891000	2.357371000	1.360423000
9	1.117325000	2.620123000	-0.452944000	9	-1.386680000	2.360386000	-1.353591000
9	-0.283220000	2.032680000	1.799633000	9	-1.417067000	0.008003000	-2.717226000
6	-2.837484000	-0.299971000	-1.514798000	6	2.347668000	1.137809000	-0.001902000
8	-1.782926000	-0.051011000	-0.971115000	7	1.636230000	0.007719000	-0.002041000
1	-2.903997000	-0.797530000	-2.503511000	6	2.346572000	-1.121982000	-0.001913000
7	-4.059342000	-0.012085000	-1.006364000	7	3.672961000	-1.246275000	-0.001748000
1	-4.903234000	-0.245645000	-1.501941000	6	4.357352000	-0.100468000	-0.001615000
1	-4.133855000	0.441787000	-0.108344000	6	3.735098000	1.141074000	-0.001623000
				1	1.775163000	-2.050016000	-0.001983000
				1	5.442592000	-0.184992000	-0.001399000
				1	4.303055000	2.064046000	-0.001477000
				1	1.781172000	2.068844000	-0.002003000
HFB:Pyridine				HFB:Furan			
6	-1.384881000	-1.438086000	0.000000000	6	1.176975000	-0.527816000	1.292149000
6	-0.689762000	-1.430192000	1.200720000	6	1.175046000	0.848146000	1.108495000
6	-0.689762000	-1.430192000	-1.200720000	6	1.187049000	-1.373045000	0.191061000
6	0.697420000	-1.419336000	1.200659000	6	1.185126000	1.375870000	-0.175594000
6	0.697420000	-1.419336000	-1.200659000	6	1.202186000	-0.845212000	-1.092953000
6	1.392495000	-1.416328000	0.000000000	6	1.201923000	0.530823000	-1.276820000

9	-2.714386000	-1.430984000	0.000000000	9	1.152877000	-1.035588000	2.519832000
9	-1.353268000	-1.406235000	-2.354255000	9	1.165023000	-2.691696000	0.365629000
9	1.360489000	-1.383241000	-2.354181000	9	1.201621000	-1.657934000	-2.144317000
9	2.721568000	-1.383234000	0.000000000	9	1.201821000	1.038627000	-2.504293000
9	1.360489000	-1.383241000	2.354181000	9	1.160980000	2.694463000	-0.350760000
9	-1.353268000	-1.406235000	2.354255000	9	1.147210000	1.660677000	2.159441000
6	-0.022663000	4.399946000	0.000000000	8	-1.788255000	-0.000199000	-0.031318000
6	-0.015108000	3.690913000	1.194797000	6	-2.596768000	-1.095193000	-0.021584000
6	-0.000232000	2.301568000	1.139209000	6	-3.900280000	-0.719736000	-0.009073000
7	0.007376000	1.604585000	0.000000000	6	-3.904281000	0.707080000	-0.009865000
6	-0.000232000	2.301568000	-1.139209000	6	-2.602741000	1.089616000	-0.022543000
6	-0.015108000	3.690913000	-1.194797000	1	-2.087295000	-2.045325000	-0.027347000
1	-0.020795000	4.200272000	2.152180000	1	-4.754289000	-1.378611000	-0.000505000
1	0.006038000	1.716031000	2.058176000	1	-4.761966000	1.361110000	-0.000649000
1	0.006038000	1.716031000	-2.058176000	1	-2.101605000	2.044279000	-0.030388000
1	-0.020795000	4.200272000	-2.152180000				
1	-0.034261000	5.485217000	0.000000000				
HFB:Imidazole				HFB:Pyrazine			
6	0.840395000	1.205721000	0.894238000	6	-1.533125000	-1.202025000	-0.565736000
6	0.928593000	1.406237000	-0.474956000	6	-1.659515000	-0.001325000	-1.249576000
6	1.121275000	-0.040370000	1.433979000	6	-1.287698000	-1.201586000	0.800110000
6	1.297380000	0.361009000	-1.308278000	6	-1.536511000	1.199892000	-0.565993000
6	1.486252000	-1.087446000	0.600653000	6	-1.168935000	-0.000350000	1.484715000
6	1.573808000	-0.887021000	-0.769566000	6	-1.291068000	1.200419000	0.799842000
9	0.450175000	2.203447000	1.686511000	9	-1.622192000	-2.355283000	-1.222980000
9	1.017796000	-0.237021000	2.745048000	9	-1.141176000	-2.354333000	1.448381000
9	1.742352000	-2.287822000	1.114034000	9	-0.915885000	0.000208000	2.789755000
9	1.914235000	-1.895273000	-1.567685000	9	-1.148019000	2.353663000	1.447976000
9	1.365667000	0.549699000	-2.622730000	9	-1.629053000	2.352727000	-1.223477000
9	0.624846000	2.596411000	-0.991685000	9	-1.876886000	-0.001774000	-2.560325000
7	-3.868267000	0.262411000	-0.072846000	6	2.304729000	1.132084000	-0.318744000
6	-3.894171000	-1.105201000	-0.208484000	7	1.600407000	0.001763000	-0.391480000
6	-2.580011000	-1.480497000	-0.269105000	6	2.304538000	-1.128587000	-0.317236000
7	-1.756084000	-0.386963000	-0.175014000	6	3.688632000	-1.127841000	-0.173270000
6	-2.562088000	0.643715000	-0.057826000	7	4.393081000	0.001718000	-0.100815000
1	-4.818005000	-1.658447000	-0.246950000	6	3.688836000	1.131296000	-0.174897000
1	-2.179764000	-2.477713000	-0.375668000	1	1.747752000	-2.062834000	-0.374391000
1	-2.265009000	1.678696000	0.040342000	1	4.244891000	2.064368000	-0.117379000
1	-4.670999000	0.867476000	0.001938000	1	1.748028000	2.066307000	-0.377081000
				1	4.244515000	-2.060928000	-0.114348000
HFB:N₃H				HFB:HO[•]			
6	0.772192000	-0.015631000	1.413319000	6	-1.086547000	1.015733000	-0.090534000
6	0.722056000	1.210054000	0.763747000	6	-1.475085000	-0.320613000	-0.048134000
6	0.879473000	-1.187217000	0.676722000	6	0.247937000	1.338697000	-0.257445000
6	0.781660000	1.264563000	-0.622096000	6	-0.531872000	-1.331659000	-0.169167000
6	0.938038000	-1.132820000	-0.709390000	6	1.199932000	0.326016000	-0.365109000
6	0.889816000	0.093208000	-1.358749000	6	0.807494000	-1.012871000	-0.335487000
9	0.704765000	-0.067875000	2.739691000	9	-1.995769000	1.974653000	0.028807000
9	0.915909000	-2.361367000	1.297629000	9	0.632907000	2.605681000	-0.298811000
9	1.032796000	-2.254820000	-1.414835000	9	2.475356000	0.638611000	-0.556593000
9	0.935801000	0.144858000	-2.685750000	9	1.711741000	-1.969415000	-0.455523000
9	0.724349000	2.438244000	-1.243823000	9	-0.911655000	-2.600597000	-0.116010000

9	0.606441000	2.331700000	1.468530000	9	-2.752362000	-0.628309000	0.120719000
7	-2.130379000	-0.130944000	-0.090849000	8	1.301784000	-0.078037000	2.113348000
7	-3.269038000	-0.126716000	-0.100466000	1	2.172622000	0.346857000	2.185170000
7	-4.485582000	-0.315257000	-0.167574000				
1	-4.984966000	0.540822000	0.077937000				
HFB:CH₃O[•]				HFB:CH₃OO[•]			
6	-0.646041000	-1.357063000	-0.278938000	6	0.104362000	1.075473000	0.856293000
6	0.564424000	-0.871593000	-0.755472000	6	0.521291000	-0.223781000	1.105966000
6	-1.630610000	-0.470880000	0.132856000	6	-1.076999000	1.304489000	0.163647000
6	0.784484000	0.499637000	-0.824457000	6	-0.236680000	-1.297395000	0.661031000
6	-1.409640000	0.900466000	0.065006000	6	-1.838477000	0.230959000	-0.278459000
6	-0.202124000	1.386434000	-0.413720000	6	-1.418930000	-1.069538000	-0.029468000
9	-0.851420000	-2.665478000	-0.200768000	9	0.853259000	2.100577000	1.256846000
9	-2.786406000	-0.930975000	0.596257000	9	-1.473828000	2.547980000	-0.081199000
9	-2.354631000	1.743966000	0.462979000	9	-2.968849000	0.447629000	-0.940779000
9	0.017014000	2.695541000	-0.469720000	9	-2.145576000	-2.094435000	-0.458997000
9	1.950190000	0.960010000	-1.268284000	9	0.181469000	-2.539182000	0.877521000
9	1.520873000	-1.712617000	-1.128499000	9	1.677741000	-0.439622000	1.731255000
8	1.471242000	-0.318828000	1.799910000	6	3.376339000	0.200966000	-1.109278000
6	2.759719000	0.103333000	1.775511000	1	3.781358000	0.614157000	-2.033423000
1	2.880605000	1.187300000	1.617272000	1	3.131230000	0.998087000	-0.406084000
1	3.178921000	-0.121018000	2.776793000	1	4.063382000	-0.516056000	-0.662850000
1	3.388689000	-0.471680000	1.074252000	8	2.176638000	-0.551718000	-1.410236000
				8	1.238444000	0.223000000	-1.911995000
HFB:HCO[•]				HFB:CH₃CO[•]			
6	-1.277260000	0.635759000	-0.433928000	6	0.501026000	-0.002567000	1.502425000
6	-1.229637000	-0.751260000	-0.398704000	6	0.672094000	1.201344000	0.833766000
6	-0.103384000	1.367550000	-0.551713000	6	0.679368000	-1.202288000	0.828096000
6	-0.008422000	-1.406309000	-0.482074000	6	1.022680000	1.205648000	-0.509222000
6	1.117699000	0.712353000	-0.635141000	6	1.029916000	-1.198189000	-0.514876000
6	1.165266000	-0.674478000	-0.600434000	6	1.201776000	0.005847000	-1.183589000
9	-2.445357000	1.262628000	-0.346813000	9	0.152414000	-0.006664000	2.785700000
9	-0.147541000	2.695577000	-0.574711000	9	0.502455000	-2.355648000	1.466062000
9	2.242545000	1.413508000	-0.736935000	9	1.191431000	-2.347487000	-1.163280000
9	2.335685000	-1.301124000	-0.668125000	9	1.527913000	0.009864000	-2.471842000
9	0.038142000	-2.734076000	-0.440191000	9	1.177559000	2.358985000	-1.152087000
9	-2.352204000	-1.451928000	-0.277763000	9	0.488382000	2.350675000	1.477109000
6	0.301420000	0.194590000	3.650595000	6	-4.456603000	-0.001353000	-0.444007000
8	0.243780000	0.078150000	2.480714000	1	-4.417984000	0.009556000	0.649680000
1	1.214228000	-0.055692000	4.263522000	1	-5.000103000	0.871562000	-0.811228000
				1	-5.005740000	-0.877930000	-0.793663000
				6	-3.094889000	-0.011748000	-1.058301000
				8	-2.033721000	-0.008859000	-0.530688000
HFB:CH₃NH[•]				HFB:HOO[•]			
6	-1.635209000	0.043464000	0.054283000	6	0.264466000	1.409109000	-0.387091000
6	-1.013094000	-1.168258000	-0.210633000	6	-0.863349000	0.695897000	-0.769628000
6	-0.955874000	1.234587000	-0.159044000	6	1.425828000	0.734281000	-0.034222000
6	0.288219000	-1.188849000	-0.693038000	6	-0.829985000	-0.691032000	-0.794933000
6	0.344240000	1.213771000	-0.643584000	6	1.459598000	-0.653511000	-0.062885000
6	0.964460000	0.002577000	-0.914033000	6	0.329988000	-1.366607000	-0.441598000
9	-2.876401000	0.062144000	0.527437000	9	0.232170000	2.737281000	-0.353938000

9	-1.546083000	2.393302000	0.110617000	9	2.505705000	1.416568000	0.331678000
9	1.006913000	2.352404000	-0.826945000	9	2.569915000	-1.299246000	0.277781000
9	2.219624000	-0.018606000	-1.357544000	9	0.354293000	-2.695544000	-0.454055000
9	0.897254000	-2.349839000	-0.923143000	9	-1.921814000	-1.374126000	-1.127356000
9	-1.657461000	-2.309965000	0.011597000	9	-1.982489000	1.338466000	-1.085965000
6	2.340677000	0.013210000	2.084375000	8	-2.100202000	0.101354000	1.962498000
1	2.890119000	0.145376000	3.028263000	1	-2.695384000	-0.277730000	2.640025000
1	2.799326000	-0.864815000	1.599094000	8	-0.880287000	-0.301565000	2.288600000
1	2.527515000	0.882673000	1.448058000				
7	0.935834000	-0.182427000	2.283136000				
1	0.837085000	-0.954222000	2.954507000				
HFB:F⁻				HFB:CH₃CO₂⁻			
6	-0.982110000	-0.968279000	-0.260338000	6	0.807513000	1.421004000	0.238030000
6	0.348019000	-1.345226000	-0.243230000	6	1.557081000	0.662702000	-0.648288000
6	-1.320186000	0.372421000	-0.269423000	6	0.092803000	0.808162000	1.252093000
6	1.339400000	-0.381192000	-0.237434000	6	1.595596000	-0.712251000	-0.517619000
6	-0.328834000	1.336320000	-0.262386000	6	0.132646000	-0.572018000	1.382899000
6	1.001104000	0.959405000	-0.246862000	6	0.880854000	-1.327762000	0.498512000
9	-1.941722000	-1.899615000	-0.228609000	9	0.760325000	2.751826000	0.095603000
9	-2.606356000	0.736542000	-0.247585000	9	-0.588202000	1.545120000	2.124535000
9	-0.657124000	2.632516000	-0.236320000	9	-0.537353000	-1.170880000	2.366276000
9	1.960585000	1.891364000	-0.208683000	9	0.903839000	-2.662193000	0.610520000
9	2.626420000	-0.745219000	-0.193055000	9	2.309499000	-1.450481000	-1.376220000
9	0.676298000	-2.641869000	-0.200861000	9	2.235412000	1.262839000	-1.634058000
9	-0.096363000	0.043982000	2.328229000	6	-2.286303000	-0.108274000	-0.961082000
				8	-1.195848000	-0.254302000	-1.566145000
				8	-2.460614000	0.164022000	0.253902000
				6	-3.575559000	-0.293439000	-1.787274000
				1	-3.367107000	-0.425211000	-2.852268000
				1	-4.119512000	-1.171844000	-1.423871000
				1	-4.241139000	0.564484000	-1.649446000
HFB:HCO₂⁻				HFB:NO₃⁻			
6	0.263176000	1.395225000	0.521562000	6	-1.686591000	-0.514505000	-0.493752000
6	1.436840000	0.779223000	0.115162000	6	-1.518236000	0.857101000	-0.428240000
6	-0.822131000	0.635715000	0.921769000	6	-0.952801000	-1.338214000	0.346355000
6	1.527742000	-0.599678000	0.115649000	6	-0.627829000	1.403723000	0.483833000
6	-0.729701000	-0.748054000	0.923256000	6	-0.065364000	-0.792272000	1.258036000
6	0.442876000	-1.361710000	0.520625000	6	0.097762000	0.582821000	1.330991000
9	0.175641000	2.731241000	0.504292000	9	-2.544732000	-1.045831000	-1.371403000
9	-1.933580000	1.233281000	1.341717000	9	-1.100466000	-2.664489000	0.269725000
9	-1.763252000	-1.487092000	1.322762000	9	0.631749000	-1.590541000	2.064907000
9	0.525816000	-2.697705000	0.497807000	9	0.911738000	1.113778000	2.236591000
9	2.654068000	-1.199477000	-0.286648000	9	-0.470640000	2.729821000	0.541684000
9	2.476407000	1.520501000	-0.285982000	9	-2.214927000	1.657311000	-1.242281000
6	-1.509591000	-0.088399000	-2.321573000	7	2.315527000	-0.097248000	-1.214063000
8	-0.260274000	-0.113968000	-2.251838000	8	1.122204000	-0.204775000	-1.610882000
1	-1.940377000	-0.169298000	-3.368870000	8	3.261699000	-0.195145000	-2.021504000
8	-2.356073000	0.012546000	-1.405084000	8	2.540492000	0.110966000	0.010148000
HFB:Cl⁻				HFB:Br⁻			
6	-0.337426000	1.339223000	-0.525857000	6	-1.268989000	0.371908000	-1.092406000
6	-1.337751000	0.381628000	-0.504622000	6	-1.018244000	1.341794000	-0.135924000

6	0.991349000	0.949404000	-0.536083000	6	-1.182290000	-0.969239000	-0.757527000
6	-1.010945000	-0.963955000	-0.495871000	6	-0.680176000	0.970376000	1.154871000
6	1.318176000	-0.396164000	-0.529765000	6	-0.844980000	-1.340696000	0.533420000
6	0.317814000	-1.353703000	-0.507818000	6	-0.593243000	-0.370795000	1.489520000
9	-0.655789000	2.635100000	-0.511750000	9	-1.578096000	0.729020000	-2.340285000
9	1.958500000	1.868704000	-0.533852000	9	-1.407952000	-1.903777000	-1.683161000
9	2.598637000	-0.768829000	-0.518710000	9	-0.739882000	-2.632001000	0.849319000
9	0.636674000	-2.649376000	-0.481769000	9	-0.244265000	-0.727872000	2.725204000
9	-1.977713000	-1.883292000	-0.453999000	9	-0.415193000	1.904300000	2.068659000
9	-2.617886000	0.754788000	-0.471205000	9	-1.083415000	2.633170000	-0.463437000
17	0.051229000	0.038090000	2.667157000	35	2.364193000	-0.001305000	-0.501669000

Table S9. Cartesian coordinates of all optimized TCB:lone pair complexes.

TCB:H₂O				TCB:N₂			
6	0.244128000	1.224683000	-0.389057000	7	0.497733000	0.860394000	1.121084000
7	1.207586000	0.345443000	-0.584118000	6	0.632366000	1.245070000	-0.134051000
7	-1.040799000	1.008194000	-0.188006000	6	0.485579000	-0.455283000	1.223975000
6	0.747473000	-0.889795000	-0.531458000	7	0.753748000	0.497481000	-1.214834000
6	-1.313261000	-0.282005000	-0.178601000	7	0.594127000	-1.356124000	0.265835000
9	1.642510000	-1.836736000	-0.689925000	6	0.720658000	-0.788058000	-0.918720000
9	-2.573386000	-0.595222000	0.022736000	9	0.346807000	-0.929660000	2.438212000
7	-0.492443000	-1.299527000	-0.348634000	9	0.828035000	-1.609252000	-1.934886000
9	0.613924000	2.484935000	-0.402223000	9	0.647536000	2.540667000	-0.333714000
8	0.660577000	-0.112492000	2.298059000	7	-2.332556000	-0.002176000	-0.237983000
1	0.243521000	-0.441299000	3.097887000	7	-3.432055000	-0.003315000	-0.298921000
1	1.533976000	0.168362000	2.582351000				
TCB:CO₂				TCB:H₂S			
6	-1.074141000	-0.905603000	-0.833212000	6	1.790176000	0.705476000	-0.058298000
7	-1.103251000	0.330994000	-1.293542000	6	0.624004000	1.408365000	-0.360454000
7	-0.990811000	-1.315598000	0.418210000	6	1.781779000	-0.706752000	-0.081657000
6	-1.025621000	1.211442000	-0.314576000	1	0.630318000	2.491179000	-0.341204000
6	-0.923101000	-0.298057000	1.255338000	6	-0.548658000	0.729639000	-0.682272000
7	-0.937384000	0.992887000	0.983634000	6	0.607487000	-1.385327000	-0.406866000
9	-1.136081000	-1.851485000	-1.739883000	1	0.601228000	-2.468203000	-0.424574000
9	-0.829884000	-0.611904000	2.525831000	6	-0.557739000	-0.682598000	-0.703404000
9	-1.039370000	2.471188000	-0.678365000	6	2.976266000	1.419352000	0.269111000
6	3.019921000	-0.008006000	-0.107061000	7	3.936514000	2.014524000	0.533338000
8	4.177546000	-0.004849000	-0.059536000	6	2.959493000	-1.445290000	0.220424000
8	1.858178000	-0.011004000	-0.156626000	7	3.912002000	-2.061211000	0.464345000
				6	-1.747416000	-1.393380000	-1.026202000
				7	-2.707802000	-1.988193000	-1.291318000
				6	-1.731665000	1.462437000	-0.978045000
				7	-2.690271000	2.069177000	-1.221513000
				16	-3.007429000	0.002219000	1.960671000
				1	-3.885332000	0.332753000	0.999270000
				1	-3.302806000	-1.302846000	1.847781000
TCB:NMe₃				TCB:OMe₂			
6	-1.209465000	-0.804314000	0.859987000	6	-0.985146000	-0.105333000	-1.095598000
6	-0.000038000	-0.676311000	1.538564000	6	0.231198000	-0.743846000	-1.325224000

6	-1.209663000	-1.082968000	-0.523798000	6	-1.013666000	1.102696000	-0.365112000
1	-0.000173000	-0.451489000	2.598371000	1	0.253169000	-1.672835000	-1.882275000
6	1.209462000	-0.804084000	0.860090000	6	1.417264000	-0.210395000	-0.825661000
6	0.000084000	-1.224196000	-1.199675000	6	0.173404000	1.640867000	0.126441000
1	0.000194000	-1.431247000	-2.263165000	1	0.150567000	2.563940000	0.692819000
6	1.209770000	-1.082610000	-0.523734000	6	1.388250000	0.994266000	-0.090260000
6	-2.431308000	-0.608683000	1.561201000	6	-2.189021000	-0.698613000	-1.566661000
7	-3.419711000	-0.427903000	2.141987000	7	-3.164787000	-1.203818000	-1.940245000
6	-2.432333000	-1.187660000	-1.242874000	6	-2.247036000	1.758952000	-0.097328000
7	-3.422159000	-1.262633000	-1.844010000	7	-3.247827000	2.296221000	0.140325000
6	2.432298000	-1.187103000	-1.243094000	6	2.585716000	1.553033000	0.435963000
7	3.421735000	-1.261916000	-1.844894000	7	3.555473000	2.022041000	0.867004000
6	2.431226000	-0.609184000	1.561620000	6	2.641153000	-0.901492000	-1.044571000
7	3.419539000	-0.428995000	2.142743000	7	3.628402000	-1.483764000	-1.225820000
7	0.000013000	2.009130000	-0.351157000	8	-0.254109000	-1.096955000	1.846333000
6	1.198356000	2.316965000	-1.111161000	6	-0.166223000	-2.482630000	1.608952000
1	2.088640000	2.035799000	-0.540022000	1	-0.943431000	-2.823288000	0.906854000
1	1.202442000	1.753027000	-2.048806000	1	0.817250000	-2.683723000	1.180795000
1	1.286477000	3.388991000	-1.363871000	1	-0.269315000	-3.058807000	2.538535000
6	-1.196278000	2.317149000	-1.114331000	6	-1.488899000	-0.747352000	2.429028000
1	-2.088063000	2.034387000	-0.546340000	1	-2.333659000	-0.978279000	1.761301000
1	-1.284371000	3.389506000	-1.365611000	1	-1.650019000	-1.273458000	3.379738000
1	-1.197066000	1.754612000	-2.052818000	1	-1.472495000	0.326419000	2.622909000
6	-0.001729000	2.708993000	0.920903000				
1	0.885534000	2.434998000	1.500015000				
1	-0.002430000	3.808199000	0.808719000				
1	-0.889415000	2.433466000	1.498653000				
TCB:Imidazole				TCB:Pyridine			
6	-0.964030000	-1.360357000	0.738433000	6	0.983652000	-1.406646000	0.836897000
6	0.223940000	-1.130034000	1.427049000	6	1.067018000	-0.188845000	1.506840000
6	-0.955029000	-1.426865000	-0.671037000	6	1.291949000	-1.470983000	-0.539423000
1	0.214983000	-1.066028000	2.508029000	1	0.822390000	-0.137643000	2.560864000
6	1.418994000	-0.954193000	0.734699000	6	1.447228000	0.966526000	0.828532000
6	0.241706000	-1.261906000	-1.363015000	6	1.675272000	-0.316329000	-1.216650000
1	0.246595000	-1.299595000	-2.445215000	1	1.898518000	-0.363514000	-2.275411000
6	1.427983000	-1.021022000	-0.675229000	6	1.753768000	0.902378000	-0.547976000
6	-2.183218000	-1.480758000	1.460658000	6	0.558174000	-2.569051000	1.538355000
7	-3.175412000	-1.561555000	2.057378000	7	0.198310000	-3.509557000	2.115272000
6	-2.165354000	-1.615826000	-1.393585000	6	1.182689000	-2.699185000	-1.249092000
7	-3.150392000	-1.754755000	-1.991452000	7	1.085500000	-3.693943000	-1.839001000
6	2.632616000	-0.813453000	-1.402482000	6	2.107461000	2.079265000	-1.264295000
7	3.607986000	-0.638244000	-2.006415000	7	2.387464000	3.037349000	-1.856348000
6	2.614437000	-0.678910000	1.454810000	6	1.487724000	2.207363000	1.523411000
7	3.581861000	-0.447666000	2.052591000	7	1.505419000	3.215974000	2.097376000
7	-1.373360000	3.621895000	-0.047936000	6	-4.212332000	0.738254000	-0.095419000
6	-0.028335000	3.902275000	-0.040866000	6	-3.332301000	1.809434000	-0.185291000
6	0.589071000	2.682513000	-0.084518000	6	-1.982810000	1.542301000	-0.386230000
7	-0.338196000	1.669887000	-0.117274000	7	-1.478344000	0.309327000	-0.497883000
6	-1.507722000	2.269601000	-0.094331000	6	-2.340289000	-0.708567000	-0.412706000
1	0.345927000	4.911969000	-0.007288000	6	-3.706658000	-0.550385000	-0.213003000
1	1.650385000	2.478346000	-0.094309000	1	-3.679644000	2.833366000	-0.101641000
1	-2.474124000	1.784705000	-0.109620000	1	-1.268906000	2.362163000	-0.462857000
1	-2.121530000	4.297272000	-0.023359000	1	-1.916952000	-1.707894000	-0.511141000

	1	-4.353833000	-1.418237000	-0.151602000
	1	-5.273272000	0.904525000	0.062187000
TCB:Furan				
6	-1.230670000	-0.346311000	0.870231000	
6	-0.011058000	0.164991000	1.307349000	
6	-1.254030000	-1.458086000	-0.001221000	
1	0.006177000	1.027760000	1.961288000	
6	1.187277000	-0.400822000	0.878722000	
6	-0.054680000	-2.030115000	-0.421683000	
1	-0.071497000	-2.877099000	-1.096082000	
6	1.166107000	-1.512011000	0.006169000	
6	-2.439431000	0.281100000	1.282042000	
7	-3.416671000	0.812042000	1.613272000	
6	-2.489930000	-1.978278000	-0.474318000	
7	-3.493974000	-2.404240000	-0.871069000	
6	2.380619000	-2.084591000	-0.462001000	
7	3.367374000	-2.551965000	-0.855486000	
6	2.420701000	0.169404000	1.300880000	
7	3.419445000	0.652168000	1.641515000	
8	0.041903000	1.356255000	-1.757106000	
6	1.158610000	1.951007000	-1.257884000	
6	0.823706000	2.982989000	-0.439243000	
6	-0.600566000	3.037703000	-0.432714000	
6	-1.021265000	2.034378000	-1.247451000	
1	2.096755000	1.529718000	-1.582716000	
1	1.511280000	3.625712000	0.088524000	
1	-1.231728000	3.731782000	0.100463000	
1	-1.991775000	1.687927000	-1.565525000	
TCB:HCO[•]				
6	-0.683068000	-0.552528000	-0.575147000	
6	0.463576000	-1.325979000	-0.401469000	
6	-0.601952000	0.855087000	-0.460606000	
1	0.404030000	-2.403798000	-0.489019000	
6	1.687202000	-0.723856000	-0.113589000	
6	0.620218000	1.456251000	-0.174803000	
1	0.680553000	2.533701000	-0.082760000	
6	1.768276000	0.682649000	0.000483000	
6	-1.926167000	-1.174644000	-0.868139000	
7	-2.950286000	-1.670472000	-1.102005000	
6	-1.770697000	1.650220000	-0.616224000	
7	-2.731904000	2.289013000	-0.736115000	
6	3.006779000	1.317467000	0.291801000	
7	4.011083000	1.848667000	0.528103000	
6	2.843679000	-1.534012000	0.060485000	
7	3.778154000	-2.207502000	0.199442000	
8	-2.654746000	-0.234583000	1.804131000	
6	-3.796586000	-0.496881000	1.707676000	
1	-4.263505000	-0.993819000	0.809943000	
TCB:CH₃O[•]				
6	1.832408000	0.700042000	-0.030102000	
6	0.654419000	1.405680000	-0.276381000	
6	1.816218000	-0.711889000	-0.040315000	
1	0.666000000	2.488556000	-0.265743000	
6	-0.535459000	0.729322000	-0.529677000	
6	0.623176000	-1.388073000	-0.296702000	
1	0.611698000	-2.470996000	-0.303140000	
6	-0.552444000	-0.682828000	-0.539408000	
6	3.037017000	1.411334000	0.227937000	
7	4.012163000	2.004735000	0.435712000	
6	3.004579000	-1.453862000	0.207015000	
7	3.965761000	-2.072451000	0.406164000	
6	-1.760583000	-1.388935000	-0.797836000	
7	-2.731765000	-1.980142000	-1.030355000	
6	-1.731364000	1.461934000	-0.768023000	
7	-2.704179000	2.062591000	-0.965970000	
8	-2.602284000	0.057690000	1.602768000	
6	-3.935811000	-0.118249000	1.464267000	
1	-4.280395000	0.702378000	0.798641000	
1	-4.183878000	-1.034600000	0.901176000	
1	-4.501956000	-0.036841000	2.403416000	
TCB:H₂PO₄⁻				
6	-1.274106000	-0.689740000	0.897049000	
6	-0.045480000	-0.366012000	1.458999000	
6	-1.328370000	-1.487226000	-0.270368000	
1	0.000637000	0.289785000	2.318284000	
6	1.139548000	-0.833426000	0.888582000	
6	-0.148137000	-1.935302000	-0.847694000	
1	-0.183470000	-2.519804000	-1.757995000	
6	1.085050000	-1.628853000	-0.272174000	
6	-2.471901000	-0.205453000	1.492045000	
7	-3.456094000	0.161713000	1.986696000	
6	-2.572243000	-1.828799000	-0.866187000	
7	-3.581411000	-2.139429000	-1.350130000	
6	2.271570000	-2.132436000	-0.873305000	
7	3.220199000	-2.583220000	-1.368413000	
6	2.384245000	-0.558369000	1.522446000	
7	3.390068000	-0.429050000	2.086165000	
15	0.268657000	2.045880000	-0.608957000	
8	0.490811000	3.425580000	-1.488314000	
8	1.430178000	1.873447000	0.328526000	
8	-1.004211000	2.461883000	0.386220000	
8	-0.204581000	0.984810000	-1.550524000	
1	1.019587000	4.027822000	-0.957332000	
1	-1.814570000	2.471829000	-0.132464000	

TCB:NO ₃ ⁻				TCB:Cl ⁻			
6	1.054980000	0.830992000	-0.035261000	6	0.894014000	1.176182000	-0.096865000
6	-0.178429000	1.461845000	-0.052779000	6	-0.384628000	1.644732000	0.232787000
6	1.151919000	-0.617182000	0.213058000	6	1.057581000	-0.148006000	-0.546462000
1	-0.204431000	2.544072000	-0.125834000	1	-0.501567000	2.652530000	0.611881000
6	-1.385528000	0.759695000	-0.021517000	6	-1.502040000	0.843435000	0.053301000
6	-0.107674000	-1.326348000	-0.010731000	6	-0.070508000	-0.965703000	-0.713395000
1	-0.075857000	-2.406903000	-0.070748000	1	0.063873000	-1.982037000	-1.057309000
6	-1.310919000	-0.668231000	-0.041734000	6	-1.344050000	-0.476329000	-0.457302000
6	2.237183000	1.596929000	-0.143527000	6	2.002936000	2.051940000	0.047289000
7	3.202420000	2.242400000	-0.245864000	7	2.880388000	2.805769000	0.158198000
6	2.285931000	-1.274248000	-0.435757000	6	2.338241000	-0.617003000	-0.959177000
7	3.147649000	-1.812569000	-0.994255000	7	3.362464000	-0.927851000	-1.409464000
6	-2.504047000	-1.442519000	-0.144263000	6	-2.475709000	-1.302035000	-0.686959000
7	-3.467566000	-2.086355000	-0.228276000	7	-3.402818000	-1.969869000	-0.899734000
6	-2.617260000	1.445846000	-0.048989000	6	-2.788570000	1.364854000	0.354694000
7	-3.625743000	2.031485000	-0.066970000	7	-3.832667000	1.814614000	0.596779000
9	1.525115000	-0.818064000	1.697015000	17	1.236619000	-2.009502000	1.644560000
TCB:Br ⁻				TCB:HCO ₂ ⁻			
6	-1.936330000	0.693529000	-0.196828000	6	0.894014000	1.176182000	-0.096865000
6	-1.026507000	1.692224000	-0.513783000	6	-0.384628000	1.644732000	0.232787000
6	-1.537874000	-0.372422000	0.659512000	6	1.057581000	-0.148005000	-0.546462000
1	-1.330093000	2.510969000	-1.154434000	1	-0.501567000	2.652530000	0.611881000
6	0.273869000	1.670227000	0.006468000	6	-1.502040000	0.843435000	0.053301000
6	-0.226751000	-0.434227000	1.113737000	6	-0.070508000	-0.965703000	-0.713395000
1	0.097923000	-1.263591000	1.727306000	1	0.063873000	-1.982037000	-1.057309000
6	0.689194000	0.581251000	0.800457000	6	-1.344050000	-0.476329000	-0.457302000
6	-3.258988000	0.769663000	-0.707418000	6	2.002936000	2.051940000	0.047289000
7	-4.339689000	0.857105000	-1.126388000	7	2.880388000	2.805769000	0.158198000
6	-2.462534000	-1.380711000	1.035308000	6	2.338241000	-0.617003000	-0.959177000
7	-3.225377000	-2.193522000	1.364605000	7	3.362464000	-0.927851000	-1.409464000
6	1.977584000	0.582658000	1.408531000	6	-2.475709000	-1.302035000	-0.686959000
7	2.974822000	0.674180000	1.996770000	7	-3.402818000	-1.969869000	-0.899734000
6	1.152944000	2.743206000	-0.294683000	6	-2.788570000	1.364854000	0.354694000
7	1.836756000	3.648813000	-0.545580000	7	-3.832667000	1.814614000	0.596779000
35	1.675398000	-1.755023000	-0.921901000	17	1.236619000	-2.009502000	1.644560000

Table S10. Cartesian coordinates of all optimized TNB:lone pair complexes.

TNB:H ₂ O				TNB:N ₂			
6	-0.835584000	1.123704000	-0.283010000	6	-1.261368000	0.626057000	-0.420212000
6	-1.374940000	-0.151604000	-0.253479000	6	-1.140658000	-0.754168000	-0.425578000
6	0.544587000	1.229339000	-0.312455000	6	-0.090110000	1.366177000	-0.422963000
6	-0.593318000	-1.294740000	-0.247946000	6	0.085968000	-1.398382000	-0.430626000
6	1.379346000	0.124590000	-0.304670000	6	1.165576000	0.780695000	-0.427808000
1	2.456193000	0.232518000	-0.313169000	1	2.066796000	1.380486000	-0.426613000
6	0.780757000	-1.124156000	-0.276879000	6	1.220936000	-0.603721000	-0.433013000
1	-1.037735000	-2.280986000	-0.218390000	1	0.154704000	-2.478744000	-0.431803000
1	-1.466231000	2.003083000	-0.276009000	1	-2.231412000	1.106661000	-0.413092000
7	-2.850973000	-0.299579000	-0.204207000	7	-2.378052000	-1.577469000	-0.416344000

8	-3.295170000	-1.435944000	-0.212158000	8	-2.235922000	-2.788820000	-0.415618000
8	-3.509921000	0.726714000	-0.159104000	8	-3.440255000	-0.978129000	-0.409996000
7	1.154210000	2.581290000	-0.313204000	7	-0.184509000	2.849391000	-0.411222000
8	0.392636000	3.533747000	-0.351707000	8	-1.304733000	3.331635000	-0.403665000
8	2.372864000	2.640126000	-0.272822000	8	0.865507000	3.469890000	-0.409749000
7	1.647006000	-2.328354000	-0.249479000	7	2.552726000	-1.263480000	-0.431704000
8	2.851940000	-2.142772000	-0.180998000	8	3.530465000	-0.534388000	-0.429116000
8	1.091371000	-3.413382000	-0.294608000	8	2.565125000	-2.483062000	-0.432994000
8	0.149256000	0.157149000	2.686659000	7	0.012245000	-0.010014000	2.696470000
1	-0.431437000	0.395008000	3.413835000	7	0.038497000	-0.033481000	3.797344000
1	0.998617000	0.008975000	3.110492000				
TNB:CO ₂				TNB:H ₂ S			
6	1.394167000	-0.159317000	-0.727166000	6	-1.829989000	0.035756000	0.086634000
6	0.812551000	1.098036000	-0.728197000	6	-1.175321000	-1.165482000	-0.134292000
6	0.543553000	-1.252696000	-0.728675000	6	-1.117748000	1.200404000	-0.151930000
6	-0.559713000	1.288081000	-0.725347000	6	0.137978000	-1.233066000	-0.570295000
6	-0.836157000	-1.127658000	-0.725894000	6	0.197014000	1.197376000	-0.588326000
1	-1.480562000	-1.997422000	-0.720382000	1	0.735682000	2.120901000	-0.756773000
6	-1.357756000	0.155767000	-0.726864000	6	0.796255000	-0.034710000	-0.791741000
1	-0.990521000	2.281102000	-0.719457000	1	0.630837000	-2.184092000	-0.725164000
1	2.469621000	-0.281985000	-0.722636000	1	-2.855620000	0.062708000	0.431760000
7	1.696899000	2.291617000	-0.714276000	7	-1.908987000	-2.433445000	0.116973000
8	1.152548000	3.383229000	-0.708623000	8	-1.299011000	-3.472172000	-0.074573000
8	2.899719000	2.088692000	-0.709193000	8	-3.064463000	-2.337469000	0.494984000
7	1.135194000	-2.615359000	-0.715056000	7	-1.788213000	2.506352000	0.080380000
8	2.352756000	-2.689724000	-0.709392000	8	-2.949160000	2.473088000	0.452235000
8	0.358145000	-3.555653000	-0.710097000	8	-1.125569000	3.510795000	-0.119217000
7	-2.833665000	0.324548000	-0.711261000	7	2.215268000	-0.071782000	-1.220995000
8	-3.506597000	-0.692871000	-0.705320000	8	2.772440000	1.000480000	-1.390741000
8	-3.259684000	1.467570000	-0.705134000	8	2.725325000	-1.171633000	-1.359030000
6	0.002613000	-0.001391000	3.515538000	16	2.887153000	-0.002409000	2.131070000
8	0.006366000	-0.000119000	4.674021000	1	3.562340000	0.967015000	1.492269000
8	-0.001137000	-0.002658000	2.352020000	1	3.580222000	-0.962239000	1.496717000
TNB:NMe ₃				TNB:OMe ₂			
6	1.269865000	0.598331000	-0.840658000	6	-1.218590000	0.912961000	-0.499910000
6	0.114498000	1.361864000	-0.843552000	6	-1.182889000	-0.448823000	-0.752181000
6	1.121451000	-0.778638000	-0.845110000	6	-0.005175000	1.570401000	-0.387431000
6	-1.152070000	0.801828000	-0.839862000	6	0.001623000	-1.155020000	-0.882224000
6	-0.117434000	-1.397572000	-0.841603000	6	1.211501000	0.919421000	-0.502239000
1	-0.208388000	-2.476146000	-0.823109000	1	2.146732000	1.453056000	-0.391427000
6	-1.235619000	-0.580593000	-0.844925000	6	1.182584000	-0.442522000	-0.754563000
1	-2.040963000	1.419543000	-0.820354000	1	0.004208000	-2.222065000	-1.064918000
1	2.249747000	1.058115000	-0.821497000	1	-2.156463000	1.441617000	-0.387503000
7	0.238543000	2.838854000	-0.782893000	7	-2.465202000	-1.191928000	-0.831996000
8	-0.798351000	3.482154000	-0.754530000	8	-2.399289000	-2.390401000	-1.053203000
8	1.368151000	3.300132000	-0.751937000	8	-3.489045000	-0.551148000	-0.657699000
7	2.338720000	-1.624332000	-0.786569000	7	-0.008752000	3.027524000	-0.103405000
8	3.414105000	-1.047729000	-0.757161000	8	-1.097199000	3.568263000	0.001905000
8	2.173820000	-2.833351000	-0.758260000	8	1.077048000	3.573687000	0.001260000
7	-2.576890000	-1.211514000	-0.786146000	7	2.468718000	-1.178638000	-0.837022000
8	-2.615816000	-2.431097000	-0.756131000	8	3.489316000	-0.532757000	-0.662491000
8	-3.541087000	-0.463632000	-0.758344000	8	2.408984000	-2.377034000	-1.060414000

7	-0.000058000	-0.002646000	2.139229000	8	0.004934000	-0.367894000	2.237490000
6	-1.253207000	-0.589035000	2.576485000	6	-1.157091000	-1.097815000	2.553780000
1	-1.341979000	-1.610210000	2.192425000	1	-1.206313000	-1.336957000	3.624978000
1	-1.350778000	-0.634488000	3.676318000	1	-2.018014000	-0.479152000	2.293667000
1	-2.094268000	-0.003386000	2.191910000	1	-1.207159000	-2.043037000	1.989899000
6	1.133303000	-0.795268000	2.578054000	6	1.173236000	-1.087540000	2.554294000
1	2.062979000	-0.361345000	2.196468000	1	1.222072000	-1.330012000	3.624749000
1	1.219196000	-0.858567000	3.677973000	1	1.233573000	-2.030390000	1.987426000
1	1.047254000	-1.815915000	2.191990000	1	2.028820000	-0.459884000	2.298169000
6	0.118509000	1.374736000	2.579703000				
1	1.046753000	1.810847000	2.197140000				
1	-0.720535000	1.963371000	2.195352000				
1	0.126421000	1.479927000	3.679736000				
TNB:Imidazole				TNB:Pyridine			
6	1.857840000	0.585285000	-0.109522000	6	-0.496802000	0.164248000	-1.262757000
6	0.796607000	1.362130000	-0.539034000	6	0.025311000	-1.093798000	-1.013836000
6	1.708752000	-0.791933000	-0.178734000	6	0.275259000	1.254940000	-0.896147000
6	-0.385907000	0.818457000	-1.020236000	6	1.271135000	-1.287602000	-0.437428000
6	0.551752000	-1.393667000	-0.641284000	6	1.527782000	1.126530000	-0.318824000
1	0.452187000	-2.471143000	-0.664460000	1	2.105023000	1.993043000	-0.022977000
6	-0.475436000	-0.563129000	-1.064036000	6	2.004531000	-0.158341000	-0.115785000
1	-1.204449000	1.448828000	-1.340355000	1	1.650346000	-2.280536000	-0.232333000
1	2.765652000	1.033891000	0.272709000	1	-1.479571000	0.291491000	-1.697636000
7	0.903296000	2.836188000	-0.433930000	7	-0.817346000	-2.278064000	-1.308901000
8	-0.098035000	3.483473000	-0.700198000	8	-0.418220000	-3.356904000	-0.900411000
8	1.978210000	3.293245000	-0.081623000	8	-1.858034000	-2.083237000	-1.915880000
7	2.820179000	-1.654629000	0.287434000	7	-0.298868000	2.612734000	-1.062281000
8	3.842749000	-1.095402000	0.647173000	8	-1.390393000	2.691522000	-1.603342000
8	2.629140000	-2.860581000	0.273608000	8	0.352417000	3.547700000	-0.625471000
7	-1.744739000	-1.175164000	-1.514133000	7	3.340140000	-0.331497000	0.509296000
8	-1.851018000	-2.388523000	-1.404074000	8	3.961060000	0.683427000	0.777079000
8	-2.609958000	-0.423788000	-1.936918000	8	3.715887000	-1.475854000	0.702948000
7	-2.774518000	-0.662547000	1.283209000	6	-3.172063000	-0.042396000	1.044478000
6	-2.793912000	0.710377000	1.270719000	6	-2.560975000	1.172821000	1.332148000
6	-1.613618000	1.086205000	1.858994000	6	-1.291530000	1.156207000	1.902819000
7	-0.874724000	-0.012173000	2.219606000	7	-0.616488000	0.037955000	2.186626000
6	-1.602589000	-1.047040000	1.864124000	6	-1.228201000	-1.120569000	1.921761000
1	-3.619248000	1.266683000	0.857048000	6	-2.494938000	-1.216479000	1.352959000
1	-1.257594000	2.090423000	2.038866000	1	-3.049171000	2.115881000	1.110197000
1	-1.339836000	-2.087395000	1.994440000	1	-0.781614000	2.091809000	2.131488000
1	-3.492808000	-1.270524000	0.916768000	1	-0.667601000	-2.022759000	2.164056000
				1	-2.930780000	-2.188920000	1.147606000
				1	-4.157487000	-0.074507000	0.590706000
TNB:Furan				TNB:HCO•			
6	-0.406489000	0.736139000	-1.016135000	6	1.619960000	0.000305000	-0.117122000
6	-0.409438000	-0.649390000	-1.022640000	6	0.911003000	1.183230000	-0.252411000
6	0.739029000	1.366081000	-0.547930000	6	0.911561000	-1.182978000	-0.252124000
6	0.664810000	-1.401740000	-0.573131000	6	-0.450786000	1.215193000	-0.505279000
6	1.847161000	0.669557000	-0.098883000	6	-0.450219000	-1.215632000	-0.504968000
1	2.728206000	1.184452000	0.262091000	1	-0.983667000	-2.153236000	-0.594007000
6	1.781013000	-0.716087000	-0.123484000	6	-1.103515000	-0.000393000	-0.628704000
1	0.631685000	-2.483763000	-0.574064000	1	-0.984667000	2.152524000	-0.594575000

1	-1.259994000	1.301263000	-1.365592000	1	2.682972000	0.000595000	0.086636000
7	-1.616977000	-1.356213000	-1.515619000	7	1.638604000	2.470790000	-0.108016000
8	-1.620588000	-2.573789000	-1.432099000	8	0.980912000	3.492502000	-0.216315000
8	-2.519731000	-0.666514000	-1.960786000	8	2.837499000	2.407703000	0.106612000
7	0.757621000	2.846377000	-0.487374000	7	1.639765000	-2.470187000	-0.107504000
8	-0.290459000	3.422906000	-0.737093000	8	2.838578000	-2.406509000	0.107404000
8	1.811977000	3.378797000	-0.181526000	8	0.982595000	-3.492215000	-0.215935000
7	2.944358000	-1.493606000	0.367744000	7	-2.571293000	-0.000774000	-0.854828000
8	3.927492000	-0.860008000	0.715306000	8	-3.118509000	-1.087927000	-0.937095000
8	2.830354000	-2.708892000	0.388231000	8	-3.119102000	1.086141000	-0.936621000
8	-1.072463000	0.257570000	2.142638000	6	-2.241736000	-0.000450000	2.362987000
6	-1.959983000	1.139549000	1.606985000	8	-1.116548000	0.001079000	2.706954000
6	-3.038399000	0.481921000	1.104285000	1	-3.125176000	-0.000537000	3.060076000
6	-2.809438000	-0.902681000	1.348655000				
6	-1.606601000	-0.982731000	1.975797000				
1	-1.682834000	2.179796000	1.669043000				
1	-3.890063000	0.928732000	0.615428000				
1	-3.446852000	-1.731123000	1.079897000				
1	-1.017804000	-1.799523000	2.361463000				
TNB:CH ₃ O [•]				TNB:H ₂ PO ₄ ⁻			
6	1.196610000	1.169449000	-0.126282000	6	-1.109903000	1.357378000	-0.503715000
6	-0.144393000	1.231411000	-0.464574000	6	-1.944919000	0.368643000	-0.015328000
6	1.759320000	-0.090415000	0.009159000	6	0.017114000	0.957967000	-1.205304000
6	-0.916756000	0.099614000	-0.666191000	6	-1.663032000	-0.982511000	-0.166582000
6	1.034357000	-1.258828000	-0.167132000	6	0.341849000	-0.376271000	-1.399571000
1	1.492377000	-2.230680000	-0.035559000	1	1.239741000	-0.674917000	-1.919717000
6	-0.301416000	-1.131350000	-0.507734000	6	-0.532397000	-1.322826000	-0.882130000
1	-1.964619000	0.174919000	-0.924953000	1	-2.299547000	-1.740116000	0.268520000
1	1.780482000	2.066659000	0.034037000	1	-1.320208000	2.403911000	-0.334637000
7	-0.800299000	2.557657000	-0.556834000	7	-3.140364000	0.761053000	0.738301000
8	-2.011270000	2.565038000	-0.716113000	8	-3.860515000	-0.133646000	1.167401000
8	-0.084620000	3.539771000	-0.457304000	8	-3.358630000	1.959025000	0.878440000
7	3.194925000	-0.192297000	0.377209000	7	0.923019000	1.991194000	-1.730943000
8	3.801764000	0.854553000	0.531984000	8	0.591006000	3.160459000	-1.589175000
8	3.657856000	-1.314827000	0.493499000	8	1.942074000	1.616534000	-2.296704000
7	-1.125705000	-2.355742000	-0.646947000	7	-0.214271000	-2.747244000	-1.076220000
8	-0.553645000	-3.426278000	-0.531890000	8	0.652296000	-3.023420000	-1.891667000
8	-2.318084000	-2.198419000	-0.858627000	8	-0.860986000	-3.562125000	-0.430190000
8	-1.915302000	-0.095014000	1.804278000	15	1.679102000	-0.109416000	1.481597000
6	-3.265845000	0.033217000	1.771653000	8	2.216295000	1.326762000	0.828530000
1	-3.777821000	-0.818064000	1.296186000	8	2.079240000	-1.206264000	0.536017000
1	-3.590398000	0.024815000	2.832422000	8	2.625672000	-0.265632000	2.825345000
1	-3.607328000	0.997828000	1.363868000	8	0.265875000	0.156753000	1.898266000
				1	3.023354000	1.151552000	0.334546000
				1	2.200553000	0.223936000	3.535043000
TNB:NO ₃ ⁻				TNB:Cl ⁻			
6	-1.730020000	-0.728126000	-0.007850000	6	-0.997885000	1.217067000	-0.152396000
6	-0.610121000	-1.357091000	-0.515482000	6	-1.666174000	0.000538000	-0.021734000
6	-1.733451000	0.663471000	0.007149000	6	0.360163000	1.192393000	-0.377986000
6	0.511466000	-0.661163000	-0.960659000	6	-0.998781000	-1.216489000	-0.152248000
6	-0.656718000	1.410388000	-0.455286000	6	1.107901000	-0.000498000	-0.389655000
1	-0.667170000	2.491172000	-0.425148000	1	2.144028000	-0.000882000	-0.686531000

6	0.440042000	0.728648000	-0.943552000	6	0.359298000	-1.192849000	-0.377808000
1	1.374310000	-1.172267000	-1.356658000	1	-1.534645000	-2.153687000	-0.093962000
1	-2.574219000	-1.295145000	0.358292000	1	-1.533008000	2.154691000	-0.094208000
7	-0.583828000	-2.827311000	-0.550669000	7	-3.102337000	0.001077000	0.194420000
8	0.376086000	-3.362339000	-1.087361000	8	-3.673736000	-1.086622000	0.279447000
8	-1.533996000	-3.425645000	-0.055370000	8	-3.672941000	1.089198000	0.279345000
7	-2.916751000	1.361441000	0.512756000	7	1.064767000	2.457823000	-0.572014000
8	-3.849217000	0.676647000	0.926753000	8	0.427018000	3.499363000	-0.425380000
8	-2.913017000	2.588638000	0.486493000	8	2.246098000	2.404295000	-0.891998000
7	1.582754000	1.499766000	-1.455540000	7	1.062918000	-2.458836000	-0.571693000
8	1.510747000	2.720990000	-1.403170000	8	2.244365000	-2.406288000	-0.891429000
8	2.510813000	0.867886000	-1.942318000	8	0.424263000	-3.499845000	-0.425220000
7	2.236807000	-0.027845000	1.743108000	17	2.046972000	-0.000139000	1.938386000
8	2.750619000	-0.160376000	2.860035000				
8	1.864289000	-1.059629000	1.101559000				
8	2.072054000	1.103468000	1.229629000				
TNB:Br ⁻				TNB:HCO ₂ ⁻			
6	1.339333000	-1.218572000	-0.194439000	6	-0.924297000	-1.215423000	-0.325804000
6	1.973642000	-0.002927000	0.058371000	6	0.442387000	-1.191551000	-0.499918000
6	0.046374000	-1.191047000	-0.668047000	6	-1.596203000	-0.001317000	-0.225565000
6	1.344093000	1.215448000	-0.192725000	6	1.190519000	0.002020000	-0.480850000
6	-0.681162000	0.002810000	-0.825195000	6	-0.927100000	1.214457000	-0.324735000
1	-1.650471000	0.005056000	-1.297088000	1	-1.466444000	2.150381000	-0.281393000
6	0.050858000	1.193664000	-0.666123000	6	0.439631000	1.193913000	-0.498864000
1	1.861567000	2.151502000	-0.034499000	1	2.227256000	0.003390000	-0.774027000
1	1.853021000	-2.156850000	-0.037098000	1	-1.461215000	-2.152771000	-0.283099000
7	3.344918000	-0.005862000	0.536653000	7	1.153067000	-2.453123000	-0.664618000
8	3.891941000	1.081523000	0.726124000	8	2.357007000	-2.404067000	-0.899797000
8	3.887750000	-1.095564000	0.724831000	8	0.506444000	-3.497240000	-0.576316000
7	-0.611676000	-2.456585000	-0.989372000	7	-3.039827000	-0.003064000	-0.056186000
8	-0.013133000	-3.498901000	-0.728582000	8	-3.612430000	-1.090577000	0.005212000
8	-1.715138000	-2.399510000	-1.518664000	8	-3.614981000	1.083077000	0.005893000
7	-0.602108000	2.462178000	-0.985750000	7	1.147520000	2.457115000	-0.662494000
8	-1.706135000	2.410308000	-1.514463000	8	0.498813000	3.499811000	-0.572417000
8	0.000950000	3.501770000	-0.724338000	8	2.351406000	2.410863000	-0.898610000
35	-2.176879000	0.000254000	1.447076000	6	1.246200000	-0.003142000	2.421809000
				8	0.016900000	-0.002534000	2.345982000
				1	1.722831000	-0.008566000	3.439544000
				8	2.112520000	0.001582000	1.488256000

Table S11. Cartesian coordinates of all optimized CNF:lone pair complexes.

CNF:H ₂ O				CNF:N ₂		
6	0.244128000	1.224683000	-0.389057000	7	0.497733000	0.860394000
7	1.207586000	0.345443000	-0.584118000	6	0.632366000	1.245070000
7	-1.040799000	1.008194000	-0.188006000	6	0.485579000	-0.455283000
6	0.747473000	-0.889795000	-0.531458000	7	0.753748000	0.497481000
6	-1.313261000	-0.282005000	-0.178601000	7	0.594127000	-1.356124000
9	1.642510000	-1.836736000	-0.689925000	6	0.720658000	-0.788058000

9	-2.573386000	-0.595222000	0.022736000	9	0.346807000	-0.929660000	2.438212000
7	-0.492443000	-1.299527000	-0.348634000	9	0.828035000	-1.609252000	-1.934886000
9	0.613924000	2.484935000	-0.402223000	9	0.647536000	2.540667000	-0.333714000
8	0.660577000	-0.112492000	2.298059000	7	-2.332556000	-0.002176000	-0.237983000
1	0.243521000	-0.441299000	3.097887000	7	-3.432055000	-0.003315000	-0.298921000
1	1.533976000	0.168362000	2.582351000				
CNF:CO ₂				CNF:H ₂ S			
6	-1.074141000	-0.905603000	-0.833212000	6	0.200508000	0.131990000	-1.361975000
7	-1.103251000	0.330994000	-1.293542000	7	0.397239000	-1.108967000	-0.959988000
7	-0.990811000	-1.315598000	0.418210000	7	0.472936000	1.256879000	-0.729947000
6	-1.025621000	1.211442000	-0.314576000	6	0.915288000	-1.143493000	0.253663000
6	-0.923101000	-0.298057000	1.255338000	6	0.984449000	1.025557000	0.464946000
7	-0.937384000	0.992887000	0.983634000	7	1.242890000	-0.134807000	1.037591000
9	-1.136081000	-1.851485000	-1.739883000	9	-0.346339000	0.264537000	-2.548512000
9	-0.829884000	-0.611904000	2.525831000	9	1.276048000	2.088229000	1.174147000
9	-1.039370000	2.471188000	-0.678365000	9	1.131931000	-2.340507000	0.744522000
6	3.019921000	-0.008006000	-0.107061000	16	-2.515451000	0.031876000	0.867136000
8	4.177546000	-0.004849000	-0.059536000	1	-2.766904000	-1.250543000	0.558391000
8	1.858178000	-0.011004000	-0.156626000	1	-2.933568000	0.454142000	-0.337370000
CNF:NMe ₃				CNF:OMe ₂			
7	-1.119533000	-0.879688000	1.053492000	7	1.088438000	-1.164666000	0.525321000
6	-1.105087000	-1.238378000	-0.215088000	6	1.201144000	0.036648000	1.060268000
6	-1.110086000	0.432925000	1.177468000	6	0.740512000	-1.094297000	-0.743711000
7	-1.117033000	-0.474163000	-1.289623000	7	1.045230000	1.212388000	0.481046000
7	-1.121430000	1.352645000	0.232992000	7	0.528077000	-0.022865000	-1.484300000
6	-1.106725000	0.803996000	-0.965644000	6	0.701145000	1.082365000	-0.784325000
9	-1.081235000	0.885711000	2.410995000	9	0.580157000	-2.246813000	-1.354802000
9	-1.073648000	1.645145000	-1.975067000	9	0.499952000	2.204769000	-1.437960000
9	-1.070840000	-2.533274000	-0.439440000	9	1.524531000	0.066266000	2.329745000
7	1.742003000	0.001946000	0.002028000	8	-1.719904000	-0.015907000	0.704070000
6	2.196876000	1.363965000	0.226707000	6	-2.404772000	1.144791000	0.290394000
1	1.815457000	1.732061000	1.183385000	1	-3.419940000	1.183621000	0.708372000
1	3.298464000	1.448907000	0.242068000	1	-1.839963000	2.005235000	0.652156000
1	1.818265000	2.020198000	-0.561927000	1	-2.478468000	1.196956000	-0.806481000
6	2.192868000	-0.874672000	1.070183000	6	-2.388126000	-1.189629000	0.299898000
1	1.810406000	-1.886794000	0.910532000	1	-3.404708000	-1.236364000	0.713632000
1	3.294216000	-0.932128000	1.139277000	1	-2.456237000	-1.254385000	-0.796675000
1	1.812343000	-0.518361000	2.031869000	1	-1.814839000	-2.039057000	0.673971000
6	2.194189000	-0.486321000	-1.290499000				
1	1.813247000	-1.496783000	-1.463038000				
1	1.813080000	0.158096000	-2.087629000				
1	3.295772000	-0.517691000	-1.373913000				
CNF:Imidazole				CNF:Pyridine			
7	1.336081000	-1.387041000	0.218627000	7	1.631609000	0.000212000	-1.395542000
6	1.412764000	-0.471069000	1.164879000	6	1.639163000	-1.087759000	-0.650887000
6	1.341629000	-0.836076000	-0.979339000	6	1.639508000	1.087863000	-0.650472000
7	1.522099000	0.836675000	1.039802000	7	1.672896000	-1.189314000	0.662714000
7	1.446081000	0.437158000	-1.302578000	7	1.673092000	1.188873000	0.663218000
6	1.515662000	1.197169000	-0.227835000	6	1.668976000	-0.000325000	1.234397000
9	1.235500000	-1.672908000	-1.988361000	9	1.609904000	2.226897000	-1.306883000
9	1.595622000	2.490977000	-0.451260000	9	1.675640000	-0.000624000	2.546725000

9	1.388936000	-0.925170000	2.397417000	9	1.609052000	-2.226495000	-1.307810000
7	-3.483308000	-0.592551000	-0.011533000	6	-3.959148000	0.000392000	-0.082650000
6	-3.510405000	0.782127000	-0.007837000	6	-3.253331000	-1.194655000	-0.021443000
6	-2.198027000	1.162950000	0.045927000	6	-1.869378000	-1.140691000	0.097103000
7	-1.375711000	0.064512000	0.075324000	7	-1.175259000	-0.000161000	0.155382000
6	-2.179215000	-0.974378000	0.039616000	6	-1.868913000	1.140642000	0.097157000
1	-4.433908000	1.335913000	-0.043001000	6	-3.252866000	1.195145000	-0.021390000
1	-1.797255000	2.165898000	0.067769000	1	-3.761447000	-2.151657000	-0.064034000
1	-1.875154000	-2.011308000	0.049829000	1	-1.285026000	-2.058053000	0.151936000
1	-4.285331000	-1.202202000	-0.044728000	1	-1.284239000	2.057808000	0.151968000
				1	-3.760603000	2.152355000	-0.063876000
				1	-5.040478000	0.000604000	-0.175573000
CNF:Furan				CNF:HCO [•]			
7	-0.415612000	-0.006942000	-1.486548000	7	-0.829382000	1.075364000	0.696452000
6	-0.811358000	1.086974000	-0.863592000	6	-0.859643000	-0.172554000	1.123023000
6	-0.819264000	-1.093125000	-0.855125000	6	-0.568959000	1.136286000	-0.595377000
7	-1.525067000	1.192687000	0.242276000	7	-0.681377000	-1.283000000	0.433213000
7	-1.533818000	-1.185223000	0.251306000	7	-0.364999000	0.144373000	-1.441412000
6	-1.834089000	0.006709000	0.732058000	6	-0.434081000	-1.026042000	-0.836860000
9	-0.473917000	-2.233729000	-1.404809000	9	-0.509897000	2.342213000	-1.108139000
9	-2.537994000	0.013560000	1.838074000	9	-0.233468000	-2.073997000	-1.600873000
9	-0.458317000	2.220797000	-1.422286000	9	-1.104591000	-0.330980000	2.402405000
8	1.242721000	-0.007762000	1.361180000	6	3.274929000	0.274988000	0.579999000
6	1.867272000	-1.095694000	0.829170000	8	2.146423000	0.024674000	0.355963000
6	2.849138000	-0.707292000	-0.023223000	1	4.117046000	-0.465737000	0.469272000
6	2.840342000	0.718788000	-0.019527000				
6	1.853780000	1.090622000	0.834837000				
1	1.491556000	-2.051709000	1.156834000				
1	3.498235000	-1.357883000	-0.587950000				
1	3.481005000	1.380292000	-0.581210000				
1	1.466044000	2.040190000	1.167249000				
CNF:CH ₃ O [•]				CNF:H ₂ PO ₄ ⁻			
6	0.919884000	-0.216615000	1.135282000	7	1.362490000	1.037059000	-0.956073000
7	0.852004000	1.052038000	0.781506000	6	1.128390000	-0.211480000	-1.321159000
7	0.808379000	-1.290862000	0.377763000	6	1.754680000	1.105492000	0.298017000
6	0.623111000	1.179919000	-0.511244000	7	1.238187000	-1.306335000	-0.587844000
6	0.584195000	-0.967368000	-0.880851000	7	1.989630000	0.131122000	1.152771000
7	0.486658000	0.232457000	-1.419611000	6	1.643025000	-1.029280000	0.633218000
9	1.135107000	-0.440892000	2.411042000	9	2.017343000	2.323774000	0.743930000
9	0.445951000	-1.976035000	-1.711180000	9	1.790134000	-2.072862000	1.432380000
9	0.525937000	2.410555000	-0.953665000	9	0.886090000	-0.399271000	-2.596541000
8	-1.992067000	0.191261000	0.243168000	15	-1.919250000	0.072249000	0.129146000
6	-3.295613000	-0.120499000	0.417299000	8	-2.804558000	-1.242550000	0.632228000
1	-3.923727000	0.744997000	0.680513000	8	-1.627808000	-0.096192000	-1.328947000
1	-3.657655000	-0.454179000	-0.577853000	8	-3.031855000	1.297662000	0.271876000
1	-3.463788000	-0.971608000	1.095708000	8	-0.855215000	0.295190000	1.162349000
				1	-3.207518000	-1.619753000	-0.154129000
				1	-2.979061000	1.617057000	1.176539000
CNF:NO ₃ ⁻				CNF:Cl ⁻			
7	1.637012000	-1.018316000	-0.072705000	6	0.977191000	-0.665466000	0.739450000
6	1.248849000	-0.460629000	1.058720000	7	1.056818000	0.642644000	0.873956000

6	1.297171000	-0.258648000	-1.095856000	7	0.570000000	-1.368744000	-0.297231000
7	0.701164000	0.715051000	1.264304000	6	0.571503000	1.255153000	-0.186883000
7	0.745150000	0.932916000	-1.103899000	6	0.125657000	-0.580649000	-1.255162000
6	0.452595000	1.337329000	0.122739000	7	0.126855000	0.735517000	-1.312763000
9	1.616802000	-0.744576000	-2.287207000	9	1.436602000	-1.369373000	1.757488000
9	0.032305000	2.579757000	0.229297000	9	-0.312905000	-1.195763000	-2.337446000
9	1.514125000	-1.163396000	2.150630000	9	0.603506000	2.574049000	-0.144241000
7	-2.204734000	-0.462763000	-0.063791000	17	-2.227449000	-0.011786000	0.934448000
8	-1.205021000	-1.230867000	-0.115214000				
8	-3.360849000	-0.915882000	-0.117340000				
8	-2.010494000	0.781423000	0.043121000				
CNF:Br ⁻				CNF:HCO ₂ ⁻			
6	-1.107446000	-1.209230000	-0.326168000	7	-1.705749000	0.008999000	-0.332964000
7	-1.139418000	-0.348331000	-1.323176000	6	-1.062426000	1.082371000	0.089512000
7	-1.124312000	-0.974765000	0.970078000	6	-1.069053000	-1.080844000	0.055407000
6	-1.110109000	0.891612000	-0.878124000	7	0.006617000	1.178118000	0.836874000
6	-1.093605000	0.319275000	1.216698000	7	-0.001239000	-1.206906000	0.800292000
7	-1.124871000	1.325077000	0.365882000	6	0.528421000	-0.020470000	1.101717000
9	-1.128477000	-2.481484000	-0.674265000	9	-1.643182000	-2.223683000	-0.317378000
9	-1.103980000	0.653710000	2.492317000	9	1.431374000	-0.038254000	2.067297000
9	-1.133476000	1.828765000	-1.805867000	9	-1.629963000	2.239739000	-0.246276000
35	2.110873000	-0.000935000	-0.007817000	6	1.888235000	0.024278000	-1.543589000
				8	0.722756000	0.036349000	-1.975210000
				1	2.720525000	0.039392000	-2.305410000
				8	2.283114000	-0.002986000	-0.346673000