Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

C-F activation of perfluorophenazine at nickel: selectivity and mechanistic investigations

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S1. NMR spectra

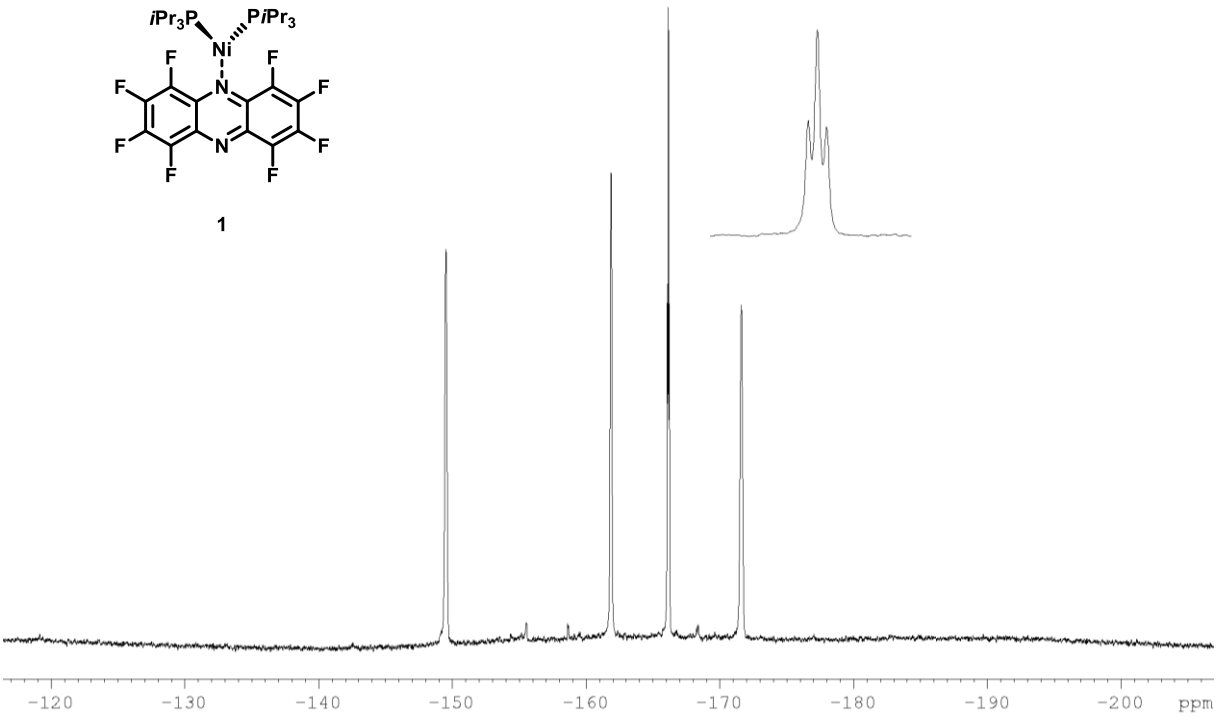


Figure S1 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of [Ni{κ-(*N*)-$C_{12}N_2F_8$}(P*i*Pr$_3$)$_2$] (**1**).

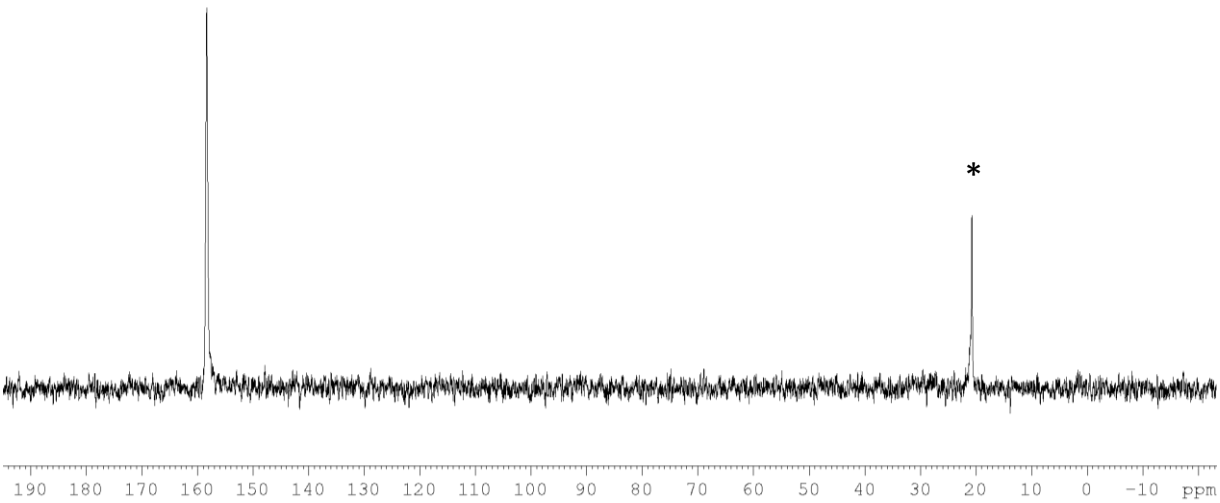


Figure S2 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of [Ni{κ-(*N*)-$C_{12}N_2F_8$}(P*i*Pr$_3$)$_2$] (**1**). *) Resonances of P*i*Pr$_3$.

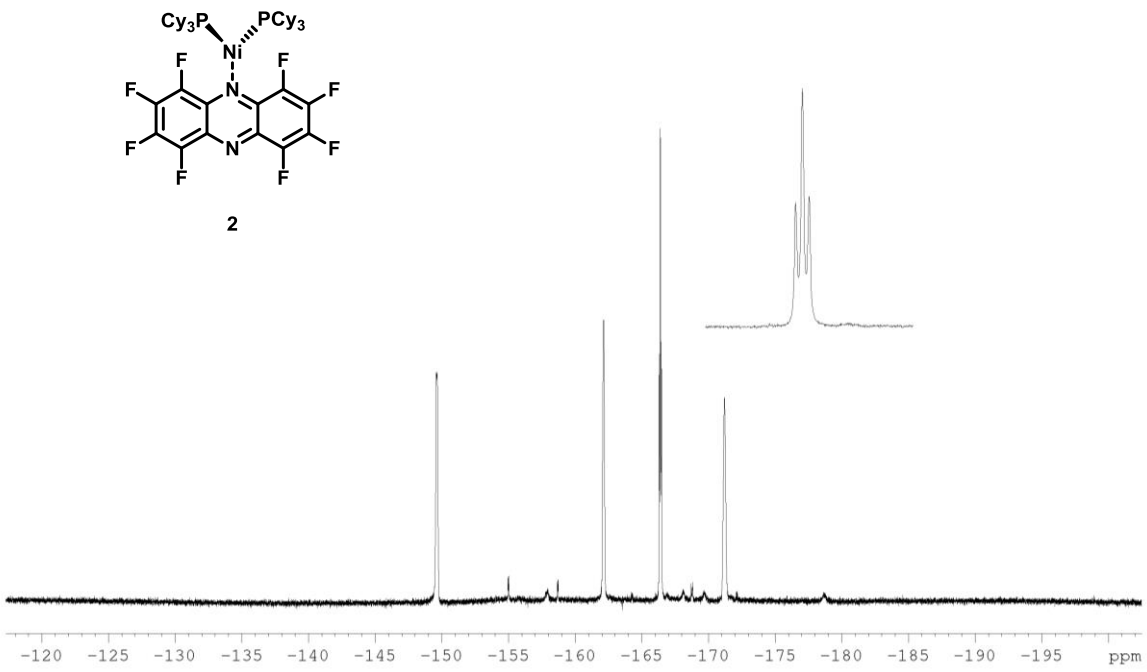


Figure S3 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of [Ni{κ-(*N*)-$C_{12}N_2F_8$}(PCy_3)$_2$] (**2**).

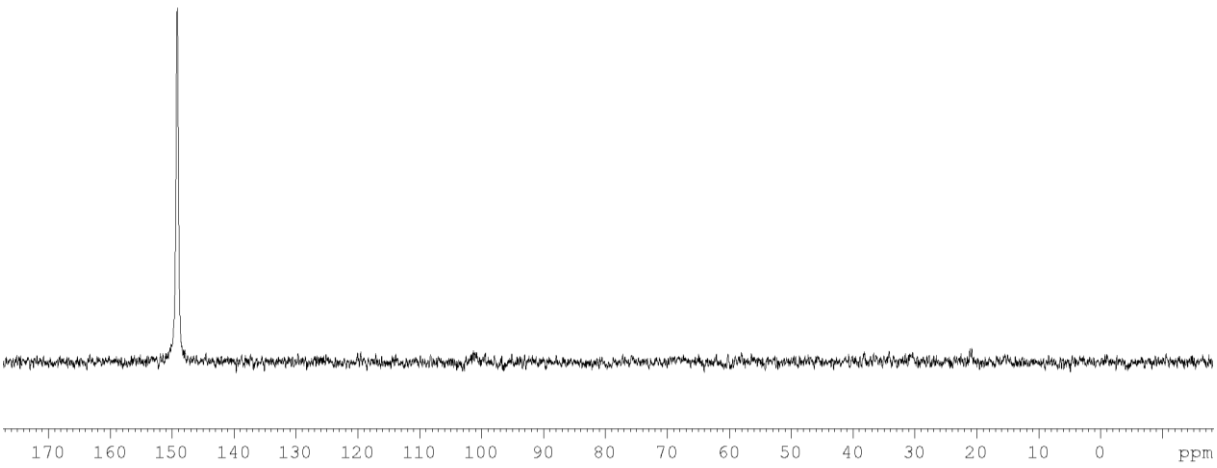


Figure S4 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of [Ni{κ-(*N*)-$C_{12}N_2F_8$}(PCy_3)$_2$] (**2**).

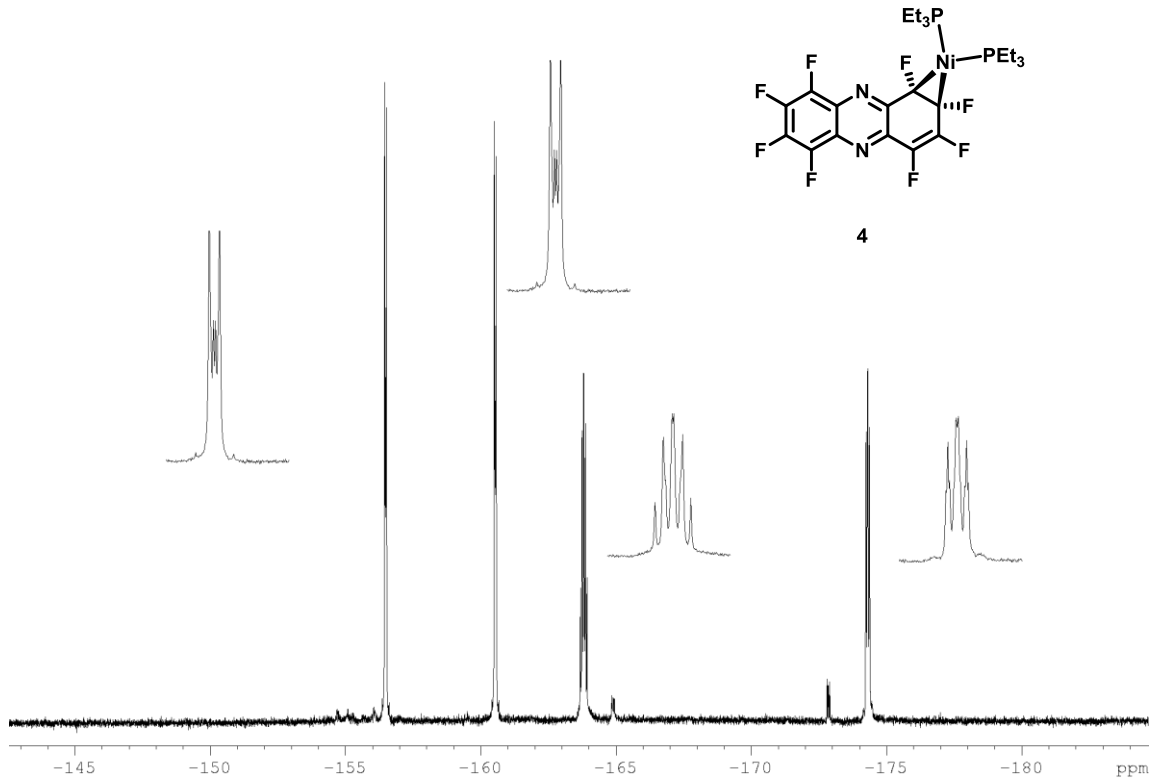


Figure S5 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of [Ni(PEt_3)$_2$(1,2-η^2-$C_{12}N_2F_8$)] (**4**).

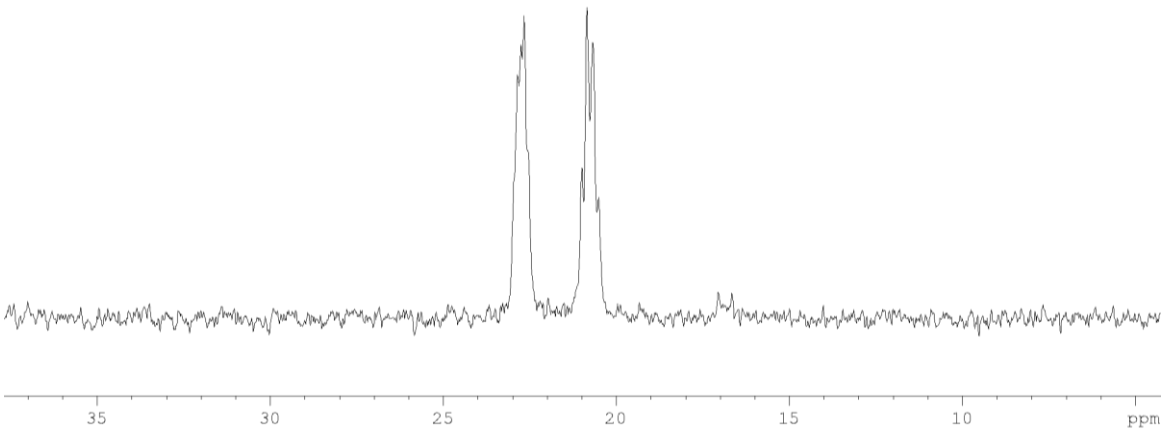


Figure S6 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of [Ni(PEt_3)$_2$(1,2-η^2-$C_{12}N_2F_8$)] (**4**).

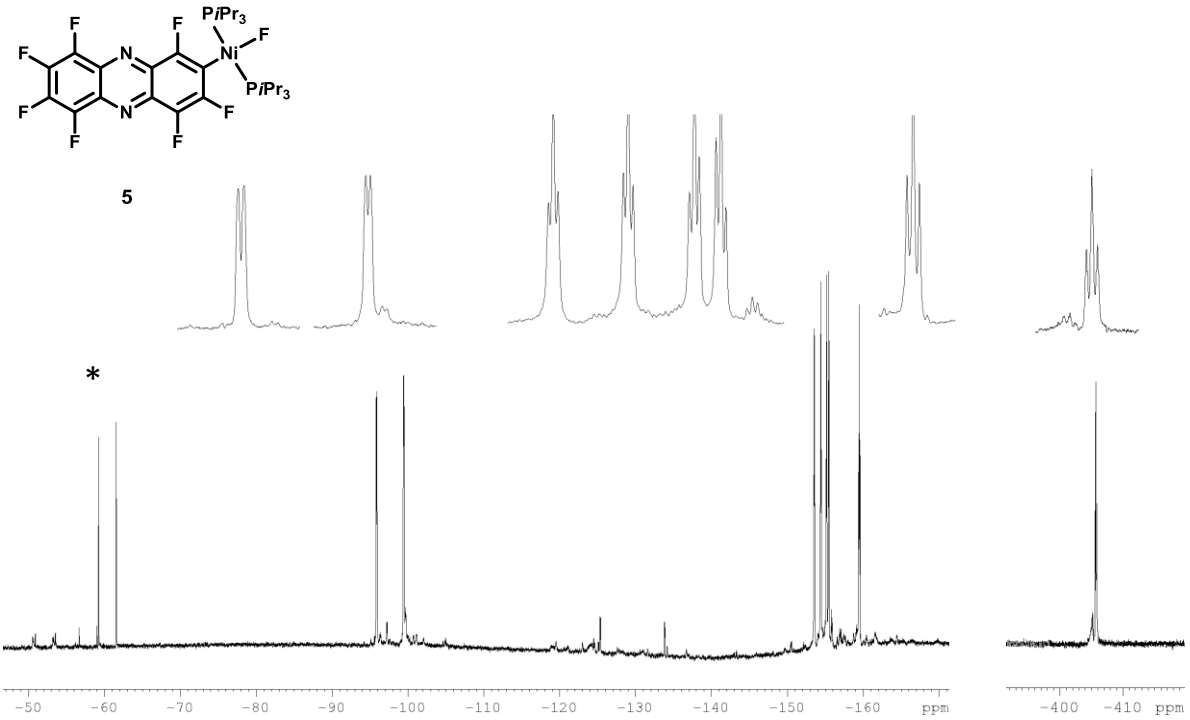


Figure S7 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of *trans*-[NiF(2-$C_{12}N_2F_7$)(P*i*Pr$_3$)$_2$] (**5**). *) Resonance of F_2P*i*Pr$_3$.

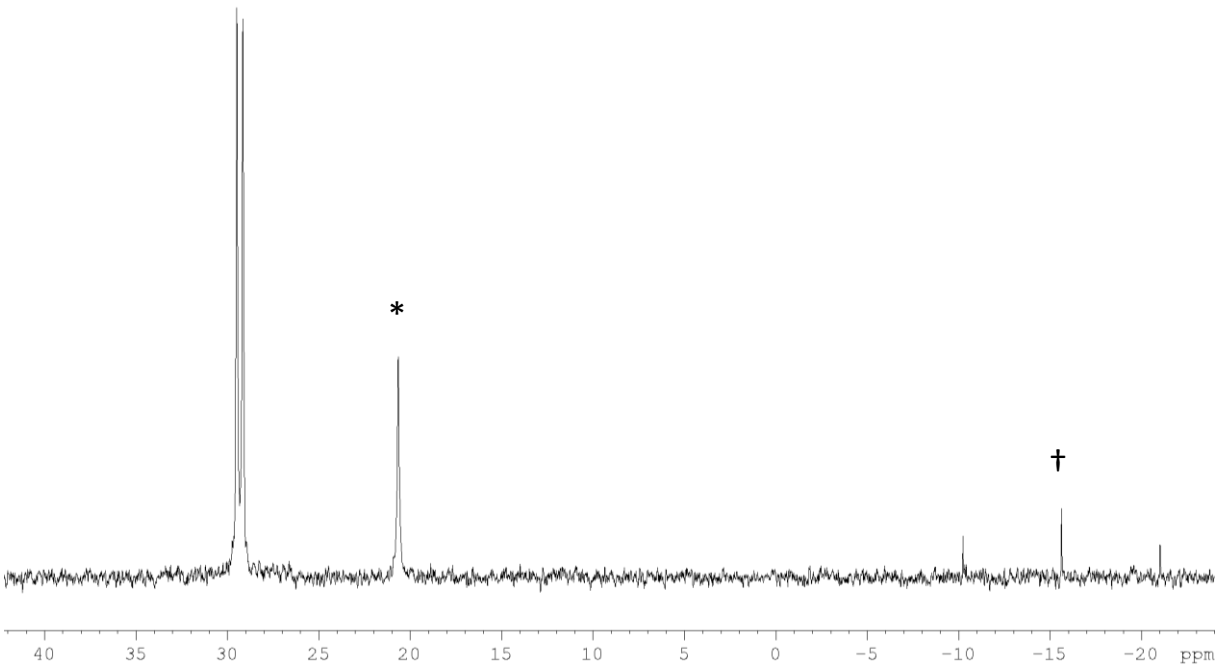


Figure S8 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of *trans*-[NiF(2-$C_{12}N_2F_7$)(P*i*Pr$_3$)$_2$] (**5**). *) Resonances of P*i*Pr$_3$. † Resonance of F_2P*i*Pr$_3$.

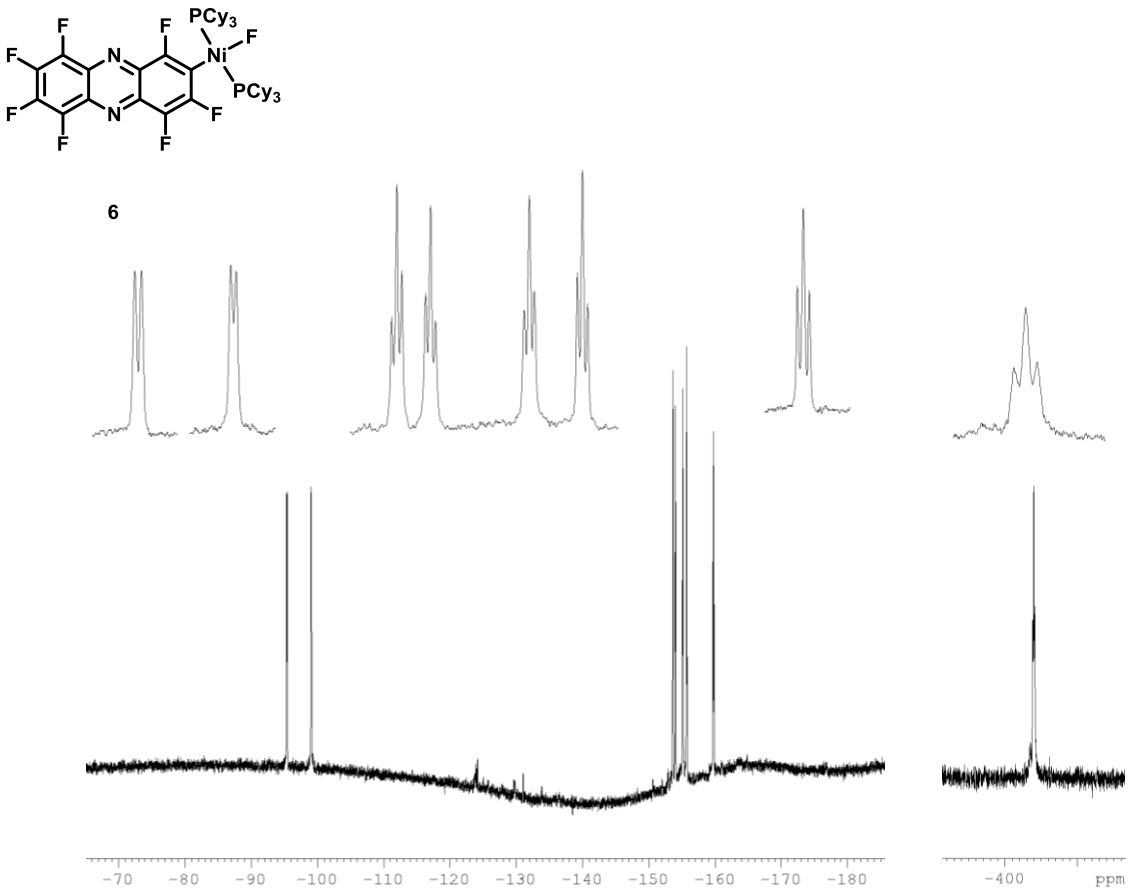


Figure S9 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of *trans*-[NiF(2-$C_{12}N_2F_7$)(PCy_3)$_2$] (**6**).

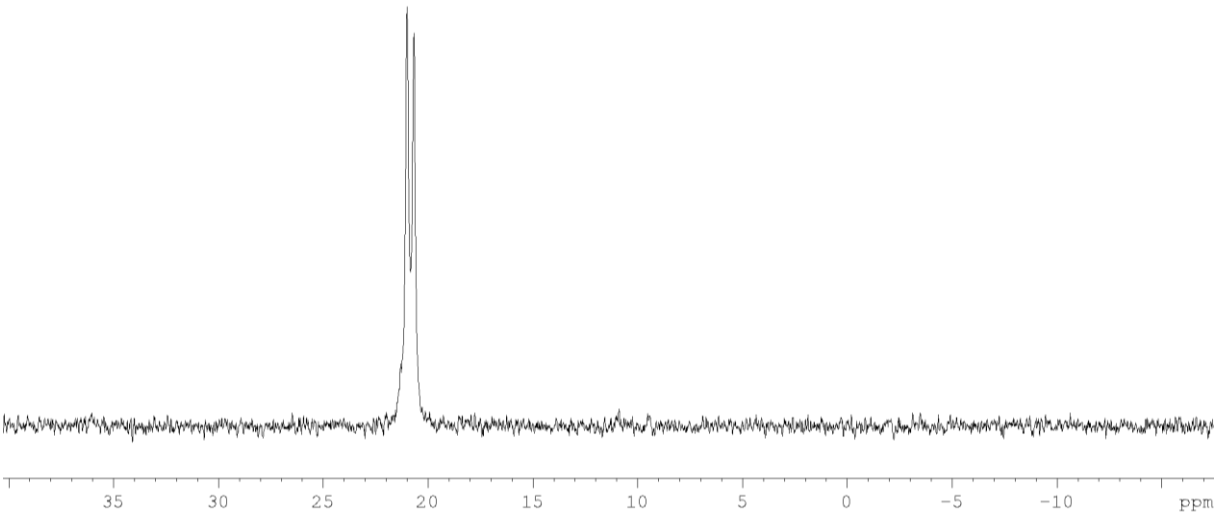


Figure S10 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of *trans*-[NiF(2-$C_{12}N_2F_7$)(PCy_3)$_2$] (**6**).

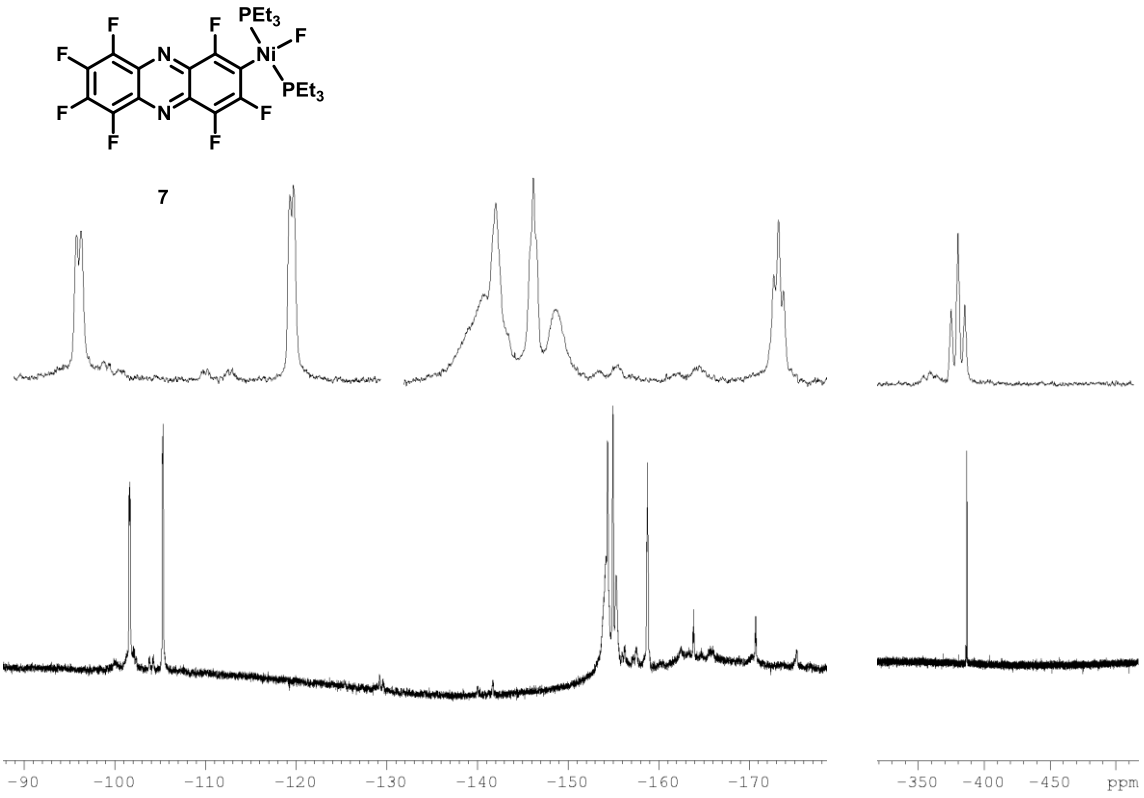


Figure S11 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of *trans*-[NiF(2-$C_{12}N_2F_7$)(PEt_3)$_2$] (**7**).

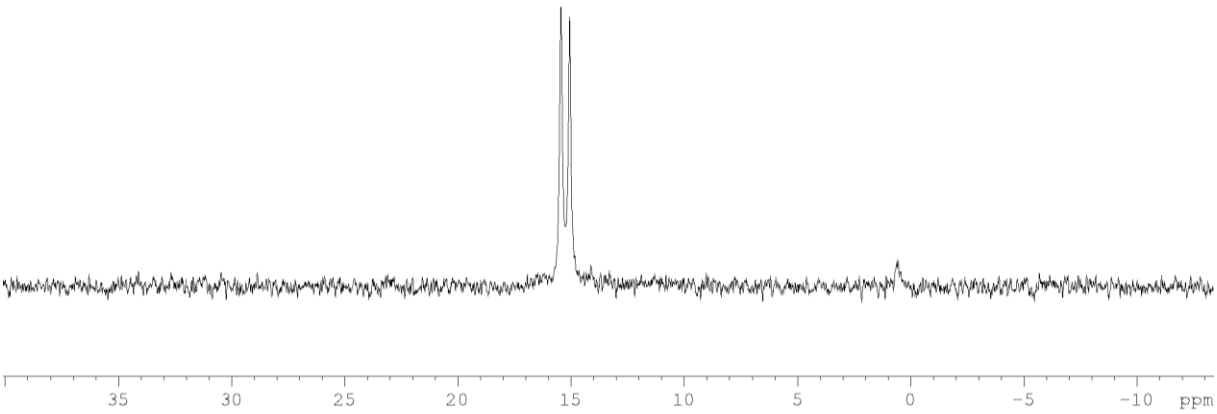
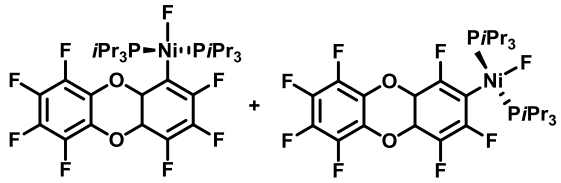


Figure S12 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of *trans*-[NiF(2-$C_{12}N_2F_7$)(PEt_3)$_2$] (**7**).



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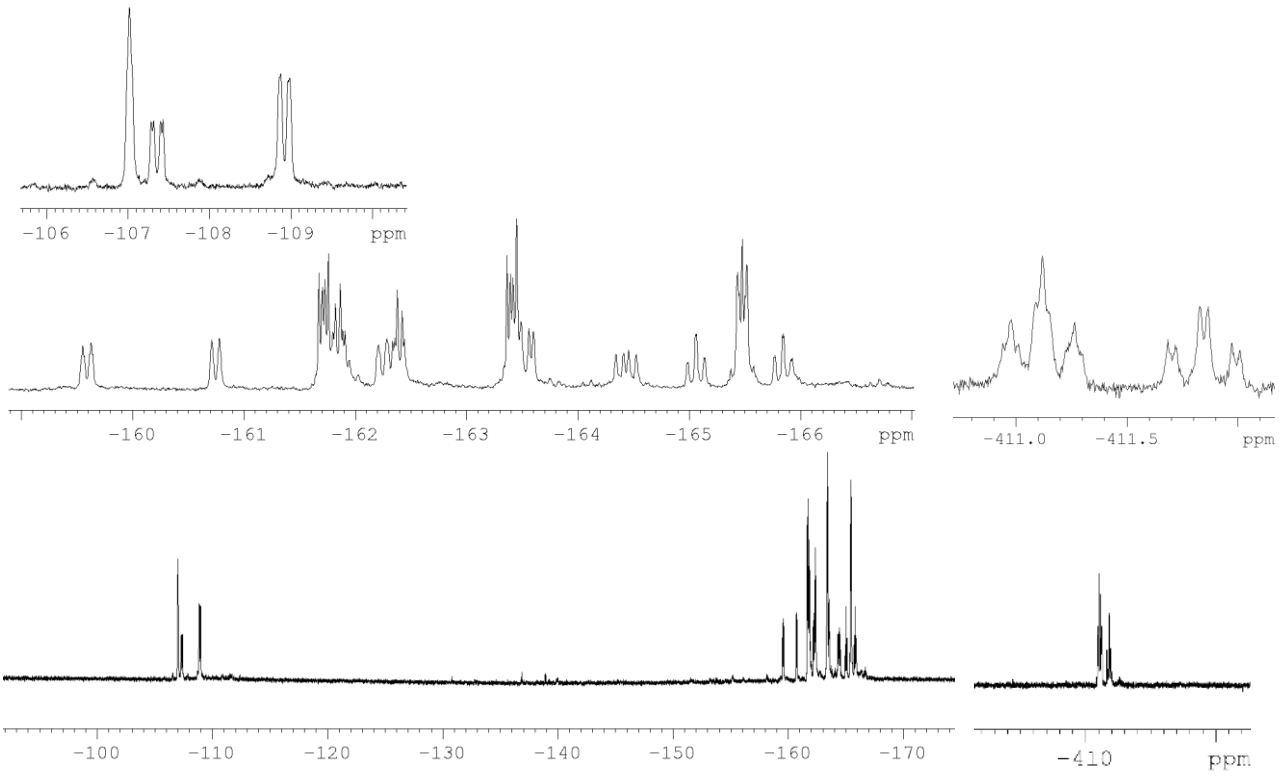


Figure S13 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of *trans*-[NiF(1-$C_{12}O_2F_7$)(P*i*Pr$_3$)$_2$] (**8**) and *trans*-[NiF(2-$C_{12}O_2F_7$)(P*i*Pr$_3$)$_2$] (**9**).

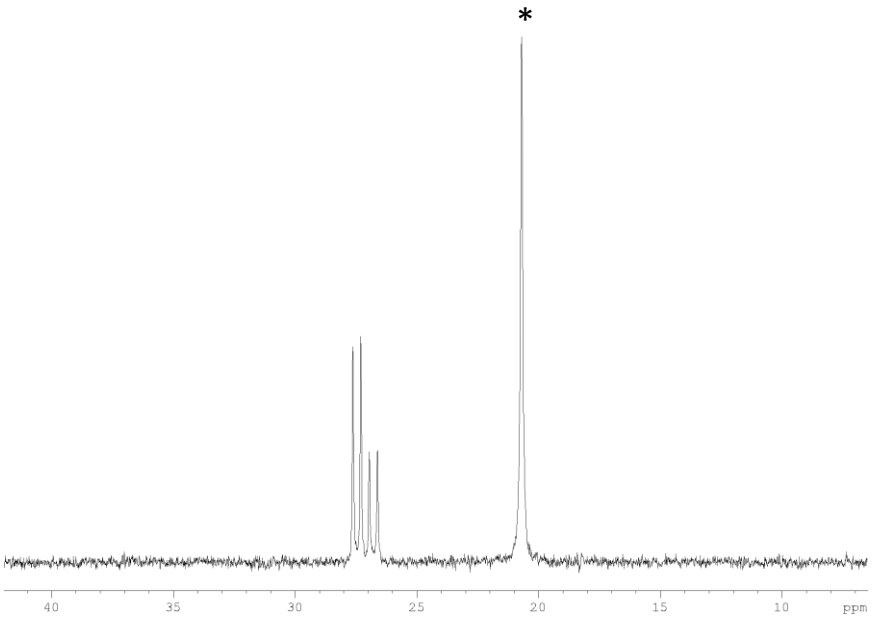
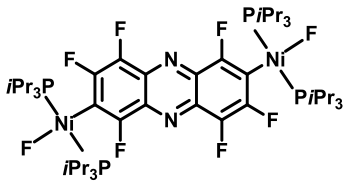


Figure S14 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of *trans*-[NiF(1-$C_{12}O_2F_7$)(P*i*Pr$_3$)$_2$] (**8**) and *trans*-[NiF(2-$C_{12}O_2F_7$)(P*i*Pr$_3$)$_2$] (**9**). *) Resonances of P*i*Pr$_3$.



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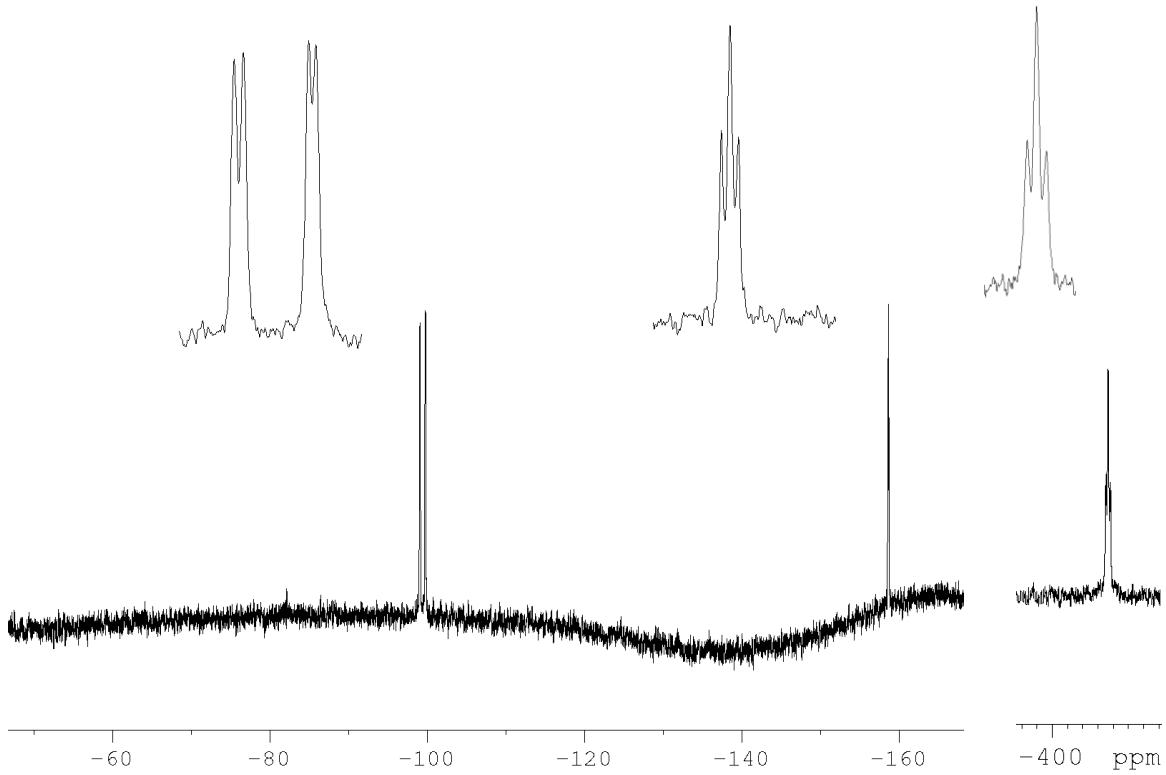

Figure S15 ^{19}F NMR (282.4 MHz, THF-d_8) spectrum of [*trans*-(P*i*Pr$_3$)$_2$NiF]$_2$(2,6-$C_{12}N_2F_6$) (**10**).

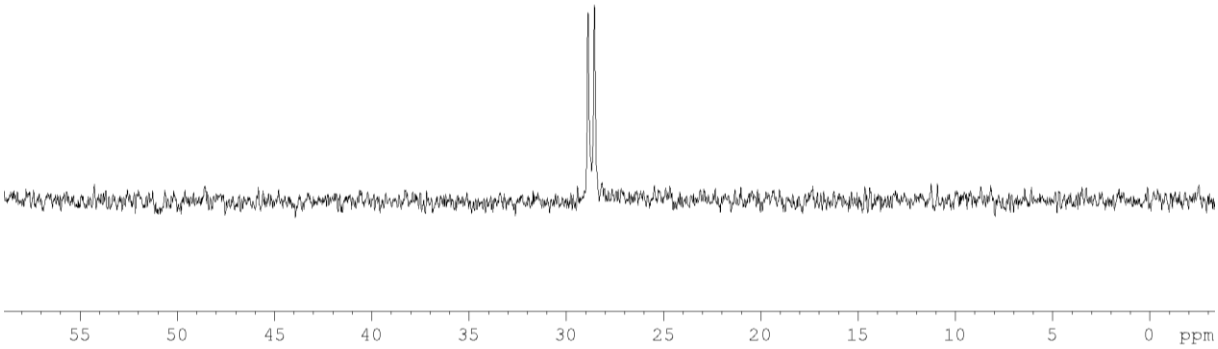

Figure S16 $^{31}P\{^1H\}$ NMR (121.5 MHz, THF-d_8) spectrum of [*trans*-(P*i*Pr$_3$)$_2$NiF]$_2$(2,6-$C_{12}N_2F_6$) (**10**).

S2. Crystal data

Table S1. Crystal data and structure refinement for [Ni{κ-(*N*)-$C_{12}N_2F_8$}(P*i*Pr$_3$)$_2$] (**1**).

Empirical formula	C30 H42 F8 N2 Ni P2
Formula weight	847.51
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.4221(6) Å
	b = 12.1060(7) Å β= 102.315(2)°.
	c = 27.1705(15) Å
Volume	3991.9(4) Å^3
Z	4
Density (calculated)	1.410 Mg/m^3
Absorption coefficient	0.639 mm^{-1}
F(000)	1784
Crystal size	0.591 x 0.331 x 0.300 mm^3
Theta range for data collection	2.277 to 25.145°.
Index ranges	-13<=h<=14, -14<=k<=14, -32<=l<=32
Reflections collected	72697
Independent reflections	7092 [R(int) = 0.1020]
Completeness to theta = 25.145°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.6571
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7092 / 0 / 490
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1371
R indices (all data)	R1 = 0.0816, wR2 = 0.1506
Extinction coefficient	n/a
Largest diff. peak and hole	1.712 and -0.523 e.Å^{-3}
CCDC	1881626

Table S2. Crystal data and structure refinement for *trans*-[NiF(2-$C_{12}N_2F_7$)(PCy_3)$_2$] (**5**).

Empirical formula	C48 H66 F8 N2 Ni P2	
Formula weight	1015.78	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.9941(6) Å	α= 72.302(2)°.
	b = 13.6197(7) Å	β= 72.776(2)°.
	c = 17.6604(10) Å	γ = 66.228(2)°.
Volume	2464.9(2) Å^3	
Z	2	
Density (calculated)	1.369 Mg/m^3	
Absorption coefficient	0.529 mm^{-1}	
F(000)	1076	
Crystal size	0.405 x 0.242 x 0.155 mm^3	
Theta range for data collection	2.279 to 28.364°.	
Index ranges	-16<=h<=16, -18<=k<=18, -23<=l<=23	
Reflections collected	68029	
Independent reflections	12275 [R(int) = 0.0469]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12275 / 8 / 641	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0555, wR2 = 0.1452	
R indices (all data)	R1 = 0.0718, wR2 = 0.1571	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.675 and -0.988 e.Å^{-3}	
CCDC	1881627	

S3. Kinetic experiments

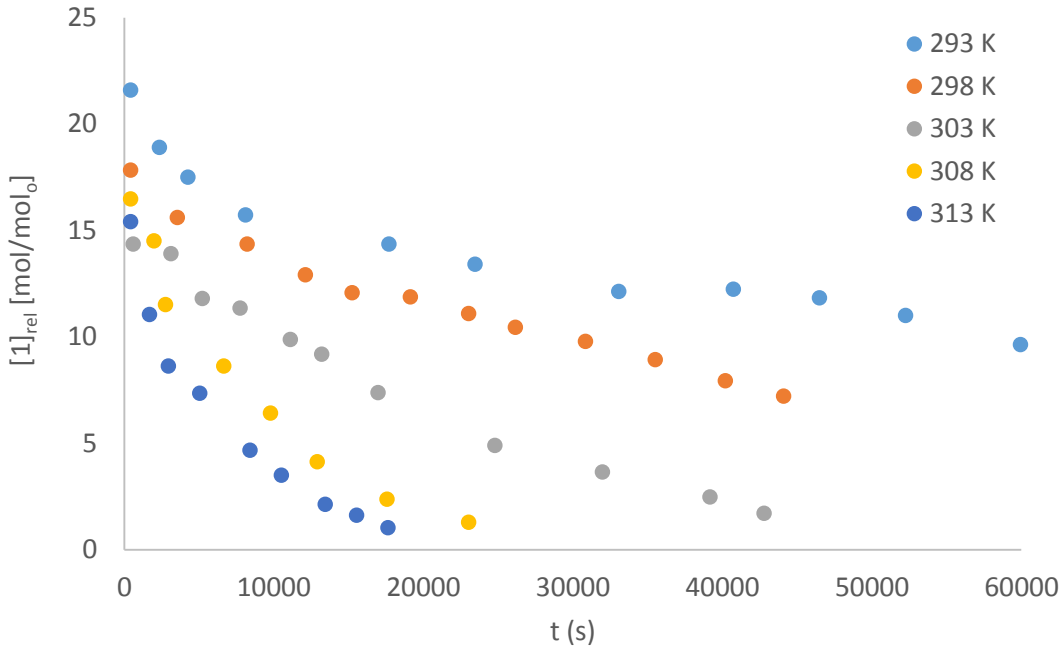

Figure S17 Kinetic trace for the loss of **1** at different temperatures; plot of $[\mathbf{1}]_{rel}$ [mol/mol$_o$] vs time.

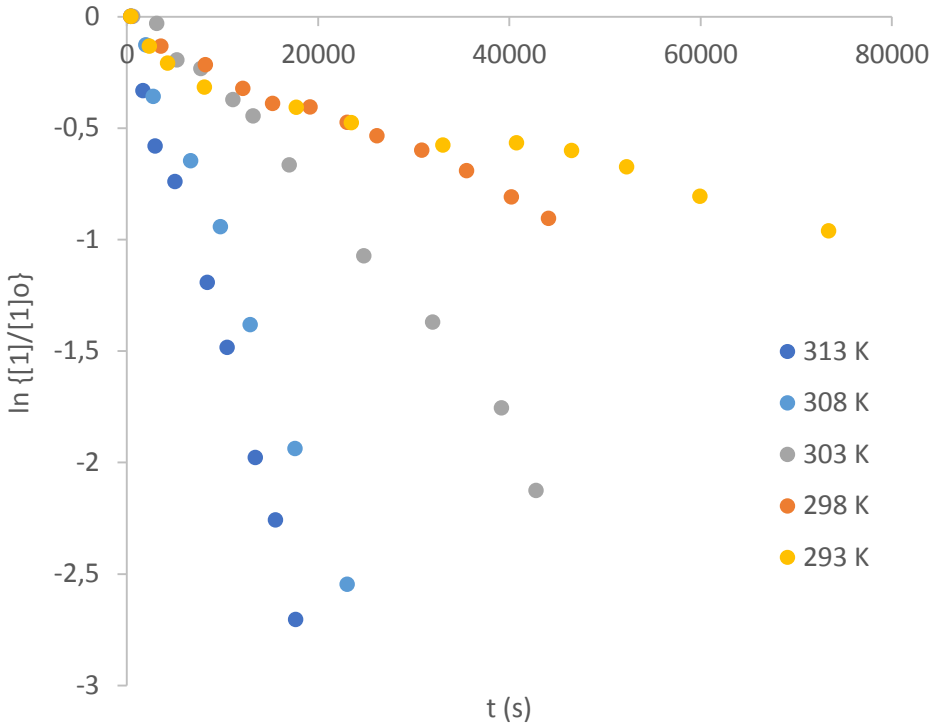

Figure S18 Kinetic trace for the loss of **1** at different temperatures; plot of ln $\{[\mathbf{1}]/[\mathbf{1}]_o\}$vs time.

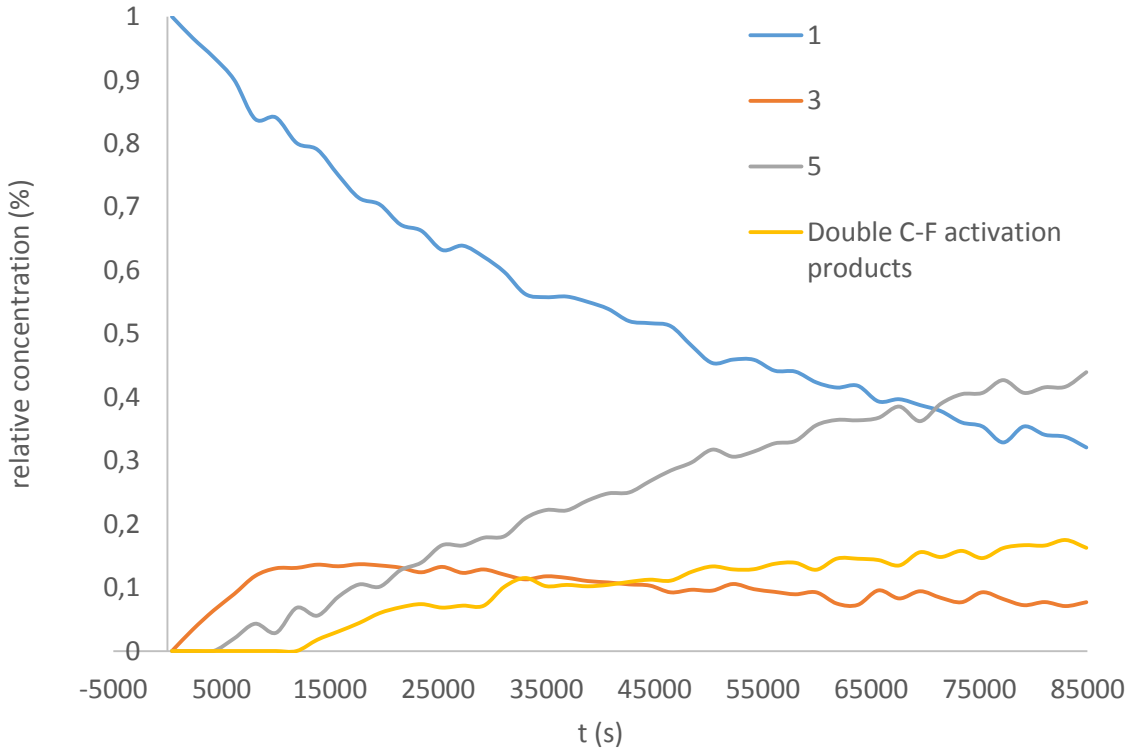

Figure S19 Kinetic trace for **1**, **3** and **5** at 293K; plot of relative concentration vs time.

S4. Optimized molecular structures of transition states

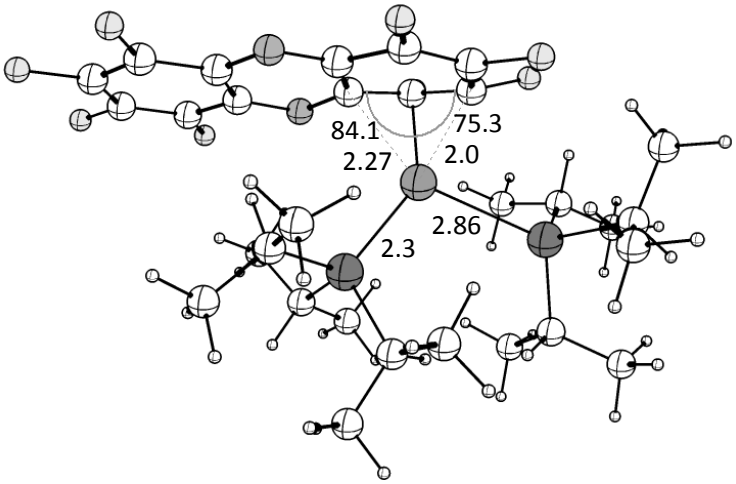

Figure S20 Optimized structure (B3LYP/cc-pVDZ) for **TSA1A2**. Distances in Å and angles in degrees.

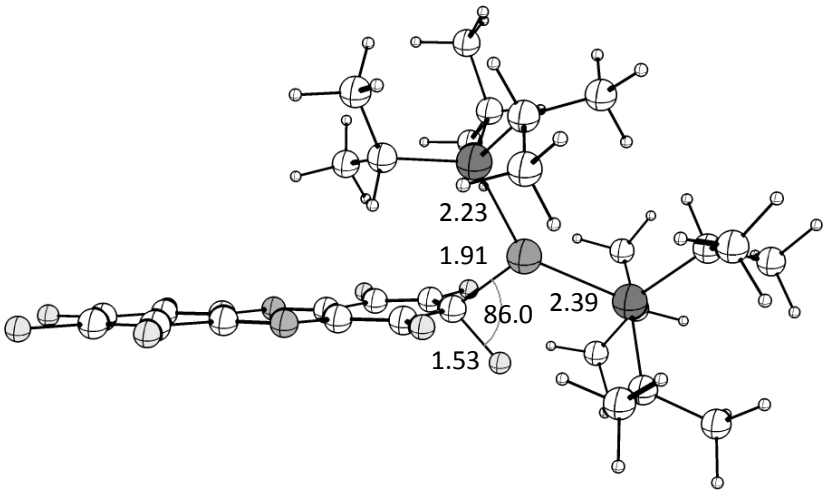

Figure S21 Optimized structure (B3LYP/cc-pVDZ) for **TSA2A3**. Distances in Å and angles in degrees.

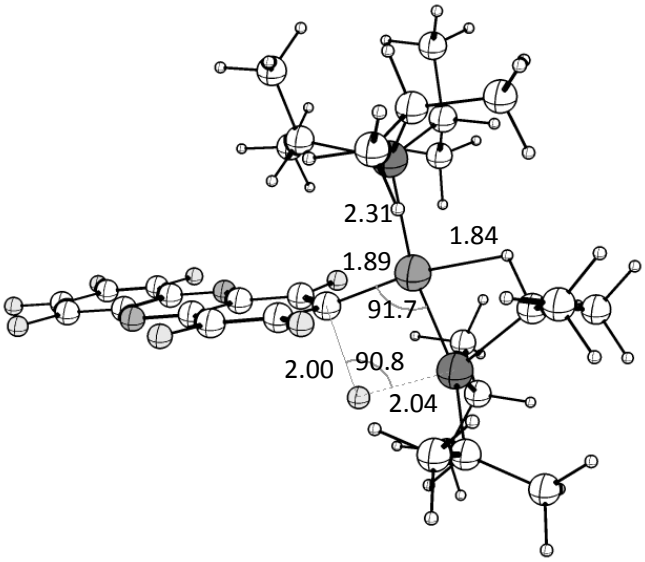

Figure S22 Optimized structure (B3LYP/cc-pVDZ) for **TSA2A3'**. Distances in Å and angles in degrees.

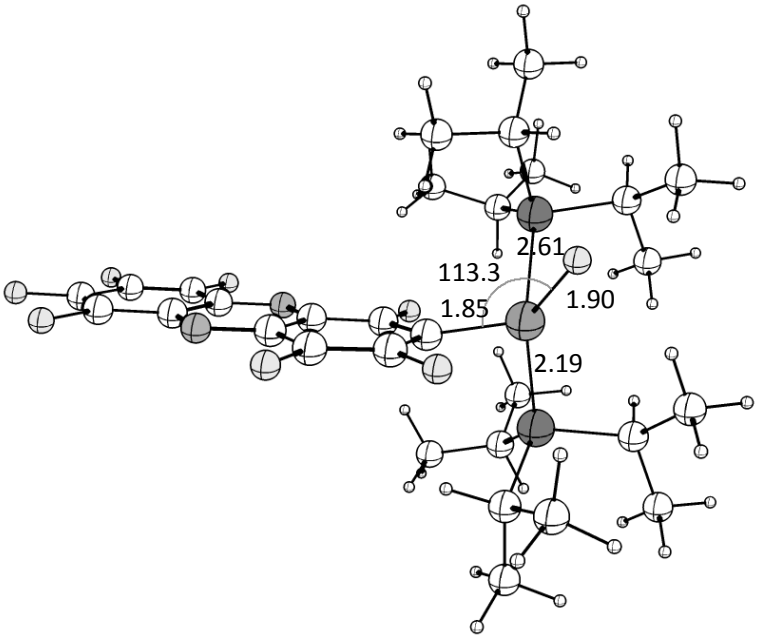

Figure S23 Optimized structure (B3LYP/cc-pVDZ) for **TSA3A4**. Distances in Å and angles in degrees.

S5. Cartesian coordinates

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A0_$C_{12}F_8N_2$, electronic energy = -1365.5529

9	-2.402328000	-2.751043000	-0.000139000
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9	-4.741484000	1.336139000	0.000052000

9	-2.402500000	2.751056000	0.000090000
9	2.402403000	-2.750971000	-0.000012000
9	2.402490000	2.751037000	-0.000005000
7	-0.000017000	-1.424326000	-0.000030000
7	-0.000041000	1.424428000	0.000006000
6	-1.139185000	-0.723559000	-0.000001000
6	-2.387373000	-1.415847000	-0.000035000
6	-3.562279000	-0.712874000	-0.000002000
6	-3.562319000	0.712803000	0.000026000
6	-2.387464000	1.415851000	0.000058000
6	-1.139199000	0.723662000	0.000056000
6	1.139225000	-0.723525000	0.000061000
6	2.387374000	-1.415798000	0.000086000
6	2.387398000	1.415856000	0.000031000
6	1.139211000	0.723629000	-0.000042000
6	3.562354000	-0.712812000	0.000106000
6	3.562355000	0.712816000	0.000120000
9	4.741351000	-1.336436000	0.000249000
9	4.741466000	1.336279000	-0.000433000

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A0_[Ni(P*i*Pr$_3$)$_2$], electronic energy = -2902.5526

28	0.000019000	0.100221000	0.000092000
15	2.156079000	0.067505000	-0.054902000
15	-2.156044000	0.067396000	0.055051000
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1	-2.469649000	0.858762000	2.281308000
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1	-4.714790000	1.910411000	2.300600000
1	-4.869866000	1.711321000	0.544585000
1	-4.841704000	0.279441000	1.605477000
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1	-3.187573000	1.645309000	-1.427524000
6	-4.412557000	-0.082057000	-1.797672000
1	-4.325163000	-1.163240000	-1.986310000
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6	-2.111467000	0.347503000	-2.751885000
1	-1.147860000	0.858323000	-2.601892000
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1	-1.246219000	-2.739425000	-0.355623000
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1	-2.593540000	-2.468840000	-1.480441000
6	3.042129000	0.555005000	1.551064000
1	3.187280000	1.642578000	1.430887000
6	4.412739000	-0.085256000	1.797344000
1	5.106078000	0.057141000	0.957506000
1	4.876774000	0.361134000	2.693398000
1	4.325640000	-1.166875000	1.983610000
6	2.111596000	0.341694000	2.752599000
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1	1.893196000	-0.728104000	2.903650000
1	2.579892000	0.723834000	3.676230000

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A1, electronic energy = -4268.1769

28	0.761140000	-0.008993000	-0.002871000
15	1.678875000	-0.177643000	2.023605000
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9	0.103295000	-2.511426000	-0.369054000
9	-1.330282000	-4.775742000	-0.468632000
9	-4.054777000	-4.702325000	-0.368905000
9	-5.354805000	-2.323162000	-0.168553000
9	0.142170000	2.520512000	-0.280670000
9	-5.310476000	2.411362000	0.067141000
7	-1.094485000	0.010132000	-0.174259000
7	-4.013994000	0.032697000	-0.075116000
6	-1.866488000	-1.151179000	-0.238998000
6	-1.245570000	-2.412777000	-0.339869000
6	-1.961989000	-3.592425000	-0.383690000
6	-3.364425000	-3.552519000	-0.326240000
6	-4.011430000	-2.340251000	-0.223744000

6	-3.301178000	-1.108341000	-0.177579000
6	-1.845814000	1.187196000	-0.144641000
6	-1.204555000	2.441733000	-0.177454000
6	-3.968125000	2.409098000	-0.009680000
6	-3.280630000	1.165357000	-0.075810000
6	3.132249000	1.763410000	-1.808457000
1	2.366100000	2.488740000	-1.488408000
6	3.677027000	2.207082000	-3.170595000
1	4.068125000	3.234980000	-3.089153000
1	4.511538000	1.568684000	-3.497180000
1	2.914175000	2.205911000	-3.961196000
6	4.249343000	1.768089000	-0.760549000
1	3.891356000	1.431260000	0.219373000
1	5.085339000	1.116572000	-1.061434000
1	4.652718000	2.786655000	-0.642080000
6	3.435360000	-1.214093000	-2.082862000
1	4.299588000	-0.887766000	-1.481693000
6	3.898383000	-1.352429000	-3.538074000
1	3.087503000	-1.713780000	-4.188386000
1	4.273232000	-0.409696000	-3.956640000
1	4.714525000	-2.091853000	-3.594041000
6	2.970991000	-2.567257000	-1.529346000
1	2.623687000	-2.485900000	-0.492611000
1	2.141886000	-2.983379000	-2.119880000
1	3.802688000	-3.290122000	-1.562625000
6	1.122502000	0.207269000	-3.323239000
1	1.829626000	0.288874000	-4.164266000
6	0.197932000	1.429354000	-3.333114000
1	-0.563214000	1.345183000	-2.545506000
1	0.734224000	2.377865000	-3.189432000
1	-0.327694000	1.485078000	-4.300493000
6	0.297237000	-1.072598000	-3.494760000
1	-0.413225000	-1.192621000	-2.664233000
1	-0.284901000	-1.016567000	-4.429375000
1	0.919834000	-1.976238000	-3.543302000
6	2.674777000	1.285958000	2.680846000
1	3.670766000	1.116820000	2.241387000
6	2.839468000	1.345284000	4.204010000
1	3.271414000	0.425176000	4.618758000
1	3.512513000	2.178046000	4.467503000
1	1.880480000	1.528902000	4.711014000
6	2.148613000	2.616350000	2.128563000
1	2.084187000	2.602536000	1.034456000
6	2.815508000	-1.675825000	2.229276000
1	2.293379000	-2.434775000	1.622616000
6	4.178449000	-1.404810000	1.583206000
1	4.717886000	-2.351338000	1.420098000
1	4.080487000	-0.899700000	0.614207000
1	4.806317000	-0.773417000	2.231564000
6	2.995514000	-2.241625000	3.642331000
1	2.043869000	-2.504188000	4.123122000
1	3.602066000	-3.161261000	3.589413000

1	3.528796000	-1.538671000	4.298926000
6	0.338729000	-0.459021000	3.316900000
1	0.851283000	-0.570102000	4.285966000
6	-0.443745000	-1.743665000	3.019403000
1	-1.102959000	-1.982479000	3.869909000
1	-1.080730000	-1.614005000	2.134954000
1	0.204628000	-2.614239000	2.844016000
6	-0.616820000	0.737031000	3.396179000
1	-0.124579000	1.644943000	3.770669000
1	-1.046688000	0.965568000	2.409656000
1	-1.449913000	0.505059000	4.080120000
6	-1.899042000	3.634015000	-0.117675000
6	-3.300064000	3.614219000	-0.027884000
9	-1.248027000	4.809500000	-0.147532000
9	-3.969008000	4.775773000	0.033573000
1	1.145492000	2.850404000	2.513891000
1	2.822148000	3.436172000	2.428229000

85

TSA1A2, electronic energy = -4268.1369

28	-0.742593000	-0.237233000	-0.314398000
15	-3.582359000	0.048925000	-0.220461000
15	0.153314000	1.634785000	0.744233000
9	-2.240756000	-2.724461000	-1.321249000
9	-0.337413000	-1.434212000	-2.827396000
9	-1.687375000	-3.530810000	1.219089000
9	3.811101000	1.073880000	-2.800647000
7	2.784144000	-2.037255000	0.756161000
7	1.934185000	-0.514284000	-1.521221000
6	-1.125440000	-2.237977000	-0.709322000
6	-0.726968000	-2.910104000	0.517359000
6	0.555571000	-2.889201000	0.975242000
6	1.562671000	-2.129976000	0.280369000
6	1.132334000	-1.378854000	-0.903591000
6	-0.136325000	-1.629372000	-1.498019000
6	3.204456000	-0.455738000	-1.061884000
6	3.641010000	-1.216326000	0.081247000
6	4.967878000	-1.078333000	0.550330000
6	5.857393000	-0.238789000	-0.085016000
6	5.444589000	0.488701000	-1.222592000
6	4.158221000	0.378869000	-1.702925000
6	-4.683189000	-1.150513000	0.755110000
1	-5.692214000	-0.716649000	0.699288000
6	-4.779929000	-2.578850000	0.211756000
1	-3.833349000	-3.122087000	0.306462000
6	-4.240780000	-1.163798000	2.222807000
1	-4.240290000	-0.159493000	2.671010000
1	-4.919763000	-1.795766000	2.819039000
6	-4.118649000	-0.245864000	-2.005781000
1	-3.903955000	-1.320446000	-2.109576000
6	-3.203562000	0.478307000	-3.003462000
1	-3.377761000	1.563505000	-3.015968000

1	-2.140869000	0.304022000	-2.776834000
6	-5.600278000	-0.018775000	-2.319536000
1	-6.261948000	-0.571404000	-1.635984000
1	-5.868921000	1.046679000	-2.264767000
6	-4.323056000	1.713340000	0.334079000
1	-3.739522000	1.929974000	1.242251000
6	-4.018563000	2.819088000	-0.682225000
1	-2.991657000	2.762168000	-1.060582000
1	-4.698131000	2.765360000	-1.545566000
6	0.682833000	3.096820000	-0.313432000
1	1.014876000	3.879447000	0.387059000
6	-0.493978000	3.635062000	-1.128789000
1	-1.307906000	4.012493000	-0.495206000
1	-0.900056000	2.850539000	-1.788119000
6	1.845509000	2.733895000	-1.235356000
1	2.735205000	2.412039000	-0.677452000
1	1.568079000	1.922202000	-1.920504000
6	1.709722000	1.190164000	1.699302000
1	2.297282000	0.705269000	0.909080000
6	1.431387000	0.136749000	2.780164000
1	0.672040000	-0.592050000	2.461790000
1	1.079391000	0.607683000	3.709878000
6	2.556976000	2.339425000	2.255777000
1	3.506883000	1.931782000	2.640373000
1	2.058185000	2.850835000	3.091170000
6	-1.083577000	2.415973000	1.926328000
6	-0.643719000	3.685439000	2.662772000
1	-0.222920000	4.446360000	1.989910000
1	0.103289000	3.462012000	3.438240000
1	-1.886870000	2.695426000	1.226319000
6	-1.660560000	1.385965000	2.904379000
1	-0.965135000	1.185391000	3.730897000
1	-1.882785000	0.430491000	2.409067000
1	-3.224844000	-1.578682000	2.317672000
1	-1.515014000	4.135063000	3.167725000
1	-2.595022000	1.767407000	3.347786000
1	-5.539431000	-3.124892000	0.796667000
1	-5.092198000	-2.611228000	-0.841651000
1	2.352677000	-0.420856000	3.007915000
1	2.808045000	3.092443000	1.495527000
1	2.131978000	3.613091000	-1.835117000
1	-0.155839000	4.467999000	-1.766251000
1	-4.154550000	3.809110000	-0.216448000
6	-5.803237000	1.749681000	0.735475000
1	-6.021058000	1.118415000	1.607930000
1	-6.072953000	2.784011000	1.008747000
1	-6.466469000	1.442559000	-0.085762000
1	-3.394174000	0.101793000	-4.022482000
9	6.334935000	1.282048000	-1.834189000
9	7.117985000	-0.098151000	0.355386000
9	5.366075000	-1.761969000	1.633891000
9	0.869601000	-3.475618000	2.141770000

1	-5.822192000	-0.360758000	-3.344808000

85

A2, electronic energy = -4268.1873

28	1.316619000	-0.167808000	0.223249000
15	3.585874000	-0.270778000	0.098701000
15	0.417177000	1.792653000	-0.544013000
9	1.643061000	-2.629957000	1.821507000
9	0.018248000	-0.605334000	2.668164000
9	1.354628000	-3.651546000	-0.746944000
9	-4.503081000	1.019838000	2.690435000
7	-2.990767000	-1.847302000	-0.871057000
7	-2.470827000	-0.440278000	1.549471000
6	0.877991000	-1.944483000	0.872781000
6	0.458919000	-2.783600000	-0.242639000
6	-0.761346000	-2.695332000	-0.832198000
6	-1.805297000	-1.872195000	-0.285060000
6	-1.512507000	-1.098965000	0.911763000
6	-0.143134000	-1.030026000	1.362168000
6	-3.689672000	-0.406889000	0.957786000
6	-3.944422000	-1.085586000	-0.278740000
6	-5.223421000	-0.971863000	-0.880519000
6	-6.210669000	-0.223152000	-0.281659000
6	-5.961355000	0.444650000	0.940550000
6	-4.729806000	0.354683000	1.548651000
6	4.305060000	-1.683104000	-0.918333000
1	5.354279000	-1.417266000	-1.108932000
6	4.304448000	-3.031664000	-0.189483000
1	3.332305000	-3.275277000	0.251175000
6	3.573788000	-1.729816000	-2.266033000
1	2.503798000	-1.945764000	-2.130881000
1	3.659983000	-0.774379000	-2.807784000
6	4.190694000	-0.607346000	1.849110000
1	3.840272000	-1.640620000	1.992848000
6	3.450682000	0.249760000	2.885116000
1	3.746381000	1.307530000	2.838177000
1	2.360826000	0.188519000	2.748622000
6	5.708468000	-0.572011000	2.049559000
1	6.243473000	-1.201288000	1.323011000
1	6.105617000	0.450574000	1.969897000
6	4.519379000	1.229589000	-0.582015000
1	3.911861000	1.496956000	-1.458835000
6	4.466629000	2.402851000	0.402386000
1	3.469235000	2.530701000	0.839597000
1	5.178952000	2.263802000	1.228399000
6	-0.116203000	3.045628000	0.751348000
1	-0.519207000	3.910607000	0.201071000
6	1.087597000	3.509311000	1.577785000
1	1.863070000	3.988390000	0.963517000
1	1.543561000	2.661491000	2.113437000
6	-1.208714000	2.495574000	1.670332000
1	-2.130043000	2.241076000	1.130319000

1	-0.871801000	1.593544000	2.197568000
6	-1.187405000	1.381882000	-1.446342000
1	-1.751873000	0.895080000	-0.637480000
6	-0.980468000	0.342109000	-2.557039000
1	-0.247419000	-0.426738000	-2.271185000
1	-0.627551000	0.812633000	-3.485084000
6	-2.025945000	2.562131000	-1.945108000
1	-1.562533000	3.048640000	-2.816027000
1	-2.188185000	3.325567000	-1.170662000
6	1.504290000	2.812553000	-1.695347000
6	1.049710000	4.238631000	-2.023676000
1	0.901790000	4.850842000	-1.122886000
1	0.116604000	4.254358000	-2.603505000
1	2.423322000	2.894018000	-1.098287000
6	1.848990000	2.031323000	-2.969647000
1	1.026477000	2.077545000	-3.697683000
1	2.055575000	0.970280000	-2.762035000
1	4.003385000	-2.516116000	-2.908051000
1	1.824980000	4.733953000	-2.632111000
1	2.739742000	2.466567000	-3.451032000
1	4.559476000	-3.831174000	-0.904517000
1	5.057302000	-3.053955000	0.611438000
1	-1.931342000	-0.166699000	-2.777552000
1	-3.016554000	2.196738000	-2.263493000
1	-1.467876000	3.256332000	2.424874000
1	0.761116000	4.245235000	2.330270000
1	4.735111000	3.340371000	-0.111220000
6	5.951417000	1.002964000	-1.082238000
1	5.992254000	0.321219000	-1.943178000
1	6.369916000	1.968091000	-1.413695000
1	6.613271000	0.608072000	-0.298571000
1	3.684641000	-0.114442000	3.899278000
9	-6.945359000	1.172720000	1.483010000
9	-7.422883000	-0.106885000	-0.839799000
9	-5.474399000	-1.594384000	-2.040009000
9	-1.013266000	-3.372633000	-1.968175000
1	5.957130000	-0.943448000	3.057747000

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TSA2A3, electronic energy = -4268.1342

28	2.121674000	0.097047000	-0.086783000
15	1.768847000	2.374981000	0.084863000
15	2.834059000	-1.879315000	-0.366949000
9	0.916797000	-2.439011000	0.056862000
9	-0.399092000	-0.067117000	-1.869599000
9	1.000202000	-0.705989000	2.623956000
9	-5.074820000	0.101047000	-2.878638000
7	-3.615230000	-0.689905000	1.648202000
7	-3.002440000	-0.246561000	-1.106066000
6	0.387127000	-0.524751000	0.320500000
6	0.010943000	-0.661964000	1.694733000
6	-1.276876000	-0.738469000	2.139273000

6	-2.359638000	-0.631520000	1.213236000
6	-2.030633000	-0.421970000	-0.193617000
6	-0.668036000	-0.352474000	-0.551593000
6	-4.267016000	-0.298927000	-0.661764000
6	-4.583267000	-0.532691000	0.725586000
6	-5.948722000	-0.583700000	1.128242000
6	-6.952236000	-0.411106000	0.210010000
6	-6.643393000	-0.177163000	-1.157167000
6	-5.341702000	-0.120824000	-1.583403000
6	2.791120000	3.091791000	1.486792000
1	2.436891000	4.120512000	1.651647000
6	2.541026000	2.265631000	2.755232000
1	2.923600000	1.239945000	2.636644000
6	4.283145000	3.150143000	1.147922000
1	4.667333000	2.168385000	0.835953000
1	4.504303000	3.873959000	0.350851000
6	-0.000500000	2.888595000	0.495619000
1	-0.340350000	2.045657000	1.118055000
6	-0.902681000	2.944312000	-0.745388000
1	-0.709982000	3.854869000	-1.333020000
1	-0.784203000	2.077172000	-1.403689000
6	-0.141993000	4.177429000	1.314187000
1	0.351266000	4.117649000	2.293989000
1	0.257897000	5.051922000	0.779054000
6	2.370515000	3.280740000	-1.442131000
1	3.449563000	3.050226000	-1.408738000
6	1.822744000	2.657137000	-2.733221000
1	1.878015000	1.558607000	-2.707807000
1	0.773436000	2.931540000	-2.906460000
6	2.750336000	-2.599593000	-2.093947000
1	3.801214000	-2.776598000	-2.371467000
6	2.140195000	-1.590200000	-3.072008000
1	2.639178000	-0.610241000	-3.036204000
1	1.080076000	-1.428593000	-2.842463000
6	1.999885000	-3.931904000	-2.159598000
1	2.485185000	-4.717712000	-1.562570000
1	0.971611000	-3.809858000	-1.795786000
6	3.357601000	-3.292824000	0.741134000
1	2.546005000	-3.999346000	0.519566000
6	3.287194000	-2.995585000	2.240553000
1	2.317753000	-2.560372000	2.508686000
1	4.080771000	-2.311249000	2.570356000
6	4.686899000	-3.926172000	0.317991000
1	5.551274000	-3.285218000	0.539829000
1	4.712026000	-4.170180000	-0.754194000
6	4.346659000	-0.652573000	-0.478420000
6	5.287535000	-0.757189000	-1.682598000
1	4.755727000	-0.730495000	-2.641916000
1	5.858556000	-1.697546000	-1.634406000
1	3.855135000	0.376638000	-0.632587000
6	5.119758000	-0.495371000	0.835572000
1	5.732988000	-1.381141000	1.047730000

1	4.448376000	-0.330056000	1.689997000
1	4.851888000	3.456322000	2.040835000
1	6.011650000	0.075474000	-1.676661000
1	5.803799000	0.366799000	0.775180000
1	3.053974000	2.726535000	3.614631000
1	1.471598000	2.188857000	3.001862000
1	3.411588000	-3.938226000	2.798617000
1	4.828178000	-4.868259000	0.873000000
1	1.975658000	-4.278823000	-3.205604000
1	2.225758000	-1.972465000	-4.102048000
1	2.408523000	3.014586000	-3.595545000
6	2.202161000	4.802347000	-1.411379000
1	2.626639000	5.250621000	-0.500745000
1	2.714568000	5.253870000	-2.276926000
1	1.141903000	5.090172000	-1.468934000
1	-1.955742000	2.977227000	-0.423197000
9	-7.659110000	-0.013465000	-2.015261000
9	-8.242568000	-0.456011000	0.571254000
9	-6.253407000	-0.800121000	2.415313000
9	-1.547636000	-0.878252000	3.451627000
1	-1.212553000	4.365124000	1.499014000

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TSA2A3‘, electronic energy = -4268.1342

28	-1.873556000	0.063534000	0.046962000
15	-3.997817000	-0.935561000	-0.384389000
15	-0.937269000	2.047683000	0.460166000
9	-1.258470000	-2.166111000	-0.450957000
9	0.344221000	-0.252249000	-2.032905000
9	-0.852706000	-1.775556000	2.315543000
9	5.024981000	0.546928000	-3.008411000
7	3.719461000	-1.361759000	1.226929000
7	3.014055000	-0.344276000	-1.354036000
6	-0.332067000	-1.071595000	0.086794000
6	0.112265000	-1.507715000	1.404562000
6	1.413944000	-1.627511000	1.759731000
6	2.463424000	-1.288546000	0.833707000
6	2.071204000	-0.797923000	-0.491478000
6	0.719785000	-0.764878000	-0.814803000
6	4.289199000	-0.418446000	-0.943864000
6	4.662198000	-0.944522000	0.344551000
6	6.031509000	-1.001105000	0.711397000
6	7.007084000	-0.553426000	-0.147174000
6	6.647291000	-0.026679000	-1.412369000
6	5.331772000	0.042430000	-1.801042000
6	-4.600151000	-1.940549000	1.080003000
1	-5.641153000	-2.234942000	0.872409000
6	-3.765025000	-3.207447000	1.291990000
1	-2.697346000	-2.969112000	1.382838000
6	-4.571186000	-1.045771000	2.326649000
1	-3.537671000	-0.741130000	2.557637000
1	-5.174144000	-0.132563000	2.203639000

6	-3.915956000	-2.144507000	-1.819043000
1	-3.299400000	-2.944540000	-1.383252000
6	-3.114678000	-1.566117000	-2.993691000
1	-3.651908000	-0.755134000	-3.506593000
1	-2.140766000	-1.181817000	-2.658571000
6	-5.252407000	-2.745651000	-2.260160000
1	-5.811944000	-3.179283000	-1.417383000
1	-5.894768000	-1.997009000	-2.747730000
6	-5.398698000	0.295387000	-0.679964000
1	-5.191268000	1.066225000	0.082217000
6	-5.275902000	0.956606000	-2.058371000
1	-4.250053000	1.286441000	-2.274538000
1	-5.586153000	0.268675000	-2.858335000
6	-1.766031000	3.238507000	-0.731344000
1	-1.253264000	4.206396000	-0.626228000
6	-3.247576000	3.446245000	-0.404447000
1	-3.391862000	3.995014000	0.536979000
1	-3.785541000	2.491275000	-0.326608000
6	-1.560345000	2.718645000	-2.160512000
1	-0.495724000	2.600792000	-2.410511000
1	-2.032550000	1.732175000	-2.292240000
6	0.899839000	2.358450000	0.194869000
1	1.130774000	1.694326000	-0.650498000
6	1.734490000	1.905777000	1.398525000
1	1.405274000	0.940486000	1.798508000
1	1.689622000	2.643010000	2.214296000
6	1.278600000	3.787262000	-0.215134000
1	0.991687000	4.528980000	0.544491000
1	0.835215000	4.084274000	-1.175112000
6	-1.460476000	2.633977000	2.164072000
6	-1.040428000	4.064516000	2.515688000
1	-1.333860000	4.789928000	1.742387000
1	0.047666000	4.139638000	2.658663000
1	-2.559328000	2.607797000	2.064723000
6	-1.090698000	1.631344000	3.265688000
1	-0.015957000	1.649397000	3.493946000
1	-1.360032000	0.602308000	2.986347000
1	-4.967737000	-1.592943000	3.197138000
1	-1.519318000	4.370501000	3.460311000
1	-1.630315000	1.886850000	4.192026000
1	-4.089588000	-3.708812000	2.218567000
1	-3.886858000	-3.925268000	0.467651000
1	2.789292000	1.804939000	1.099115000
1	2.373437000	3.839184000	-0.332395000
1	-2.006794000	3.416752000	-2.886561000
1	-3.726494000	4.029726000	-1.206947000
1	-5.931127000	1.841073000	-2.108071000
6	-6.824473000	-0.213476000	-0.436320000
1	-6.976620000	-0.557056000	0.596296000
1	-7.536184000	0.609552000	-0.615672000
1	-7.091810000	-1.036295000	-1.113620000
1	-2.928274000	-2.359418000	-3.736608000

9	7.625654000	0.403120000	-2.223048000
9	8.307896000	-0.600122000	0.186463000
9	6.380040000	-1.492602000	1.910578000
9	1.748268000	-2.003045000	3.006674000
1	-5.073912000	-3.551894000	-2.991027000

85

A3, electronic energy = -4268.2015

28	1.664357000	-0.123688000	-0.400698000
15	3.675117000	-1.423654000	-0.303351000
15	1.907026000	1.746966000	0.856704000
9	1.350712000	-1.370922000	-1.744275000
9	-0.744251000	-0.762869000	1.434515000
9	0.189368000	1.191842000	-2.779396000
9	-5.276756000	-1.614501000	2.696820000
7	-4.305114000	0.369545000	-1.587581000
7	-3.409790000	-0.697716000	0.901487000
6	-0.203749000	0.216529000	-0.642810000
6	-0.701013000	0.716085000	-1.876223000
6	-2.029773000	0.783134000	-2.200434000
6	-3.005895000	0.305724000	-1.278646000
6	-2.546390000	-0.236343000	-0.011116000
6	-1.141289000	-0.253353000	0.233538000
6	-4.711754000	-0.635077000	0.589667000
6	-5.165509000	-0.094601000	-0.670502000
6	-6.566184000	-0.054293000	-0.940242000
6	-7.462319000	-0.522873000	-0.016587000
6	-7.015381000	-1.055788000	1.225630000
6	-5.679900000	-1.111529000	1.524042000
6	4.685216000	-1.279253000	-1.883336000
1	5.465562000	-2.051863000	-1.799643000
6	3.887566000	-1.544155000	-3.162494000
1	3.057622000	-0.833595000	-3.269504000
6	5.362107000	0.095005000	-1.946551000
1	4.612390000	0.885567000	-2.080118000
1	5.946126000	0.331130000	-1.044483000
6	2.988242000	-3.177009000	-0.347051000
1	2.446743000	-3.136426000	-1.300408000
6	1.932502000	-3.414456000	0.742584000
1	2.380330000	-3.543853000	1.738256000
1	1.207048000	-2.589491000	0.796570000
6	4.015365000	-4.310311000	-0.404077000
1	4.761750000	-4.163258000	-1.199131000
1	4.550391000	-4.438516000	0.549024000
6	5.027470000	-1.382203000	1.017975000
1	5.208518000	-0.303538000	1.145649000
6	4.520078000	-1.952537000	2.349403000
1	3.516088000	-1.592257000	2.610727000
1	4.483154000	-3.050218000	2.313678000
6	2.341125000	1.591584000	2.679078000
1	2.063238000	2.559889000	3.116553000
6	3.825136000	1.378502000	2.970576000

1	4.439743000	2.235538000	2.663573000
1	4.213854000	0.487558000	2.474551000
6	1.459746000	0.504139000	3.303739000
1	0.388994000	0.712548000	3.166656000
1	1.655310000	-0.476187000	2.843425000
6	0.337161000	2.811875000	0.932625000
1	-0.446891000	2.051219000	1.046172000
6	0.073235000	3.564383000	-0.378812000
1	0.267695000	2.959998000	-1.270624000
1	0.693753000	4.470968000	-0.443258000
6	0.219046000	3.774791000	2.121649000
1	1.050738000	4.492921000	2.169671000
1	0.153602000	3.252096000	3.085515000
6	3.285740000	2.772755000	0.104119000
6	3.528799000	4.132593000	0.769218000
1	3.645336000	4.062465000	1.859768000
1	2.705116000	4.830620000	0.560400000
1	4.160374000	2.126582000	0.291120000
6	3.141157000	2.922743000	-1.418066000
1	2.416212000	3.704648000	-1.677777000
1	2.812307000	1.990067000	-1.898585000
1	6.049447000	0.135740000	-2.807185000
1	4.450356000	4.580716000	0.362653000
1	4.110409000	3.212513000	-1.853565000
1	4.561632000	-1.446653000	-4.030143000
1	3.458353000	-2.555590000	-3.179327000
1	-0.980396000	3.884102000	-0.409574000
1	-0.710426000	4.356375000	2.007066000
1	1.660668000	0.428917000	4.384470000
1	3.965215000	1.240924000	4.055046000
1	5.203520000	-1.669436000	3.165922000
6	6.376623000	-2.019022000	0.654080000
1	6.856252000	-1.539596000	-0.209327000
1	7.061950000	-1.907495000	1.511038000
1	6.286699000	-3.092945000	0.443582000
1	1.372734000	-4.336290000	0.511923000
9	-7.937564000	-1.497221000	2.087818000
9	-8.778678000	-0.494182000	-0.250832000
9	-7.002070000	0.445260000	-2.102406000
9	-2.432859000	1.296189000	-3.376703000
1	3.494601000	-5.259718000	-0.614168000

85

A3‘, electronic energy = -4268.1596

28	2.067320000	-0.015878000	-0.011632000
15	2.060906000	2.318113000	-0.047043000
15	2.514193000	-2.101442000	-0.303811000
9	0.831242000	-2.788547000	-0.376381000
9	-0.479173000	-0.122191000	-1.807953000
9	0.863421000	-0.287951000	2.733004000
9	-5.131412000	-0.096962000	-2.905224000
7	-3.749040000	-0.344872000	1.705773000

7	-3.092929000	-0.195356000	-1.066758000
6	0.260105000	-0.179566000	0.431207000
6	-0.120228000	-0.275199000	1.797314000
6	-1.416810000	-0.340174000	2.234485000
6	-2.480562000	-0.313268000	1.286588000
6	-2.139992000	-0.239705000	-0.125523000
6	-0.763136000	-0.196600000	-0.475875000
6	-4.363749000	-0.223195000	-0.643932000
6	-4.697598000	-0.300720000	0.759277000
6	-6.071922000	-0.324177000	1.142681000
6	-7.056710000	-0.271767000	0.192267000
6	-6.728321000	-0.194512000	-1.190896000
6	-5.421868000	-0.171084000	-1.600824000
6	3.198356000	3.079604000	1.237949000
1	2.965199000	4.154543000	1.269737000
6	2.885722000	2.462997000	2.607310000
1	3.138843000	1.393055000	2.620452000
6	4.679315000	2.927862000	0.876434000
1	4.949706000	1.881022000	0.677702000
1	4.956567000	3.523609000	-0.004567000
6	0.380240000	3.097035000	0.321002000
1	-0.042021000	2.395228000	1.057435000
6	-0.542412000	3.093146000	-0.905968000
1	-0.266156000	3.895763000	-1.606486000
1	-0.528665000	2.144226000	-1.453397000
6	0.413342000	4.491979000	0.956344000
1	0.926947000	4.506032000	1.927399000
1	0.893795000	5.233575000	0.300550000
6	2.718383000	2.963270000	-1.681152000
1	3.747307000	2.563356000	-1.660448000
6	2.014210000	2.326795000	-2.888343000
1	1.804270000	1.260874000	-2.725265000
1	1.059673000	2.823636000	-3.108323000
6	2.862105000	-2.661938000	-2.061429000
1	3.952466000	-2.780712000	-2.123705000
6	2.427173000	-1.566620000	-3.040605000
1	2.935024000	-0.611463000	-2.840007000
1	1.344383000	-1.389345000	-2.966671000
6	2.222114000	-4.005723000	-2.419115000
1	2.538576000	-4.811580000	-1.739876000
1	1.127287000	-3.943269000	-2.382468000
6	2.952760000	-3.535275000	0.828942000
1	2.235607000	-4.276664000	0.451431000
6	2.581816000	-3.273564000	2.293260000
1	1.576084000	-2.838234000	2.373458000
1	3.287322000	-2.593495000	2.788249000
6	4.354083000	-4.124013000	0.649518000
1	5.151378000	-3.470897000	1.025387000
1	4.572793000	-4.353341000	-0.404162000
6	4.191379000	-0.865196000	-0.076854000
6	5.349452000	-1.070721000	-1.058166000
1	5.047785000	-0.927771000	-2.104328000

1	5.780336000	-2.079246000	-0.962536000
1	3.888044000	0.200613000	-0.328150000
6	4.673917000	-0.782622000	1.375562000
1	5.187599000	-1.700811000	1.687770000
1	3.844237000	-0.610725000	2.076531000
1	5.300675000	3.272495000	1.718798000
1	6.159530000	-0.346999000	-0.850961000
1	5.391639000	0.045151000	1.508227000
1	3.474670000	2.965201000	3.391638000
1	1.822201000	2.552534000	2.874523000
1	2.590030000	-4.225359000	2.849715000
1	4.416072000	-5.071559000	1.210577000
1	2.530126000	-4.291124000	-3.439018000
1	2.664382000	-1.862614000	-4.075639000
1	2.651341000	2.421635000	-3.782357000
6	2.797066000	4.487961000	-1.805700000
1	3.328632000	4.954541000	-0.963397000
1	3.334095000	4.758189000	-2.730098000
1	1.794303000	4.937010000	-1.866297000
1	-1.578567000	3.281155000	-0.581818000
9	-7.732289000	-0.145309000	-2.073359000
9	-8.350732000	-0.290881000	0.531372000
9	-6.395967000	-0.395624000	2.439279000
9	-1.704919000	-0.419271000	3.546027000
1	-0.622113000	4.828444000	1.130350000

85

TSA3A4, electronic energy = -4268.1729

28	-2.102021000	-0.273138000	-0.635547000
15	-2.222487000	2.312993000	-0.264138000
15	-2.490113000	-1.836834000	0.853877000
9	-2.807757000	0.092547000	-2.358957000
9	0.234324000	0.652040000	1.201815000
9	-0.647889000	-2.125339000	-2.542804000
9	4.720483000	1.652040000	2.411159000
7	3.826199000	-1.213290000	-1.359513000
7	2.887255000	0.396159000	0.800149000
6	-0.298877000	-0.702481000	-0.656185000
6	0.218468000	-1.509536000	-1.716252000
6	1.556932000	-1.686443000	-1.954601000
6	2.520926000	-1.051535000	-1.119778000
6	2.040971000	-0.236187000	-0.022335000
6	0.633584000	-0.116544000	0.159178000
6	4.195062000	0.239214000	0.556868000
6	4.671426000	-0.577398000	-0.536748000
6	6.077883000	-0.703693000	-0.742269000
6	6.957504000	-0.058220000	0.085796000
6	6.488032000	0.746816000	1.162881000
6	5.146461000	0.893405000	1.395569000
6	-4.049660000	2.788237000	-0.218355000
1	-4.114620000	3.877594000	-0.075744000
6	-4.778881000	2.424754000	-1.517549000

1	-4.534019000	1.403038000	-1.842076000
6	-4.702077000	2.095180000	0.983324000
1	-4.740686000	1.008670000	0.816376000
1	-4.156784000	2.269451000	1.923910000
6	-1.654689000	3.052371000	-1.899911000
1	-2.329215000	2.516932000	-2.586183000
6	-0.230698000	2.619388000	-2.274935000
1	0.533355000	3.096103000	-1.644391000
1	-0.108418000	1.530521000	-2.192997000
6	-1.857334000	4.560100000	-2.070173000
1	-2.884367000	4.873262000	-1.830341000
1	-1.171630000	5.137377000	-1.431512000
6	-1.494202000	3.355718000	1.154039000
1	-1.566612000	2.665558000	2.012417000
6	-0.006088000	3.676158000	0.951118000
1	0.584809000	2.794767000	0.678330000
1	0.133348000	4.444599000	0.176149000
6	-1.893266000	-1.683536000	2.623957000
1	-2.463632000	-2.459600000	3.160968000
6	-2.252666000	-0.312384000	3.207150000
1	-3.334140000	-0.115266000	3.188793000
1	-1.744128000	0.487446000	2.650486000
6	-0.397234000	-1.980311000	2.807474000
1	-0.061119000	-2.875397000	2.266506000
1	0.216499000	-1.132418000	2.484860000
6	-1.944398000	-3.542245000	0.289161000
1	-0.875312000	-3.374349000	0.076205000
6	-2.638010000	-3.933388000	-1.022596000
1	-2.672259000	-3.102433000	-1.738849000
1	-3.666138000	-4.277020000	-0.833930000
6	-2.057064000	-4.667513000	1.325789000
1	-3.104135000	-4.905379000	1.556570000
1	-1.543028000	-4.439507000	2.268757000
6	-4.366478000	-1.785078000	1.028125000
6	-4.986345000	-2.913517000	1.859268000
1	-4.489912000	-3.055299000	2.829663000
1	-4.966014000	-3.869115000	1.315497000
1	-4.501890000	-0.843096000	1.583037000
6	-5.085821000	-1.635794000	-0.320845000
1	-5.081530000	-2.579393000	-0.883137000
1	-4.637712000	-0.868361000	-0.968089000
1	-5.736893000	2.449942000	1.121112000
1	-6.043088000	-2.672036000	2.059380000
1	-6.136631000	-1.357033000	-0.142500000
1	-5.868711000	2.506445000	-1.367736000
1	-4.506554000	3.103617000	-2.339295000
1	-2.092365000	-4.766015000	-1.493795000
1	-1.595841000	-5.579038000	0.911505000
1	-0.195846000	-2.145697000	3.878011000
1	-1.923339000	-0.261198000	4.257249000
1	0.411485000	4.079102000	1.889070000
6	-2.253253000	4.637872000	1.519058000

1	-3.285160000	4.445613000	1.843689000
1	-1.736963000	5.140180000	2.354992000
1	-2.286181000	5.347657000	0.678520000
1	-0.021706000	2.903848000	-3.320034000
9	7.395154000	1.351586000	1.935389000
9	8.277956000	-0.162248000	-0.090181000
9	6.534450000	-1.454704000	-1.749929000
9	1.975909000	-2.449509000	-2.976361000
1	-1.656459000	4.853139000	-3.115161000

85

A4, electronic energy = -4267.8525

28	2.151107000	0.011354000	0.125825000
15	2.534480000	-2.173635000	-0.082582000
15	2.201537000	2.228489000	0.449083000
9	3.917727000	0.091705000	0.623325000
9	-0.428377000	-0.306640000	1.826406000
9	0.901834000	0.104353000	-2.675466000
9	-5.097385000	-0.714128000	2.815693000
7	-3.692082000	0.207980000	-1.652498000
7	-3.038231000	-0.317994000	1.068923000
6	0.346123000	-0.069550000	-0.376028000
6	-0.066651000	0.051112000	-1.731885000
6	-1.357347000	0.170985000	-2.157900000
6	-2.424924000	0.083105000	-1.237870000
6	-2.086620000	-0.139516000	0.150502000
6	-0.702463000	-0.179837000	0.498059000
6	-4.311716000	-0.218447000	0.639813000
6	-4.643217000	0.071187000	-0.710700000
6	-6.014261000	0.185474000	-1.089702000
6	-6.979124000	0.048541000	-0.155960000
6	-6.667414000	-0.303006000	1.158627000
6	-5.387859000	-0.397390000	1.551844000
6	3.811716000	-2.527929000	-1.380030000
1	3.846138000	-3.520821000	-1.494414000
6	3.354348000	-1.936217000	-2.717848000
1	3.364218000	-0.946485000	-2.731097000
6	5.236639000	-2.063070000	-1.040749000
1	5.247532000	-1.080462000	-0.921542000
1	5.530866000	-2.480748000	-0.192778000
6	1.126323000	-3.308357000	-0.535692000
1	0.572012000	-2.802243000	-1.196328000
6	0.201261000	-3.580109000	0.663560000
1	0.689976000	-4.113512000	1.339153000
1	-0.054740000	-2.719484000	1.080566000
6	1.492086000	-4.634980000	-1.225833000
1	2.047241000	-4.452574000	-2.025124000
1	2.019429000	-5.198763000	-0.606230000
6	3.301886000	-2.667095000	1.519807000
1	4.150173000	-2.139367000	1.573557000
6	2.464490000	-2.195346000	2.721614000
1	2.255883000	-1.232660000	2.623103000

1	1.609861000	-2.694587000	2.746097000
6	2.551792000	2.688772000	2.211257000
1	2.544930000	3.687932000	2.258429000
6	3.907850000	2.229059000	2.729759000
1	4.625097000	2.594256000	2.153616000
1	3.958261000	1.240952000	2.695520000
6	1.416639000	2.187697000	3.119071000
1	0.550475000	2.527144000	2.781146000
1	1.389252000	1.198653000	3.096569000
6	0.692041000	3.232698000	0.041478000
1	-0.081336000	2.703719000	0.391884000
6	0.453690000	3.350830000	-1.469518000
1	0.536731000	2.457278000	-1.887488000
1	1.142567000	3.940533000	-1.866869000
6	0.551647000	4.616334000	0.667064000
1	1.258104000	5.211545000	0.309986000
1	0.675909000	4.548621000	1.647029000
6	3.670807000	2.805157000	-0.503790000
6	4.077705000	4.167283000	-0.674967000
1	4.139127000	4.597341000	0.214304000
1	3.462417000	4.846984000	-1.049845000
1	4.450386000	2.299335000	-0.134461000
6	3.708742000	2.608901000	-1.876817000
1	3.003000000	3.156000000	-2.305813000
1	3.523401000	1.658201000	-2.078523000
1	5.896342000	-2.348966000	-1.846637000
1	5.022355000	4.603490000	-0.964379000
1	4.683422000	2.889835000	-2.247593000
1	3.978543000	-2.243863000	-3.543762000
1	2.519960000	-2.318532000	-3.082087000
1	-0.532872000	3.755962000	-1.639704000
1	-0.427194000	5.010364000	0.436823000
1	1.590169000	2.536433000	4.126380000
1	4.029777000	2.576251000	3.745137000
1	3.025772000	-2.366625000	3.628270000
6	3.458222000	-4.198397000	1.567509000
1	3.531940000	-4.780220000	0.660620000
1	4.238008000	-4.567227000	2.217353000
1	2.747675000	-4.865217000	2.033205000
1	-0.675305000	-4.111556000	0.323565000
9	-7.681793000	-0.555113000	2.059668000
9	-8.296942000	0.259749000	-0.506885000
9	-6.351859000	0.434753000	-2.404346000
9	-1.621059000	0.379420000	-3.496336000
1	0.581646000	-5.141779000	-1.509830000