Supporting Information:

Trigonal Bipyramidal or Square Planar? Density Functional Theory calculations of iron bis(dithiolene) N-heterocyclic carbene complexes

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Contents

Information About Computed Properties:

The Microsoft Excel sheet titled “Research Data Compilation-simplified.xlsx” contains all of the computed properties utilized in this study. The table includes the properties and their normalized values. For chemical shifts, isotropic shielding tensors are included and the chemical shift (δ) calculated from the isotropic shielding tensor as compared to a reference are indicated. For example for the HEP values, the column titled “HEP” is the HEP isotropic shielding tensor, the column titled "HEP-CS” is the HEP value as a chemical shift when referenced to TMS, and the column “N(HEP)” is the normalized value of the HEP chemical shift.

Information About Regression Models:

The excel sheet titled “NormalizedRegressionModels.xlsx”, data associated with the multivariable regression models can be found. Sheet 1 includes the model number, the number of variables in the model, the variables included in the model, the R^2 value, the adjusted r^2 value, the root-mean-square error, and the associated p-value for the regression model. Sheet 2 includes all AIC and BIC values for each regression model.

Benchmarking to Experimental Data:

R1	R2	HEP Calc	HEP Exp
CH_3	H	209.64	179.91[1]
$C(CH_3)_3$	H	217.11	177.66[1]
CH_3	CH_3	206.41	180.80[2]
CH_3	Cl	204.41	177.56[2]
CH_3	Br	204.68	177.36[2]

R1	R2	TEP Calc	TEP Exp
CH_3	H	2032.43	2055[3]

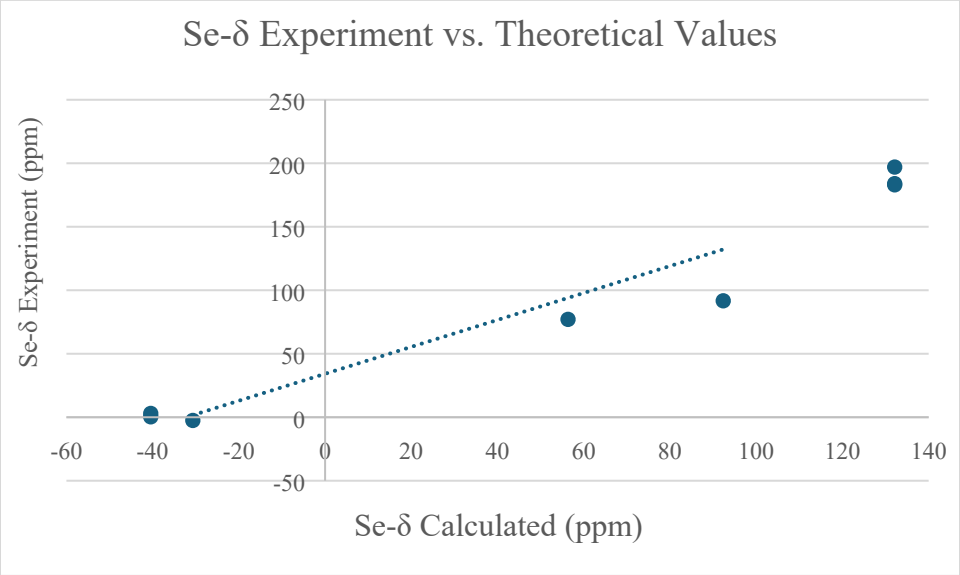
R1	R2	^{31}P-δ Calc	^{31}P-δ Exp
CH_3	CH_3	-53.66	-53.5[3,4], -49.1[5]

R1	R2	^{77}Se-δ Calc	^{77}Se-δ Exp
CH_3	H	-30.68	-2.53[1]
$C(CH_3)_3$	H	132.12	183.95[1],197[3], 183[3]
CH_3	CH_3	-40.44	0.33[2],3[3]
CH_3	Cl	56.35	77.07[2]
CH_3	Br	92.35	91.69[2]

The tables preceding this text contain experimental values obtained from literature (Exp) and our predicted values from DFT (Calc). Due to the limited amount of experimental

data from some of these properties, a comparison is not valid. Deviations may be the result of our DFT calculations being conducted in the gas-phase with the neglect of solvent. Others have studied the impact of solvation models on the calculation of Se-NMR chemical shifts and have noted its sensitivity to solvent.[6] This leaves a significant opportunity for a benchmarking study of these properties.

However, despite the deviation in values the general trends are conserved when considering changes in chemical shifts for Se-NMR. A plot of the experimental Se chemical shifts vs. our calculated values yields a R^2 value of 0.9467 when fit with a simple linear regression. To make a definitive/conclusive argument, more benchmarking is needed.



(1) Barnett, C.; Cole, M. L.; Harper, J. B. Steric Properties of *N* -Heterocyclic Carbenes Affect the Performance of Electronic Probes. *Eur. J. Inorg. Chem.* **2021**, *2021* (47), 4954–4958. https://doi.org/10.1002/ejic.202100796.

(2) Barnett, C.; Harper, J. B.; Cole, M. L. Correlating Electronic Properties of *N* -Heterocyclic Carbenes with Structure, and the Implications of Using Different Probes. *ChemistrySelect* **2022**, *7* (2), e202104348. https://doi.org/10.1002/slct.202104348.

(3) Huynh, H. V. Electronic Properties of N-Heterocyclic Carbenes and Their Experimental Determination. *Chem. Rev.* **2018**, *118* (19), 9457–9492. https://doi.org/10.1021/acs.chemrev.8b00067.

(4) Back, O.; Henry-Ellinger, M.; Martin, C. D.; Martin, D.; Bertrand, G. ^{31} P NMR Chemical Shifts of Carbene–Phosphinidene Adducts as an Indicator of the π-Accepting Properties of Carbenes. *Angew. Chem. Int. Ed.* **2013**, *52* (10), 2939–2943. https://doi.org/10.1002/anie.201209109.

(5) Krachko, T.; Slootweg, J. C. N-Heterocyclic Carbene–Phosphinidene Adducts: Synthesis, Properties, and Applications. *Eur. J. Inorg. Chem.* **2018**, *2018* (24), 2734–2754. https://doi.org/10.1002/ejic.201800459.

(6) Kondrashova, S. A.; Latypov, S. K. NMR “Finger Prints” of N-Heterocyclic Carbenes, DFT Analysis: Scopes and Limitations. *Molecules* **2023**, *28* (23), 7729. https://doi.org/10.3390/molecules28237729.

Optimized Coordinates:

TURBOMOLE Coordinates

Fe-adduct R_1=H R_2=H

```
22
 Energy =   -3238.3286544420
Fe    1.5668643   10.4941289   23.6426306
 S    3.7088708   10.1683863   23.4496571
 C    4.3197019   10.2231937   25.0452435
 C    3.4706895   10.4931662   26.0953626
 S    1.8091835   10.7737024   25.7934589
 S    1.4836537   10.7503024   21.4762916
 C   -0.0561052   11.4315380   21.1667611
 C   -0.8933844   11.7338683   22.2172589
 C    1.0311774    8.7047980   23.6928186
 N    1.3527779    7.7471092   24.6128219
 C    0.7680709    6.5223391   24.3211791
 H    0.9091325    5.6434858   24.9369671
 C    0.0504054    6.7044063   23.1791430
 H   -0.5558982    6.0149972   22.6058953
 N    0.2242953    8.0333945   22.8176920
 S   -0.3922464   11.4223439   23.8214937
 H   -0.3254764   11.6450901   20.1295476
 H   -1.8700338   12.1998852   22.0658496
 H    5.3919302   10.0702979   25.1895182
 H    3.8269767   10.5720815   27.1252583
 H    1.9312654    7.9605537   25.4187360
 H   -0.1543207    8.4859414   21.9921853
```

Fe-adduct R_1=NH_2 R_2=H

```
26
 Energy =   -3349.0222629640
Fe    1.4699234   10.1755669   23.6650585
 S    3.6425724   10.0750617   23.6734646
 C    4.1174378   10.4826368   25.2686604
 C    3.1590482   10.7453186   26.2189563
 S    1.5013509   10.6738862   25.7986561
 S    1.6364998   10.3657068   21.4878292
 C    0.2654074   11.2714814   21.0093953
```

C	-0.6500118	11.6768903	21.9517415
C	0.9409584	8.3514051	23.7779912
N	1.4710972	7.3411817	24.5546374
C	0.8149895	6.1333533	24.3696432
H	1.1188558	5.2472338	24.9103696
C	-0.1636005	6.3608360	23.4573370
H	-0.9148226	5.7198298	23.0160443
N	-0.0748378	7.7002895	23.1085594
S	-0.4148742	11.2607148	23.5973137
N	-0.9769620	8.2412949	22.1748425
N	2.5557304	7.4174850	25.4469231
H	0.1677580	11.5308913	19.9525474
H	-1.5189622	12.2882870	21.6982322
H	5.1865884	10.5528991	25.4814651
H	3.4151631	11.0295665	27.2424334
H	3.3655995	7.7465836	24.9099540
H	2.3425058	8.1644166	26.1172643
H	-1.4507992	9.0267665	22.6341071
H	-0.4177054	8.6545771	21.4202433

Fe-adduct R_1=H R_2=OH

24

Energy = -3388.8437154960

Fe	1.5269522	10.5040994	23.6454141
S	3.6648308	10.1301676	23.4270666
C	4.2987561	10.2258765	25.0141385
C	3.4682553	10.5492316	26.0643075
S	1.8093916	10.8450173	25.7757044
S	1.4229755	10.7646554	21.4874769
C	-0.1268354	11.4202850	21.1876247
C	-0.9641868	11.7099809	22.2423518
C	0.9841575	8.7170164	23.7194222
N	1.6354080	7.6555455	24.2704711
C	0.8964308	6.4694006	24.1503528
C	-0.2432102	6.8057367	23.4809512
N	-0.1745163	8.1662363	23.2334315
S	-0.4458223	11.4112790	23.8452449
H	-0.4070052	11.6246807	20.1514891
H	-1.9479409	12.1623877	22.0953967
H	5.3705288	10.0612017	25.1494910
H	3.8386864	10.6587106	27.0863664
H	2.5679369	7.7337554	24.6642897
H	-0.8929856	8.7169760	22.7737501
O	1.3542402	5.2397638	24.5273426
H	1.2293666	5.1139381	25.4874236
O	-1.3194092	6.0957592	23.0650189
H	-1.1278750	5.1479585	23.1884838

Fe-adduct R_1=H R_2=NH_2

26

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 Energy =   -3349.0978575880
Fe     1.5435944   10.3635071   23.6204262
 S     3.6713255    9.9540535   23.4101306
 C     4.2922553    9.9685618   25.0036724
 C     3.4580147   10.2563042   26.0612822
 S     1.8063512   10.5974055   25.7720824
 S     1.4611241   10.6591936   21.4624275
 C    -0.0665833   11.3720803   21.1688203
 C    -0.8924939   11.6808445   22.2272972
 C     0.9275358    8.5959497   23.6361453
 N     1.3392310    7.5562419   24.4023401
 C     0.6070930    6.3744521   24.1401093
 C    -0.2813747    6.7107110   23.1535530
 N    -0.0669778    8.0521005   22.8639097
 S    -0.3872540   11.3444278   23.8259948
 H    -0.3369383   11.6018697   20.1353816
 H    -1.8586399   12.1711857   22.0855119
 H     5.3595250    9.7780023   25.1411667
 H     3.8221457   10.3100087   27.0901565
 H     2.0718534    7.6555319   25.0972781
 H    -0.5279690    8.5817169   22.1307023
 N     0.7756345    5.1293590   24.7586596
 H     0.5953694    5.1291119   25.7635360
 H     1.6746753    4.6817953   24.5733107
 N    -1.1778328    5.9259776   22.4327544
 H    -1.1747647    4.9685723   22.7860145
 H    -2.1324799    6.2885954   22.4304970
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Fe-adduct R_1=H R_2=CH_3

```
28
 Energy =   -3316.9978613800
Fe     1.5590135   10.5286704   23.6444936
 S     3.6856004   10.1191999   23.4118837
 C     4.3246603   10.1527760   24.9985606
 C     3.5033228   10.4600197   26.0609882
 S     1.8508552   10.8057458   25.7851530
 S     1.4501308   10.8030769   21.4864256
 C    -0.0805606   11.5112090   21.2011411
 C    -0.9007968   11.8190879   22.2641758
 C     0.9679898    8.7548058   23.7063095
 N     1.4818199    7.7161388   24.4224025
 C     0.7771810    6.5259753   24.2225784
 C    -0.2260294    6.8276274   23.3418637
 N    -0.0810335    8.1863118   23.0481115
 S    -0.3823098   11.4904414   23.8605611
 H    -0.3588319   11.7361107   20.1686560
 H    -1.8708053   12.3033483   22.1278913
 H     5.3926970    9.9607289   25.1273879
 H     3.8791444   10.5263696   27.0848863
 H     2.2874084    7.8323520   25.0283953
 H    -0.6720327    8.7222525   22.4211502
 C     1.1532916    5.2556678   24.9016828
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H	1.0935442	5.3475902	25.9975504
H	2.1797939	4.9478496	24.6482277
H	0.4792664	4.4451877	24.5990817
C	-1.3045506	5.9945515	22.7425787
H	-1.2525286	4.9677267	23.1238310
H	-1.2212955	5.9478725	21.6454540
H	-2.3038049	6.3895358	22.9840079

Fe-adduct R_1=F R_2=H

22
Energy = -3436.7247392010

Fe	1.5342417	10.4169820	23.6539704
S	3.6994895	10.1661908	23.5475858
C	4.2682719	10.4478569	25.1297825
C	3.3765141	10.7583185	26.1320561
S	1.7106529	10.8580292	25.7832584
S	1.5974189	10.7556380	21.4997798
C	0.1574836	11.5887573	21.1273110
C	-0.7370027	11.8907668	22.1298768
C	0.9896723	8.6379991	23.7090035
N	1.4407821	7.5703780	24.4514062
C	0.8071615	6.3631744	24.2547025
H	1.0801827	5.4598655	24.7830348
C	-0.1425992	6.6224234	23.3076061
H	-0.8815503	5.9951388	22.8277131
N	0.0070167	7.9617182	23.0223903
S	-0.3970889	11.4310808	23.7360551
F	-0.7981411	8.5670572	22.1071286
F	2.4525008	7.6806251	25.3547979
H	-0.0097156	11.8846183	20.0889832
H	-1.6608338	12.4418165	21.9389956
H	5.3454475	10.3949052	25.3045323
H	3.6998952	10.9687500	27.1540302

Fe-adduct R_1=Cl R_2=H

22
Energy = -4157.5436811280

Fe	1.4716498	10.3117414	23.6575274
S	3.6297732	10.1190032	23.3536965
C	4.3362678	10.5640963	24.8400692
C	3.5335761	10.8967429	25.9076511
S	1.8366736	10.8550190	25.7382705
S	1.4071278	10.7618987	21.5242981
C	0.0081966	11.7123726	21.3012511
C	-0.8140591	11.9814965	22.3718089
C	0.9300778	8.5174963	23.7550053
N	1.4500148	7.4561385	24.4929710
C	0.7802841	6.2514259	24.3165238
H	1.0769085	5.3468997	24.8299718
C	-0.2173207	6.5039649	23.4360281

H	-0.9822872	5.8680472	23.0112791
N	-0.1129583	7.8518707	23.1145087
S	-0.4273195	11.3674622	23.9145902
H	-0.1868203	12.1083168	20.3018273
H	-1.7087772	12.6017695	22.2781342
H	5.4267950	10.5952650	24.8989597
H	3.9433601	11.2146560	26.8692251
Cl	2.7795043	7.5467915	25.5375894
Cl	-1.1981773	8.5535054	22.0204437

Fe-adduct R_1=CHO R_2=H

26
Energy = -3465.0842644890

Fe	1.4589008	10.2388807	23.6508087
S	3.6347712	10.1123178	23.6225086
C	4.1375381	10.6068901	25.1800141
C	3.1978024	10.9256636	26.1322790
S	1.5343948	10.8274596	25.7496219
S	1.6539812	10.5710870	21.5039950
C	0.2962986	11.5129368	21.0669416
C	-0.6413783	11.8426753	22.0174276
C	0.9297706	8.4490978	23.7503747
N	1.4156591	7.4338405	24.5804657
C	0.7471515	6.2175907	24.3615648
H	1.0147933	5.3387514	24.9335159
C	-0.1640241	6.4324278	23.3991045
H	-0.8895192	5.7872203	22.9208947
N	-0.0593306	7.7815601	23.0212559
S	-0.4408862	11.3091054	23.6289378
C	-0.9022013	8.3085409	22.0090722
C	2.4475885	7.5167948	25.5508662
H	0.2191671	11.8452191	20.0293684
H	-1.5164097	12.4545395	21.7880584
H	5.2108705	10.6714929	25.3723765
H	3.4718903	11.2595810	27.1355995
H	2.8967561	8.5164972	25.6238995
H	-0.7171260	9.3709337	21.7997086
O	2.7693767	6.5511493	26.2101506
O	-1.7295653	7.6158370	21.4554001

Fe-adduct R_1=H R_2=Cl

22
Energy = -4157.6491516220

Fe	1.5160118	10.4060766	23.6114022
S	3.6380083	9.9771897	23.3723835
C	4.2772152	9.9774838	24.9577440
C	3.4599052	10.2757848	26.0263609
S	1.8113453	10.6419158	25.7584640

S	1.4135340	10.7183861	21.4567796
C	-0.1054295	11.4539334	21.1839779
C	-0.9183274	11.7629149	22.2528120
C	0.8963107	8.6542245	23.6352904
N	1.3579690	7.5989717	24.3740419
C	0.6409112	6.4343637	24.1233175
C	-0.3079838	6.7598118	23.1958307
N	-0.1331490	8.1102271	22.9155986
S	-0.4041300	11.4059325	23.8429372
H	-0.3822873	11.6953950	20.1550196
H	-1.8806344	12.2642291	22.1248013
H	5.3425464	9.7685110	25.0817150
H	3.8362768	10.3198122	27.0512853
H	2.1296328	7.6830154	25.0287236
H	-0.6844282	8.6477158	22.2533046
Cl	0.9757906	4.9546390	24.8892892
Cl	-1.5079077	5.8068060	22.4605509

Fe-adduct R_1=H R_2= (C(=O)OH)

28
Energy = -3615.6655686450

Fe	1.4825826	10.2660849	23.6377064
S	3.6134465	9.8628096	23.4307272
C	4.2318218	9.8810149	25.0231321
C	3.3958845	10.1670566	26.0797610
S	1.7452480	10.5025495	25.7897157
S	1.4215832	10.6093452	21.4857426
C	-0.0879855	11.3540437	21.1934821
C	-0.9226328	11.6472242	22.2495595
C	0.8706922	8.5297876	23.6374933
N	1.3050258	7.4629897	24.3839267
C	0.5876048	6.3084007	24.1329754
C	-0.3406584	6.6403316	23.1548939
N	-0.1433381	7.9791889	22.8940111
S	-0.4426125	11.2649556	23.8432890
H	-0.3438278	11.6077362	20.1621433
H	-1.8838325	12.1471355	22.1094895
H	5.2982852	9.6883186	25.1608914
H	3.7567336	10.2175691	27.1096662
H	2.0691137	7.5203863	25.0534226
H	-0.6871498	8.4887935	22.1995665
C	0.9460034	5.0639623	24.8303007
C	-1.3605104	5.9308647	22.3403710
O	2.0366882	4.8696792	25.3129369
O	-2.1240583	6.5582942	21.6362009
O	-1.4100317	4.5764637	22.3883297
O	-0.0328505	4.0866964	24.8820640
H	-0.9188941	4.5033705	24.9000822
H	-0.6798413	4.2009071	22.9286090

HEP complex R_1=H R_2=H

```
45
 Energy =   -6119.4131576040
 H    -2.5744744   -5.5547380    3.0413380
 C    -2.8680623   -5.8947011    2.0486752
 C    -4.1171311   -5.5646612    1.5205912
 H    -4.8053758   -4.9625979    2.1143398
 C    -4.5011807   -5.9913519    0.2379323
 H    -5.4836775   -5.7157736   -0.1460779
 C    -3.6513230   -6.7603390   -0.5583747
 H    -3.9634974   -7.0816320   -1.5498775
 C    -2.3976162   -7.0936469   -0.0346466
 C    -2.0177070   -6.6667403    1.2537140
 N    -1.3164815   -7.8236045   -0.5293758
 N    -0.7328600   -7.1656647    1.4772936
 C    -1.2184941   -8.4697858   -1.8590099
 C    -1.2442598   -7.4296079   -2.9812674
 H    -2.2056063   -6.9007801   -3.0388657
 H    -0.4449800   -6.6904687   -2.8384981
 H    -1.0794429   -7.9313619   -3.9447744
 C    -2.2538671   -9.5853302   -2.0159139
 H    -3.2841716   -9.2037005   -2.0156284
 H    -2.0881535  -10.1007260   -2.9720958
 H    -2.1500365  -10.3210669   -1.2074206
 C     0.0275019   -6.8375936    2.7097639
 C     0.8058401   -5.5315463    2.5212606
 H     1.5769841   -5.6531488    1.7479760
 H     0.1417344   -4.7094750    2.2203802
 H     1.2930635   -5.2503494    3.4656111
 C     0.9112989   -7.9845553    3.1893614
 H    -0.7542587   -6.6816895    3.4689476
 H     1.7522812   -8.1586030    2.5023444
 H     1.3205157   -7.7217435    4.1752695
 H     0.3500452   -8.9230224    3.2771208
 C    -0.3018674   -7.8631707    0.3859978
 H    -0.2174441   -8.9305087   -1.8393822
Pd     1.4592022   -8.8186897    0.0305970
Br     2.4129756   -6.7065872   -0.8826730
Br     0.4726205  -10.9652022    0.8371697
 C     3.1941137   -9.7855324   -0.3933681
 N     4.3239026   -9.2751872   -0.9422543
 N     3.4863817  -11.0972645   -0.2150628
 C     5.3018476  -10.2400910   -1.1088155
 H     4.3582732   -8.2813080   -1.1879898
 C     4.7653432  -11.4070564   -0.6429620
 H     6.2746519  -10.0268243   -1.5337233
 H     5.1816648  -12.4049222   -0.5845812
 H     2.7772168  -11.7186999    0.1864646
```

HEP complex R_1=NH_2 R_2=H

```
49
```

```
 Energy =   -6230.1057498840
 H    -3.2568775   -5.4018413    3.4030379
 C    -3.4612966   -5.6704242    2.3671831
 C    -4.5844599   -5.1685554    1.7085683
 H    -5.2632003   -4.5031559    2.2423944
 C    -4.8530420   -5.5015085    0.3702624
 H    -5.7388369   -5.0918285   -0.1156892
 C    -4.0085518   -6.3446178   -0.3531359
 H    -4.2297535   -6.5906213   -1.3896623
 C    -2.8805801   -6.8502416    0.3020999
 C    -2.6175967   -6.5186369    1.6456873
 N    -1.8417717   -7.6929960   -0.0933951
 N    -1.4408545   -7.1836470    1.9981752
 C    -1.6618999   -8.3039192   -1.4297559
 C    -1.4254497   -7.2347100   -2.4999782
 H    -2.3019112   -6.5880097   -2.6444507
 H    -0.5660548   -6.6058133   -2.2315354
 H    -1.2082392   -7.7227988   -3.4602656
 C    -2.7967278   -9.2788987   -1.7542486
 H    -2.8802277  -10.0422788   -0.9690681
 H    -2.5810779   -9.7844917   -2.7058451
 H    -3.7660120   -8.7726287   -1.8584136
 C    -0.8067911   -6.9895972    3.3256847
 C     0.1490385   -5.7926879    3.2859426
 H     0.9802153   -5.9887621    2.5943470
 H    -0.3671710   -4.8810453    2.9544192
 H     0.5566175   -5.6091089    4.2902031
 C    -0.1462717   -8.2563979    3.8596534
 H    -1.6503884   -6.7504991    3.9914488
 H     0.7310539   -8.5297204    3.2537443
 H     0.1838383   -8.0722581    4.8919569
 H    -0.8342501   -9.1110386    3.8517515
 C    -0.9629786   -7.8949146    0.9342023
 H    -0.7317826   -8.8836525   -1.3114376
Pd     0.6877754   -9.0833371    0.7557113
Br    -0.7042705  -11.0692509    1.3328565
Br     2.0504490   -7.1105672    0.0928466
 C     2.3176534  -10.2823290    0.5157405
 N     2.4654843  -11.3509425   -0.3193314
 N     3.5298594  -10.2059132    1.1366003
 C     3.7229191  -11.9241570   -0.2199656
 C     4.4053064  -11.1879815    0.7011433
 H     3.9957173  -12.7894810   -0.8094911
 H     5.4134997  -11.2569179    1.0876020
 N     3.9220343   -9.2328224    2.0792480
 H     3.3670690   -9.3884011    2.9269530
 H     3.6211986   -8.3255837    1.6876518
 N     1.4804001  -11.8803539   -1.1792316
 H     1.3089492  -11.1800183   -1.9078616
 H     0.6164671  -11.9360274   -0.6141929
```

HEP complex R_1=H R_2=OH

47
 Energy =   -6269.9287300310
 H   -2.5858992   -5.5107221   2.8984320
 C   -2.8775642   -5.9064775   1.9262332
 C   -4.1608892   -5.6910685   1.4219337
 H   -4.8757184   -5.1145382   2.0096469
 C   -4.5481106   -6.2066611   0.1733867
 H   -5.5585482   -6.0221818   -0.1924075
 C   -3.6676549   -6.9536854   -0.6109020
 H   -3.9838311   -7.3469815   -1.5748316
 C   -2.3799740   -7.1733238   -0.1104292
 C   -1.9943332   -6.6503581   1.1401668
 N   -1.2653462   -7.8564018   -0.5984831
 N   -0.6672463   -7.0343062   1.3426221
 C   -1.1595397   -8.5692762   -1.8927830
 C   -1.2953454   -7.6026254   -3.0716887
 H   -2.2940861   -7.1479223   -3.1265433
 H   -0.5454203   -6.8036187   -2.9978152
 H   -1.1231478   -8.1486839   -4.0096008
 C   -2.1162293   -9.7627215   -1.9508381
 H   -3.1708812   -9.4539385   -1.9467822
 H   -1.9365221 -10.3259839   -2.8768835
 H   -1.9452028 -10.4363171   -1.1007466
 C   0.0508171   -6.7186270   2.6034815
 C   1.5322274   -6.4234945   2.3897812
 H   2.0810372   -7.3272570   2.0841005
 H   1.6891961   -5.6575209   1.6198337
 H   1.9577135   -6.0666215   3.3386153
 C   -0.1890682   -7.8178150   3.6434724
 H   -0.4255132   -5.7892121   2.9510045
 H   0.2662820   -8.7623847   3.3147459
 H   0.2587229   -7.5239138   4.6034411
 H   -1.2627830   -7.9888910   3.8038006
 C   -0.2262119   -7.7791291   0.2866530
 H   -0.1272625   -8.9547876   -1.8818087
Pd   1.5794966   -8.6559256   -0.0388264
Br   2.2802995   -6.6820571   -1.3961141
Br   0.8540781 -10.6829570   1.2102587
 C   3.3740842   -9.5369389   -0.4032392
 N   4.4131721   -9.0383032   -1.1105470
 N   3.8015635 -10.7650467   0.0016220
 C   5.4726366   -9.9430862   -1.1759723
 C   5.0742889 -11.0366135   -0.4535744
 O   6.6913581   -9.6861930   -1.7379885
 O   5.6821159 -12.2092089   -0.1500972
 H   4.3432316   -8.1030150   -1.5266351
 H   3.1866355 -11.3648127   0.5620019
 H   6.6263437   -9.7209377   -2.7110267
 H   6.6033386 -12.1637465   -0.4658293

HEP complex R_1=H R_2=NH_2

49

```
 Energy =   -6230.1822188910
 H   -2.2411995   -6.1407456    3.0766126
 C   -2.5362989   -6.2488319    2.0331040
 C   -3.6995811   -5.6443682    1.5545883
 H   -4.3184282   -5.0639092    2.2389494
 C   -4.0855648   -5.7718871    0.2096358
 H   -5.0005982   -5.2862286   -0.1325571
 C   -3.3241409   -6.5081179   -0.6997339
 H   -3.6355620   -6.5978499   -1.7380397
 C   -2.1581760   -7.1169286   -0.2247038
 C   -1.7742399   -6.9880211    1.1253861
 N   -1.1771199   -7.9046769   -0.8276200
 N   -0.5874316   -7.7089632    1.2736835
 C   -1.1169453   -8.3076337   -2.2516015
 C   -0.9240557   -7.0912329   -3.1607238
 H   -1.7798604   -6.4014190   -3.1378553
 H   -0.0216444   -6.5407657   -2.8643116
 H   -0.7933472   -7.4288724   -4.1976328
 C   -2.3010612   -9.1981595   -2.6338039
 H   -3.2575127   -8.6598221   -2.5912712
 H   -2.1632788   -9.5589211   -3.6625938
 H   -2.3539428  -10.0705655   -1.9697057
 C    0.1660436   -7.7218442    2.5535732
 C    1.1455913   -6.5447702    2.6028760
 H    1.9118438   -6.6510142    1.8219582
 H    0.6281513   -5.5868940    2.4517736
 H    1.6412308   -6.5165202    3.5838538
 C    0.8394973   -9.0604384    2.8369970
 H   -0.6105007   -7.5719825    3.3196908
 H    1.6731282   -9.2461752    2.1437784
 H    1.2391779   -9.0408737    3.8613937
 H    0.1363284   -9.8978144    2.7461482
 C   -0.2174578   -8.2589717    0.0799926
 H   -0.2007847   -8.9186719   -2.2984133
Pd    1.4036103   -9.3896199   -0.4109135
Br    2.6867621   -7.3205578   -0.9494423
Br    0.0822804  -11.4714446   -0.0068815
 C    3.0104532  -10.5123893   -0.9467473
 N    3.1076648  -11.8722627   -0.9627619
 N    4.2164590  -10.0919241   -1.3749393
 C    4.3437254  -12.2982078   -1.4157277
 H    2.3072186  -12.4379400   -0.6627083
 C    5.0711595  -11.1630759   -1.6890995
 H    4.4038945   -9.0882740   -1.4581508
 N    6.3880445  -11.0842748   -2.1688448
 H    7.0517568  -10.6905527   -1.4996731
 H    6.4758556  -10.5853782   -3.0552263
 N    4.7275645  -13.6355034   -1.4448381
 H    4.0600852  -14.2520167   -1.9104755
 H    5.6519656  -13.7317972   -1.8660280
```

HEP complex R_1=H R_2=CH_3

```
51
 Energy =   -6198.0816498110
 H    -2.2868344   -6.2007818    3.1190727
 C    -2.5874494   -6.2962806    2.0761131
 C    -3.7675007   -5.7109637    1.6149791
 H    -4.3965421   -5.1536419    2.3095106
 C    -4.1577116   -5.8235878    0.2700090
 H    -5.0858619   -5.3546674   -0.0578688
 C    -3.3839996   -6.5232887   -0.6573857
 H    -3.6995711   -6.5974374   -1.6958619
 C    -2.2021100   -7.1154034   -0.1998026
 C    -1.8143869   -7.0014708    1.1505729
 N    -1.2078018   -7.8716893   -0.8205478
 N    -0.6118626   -7.6994148    1.2805443
 C    -1.1439932   -8.2474625   -2.2522789
 C    -0.9619595   -7.0115894   -3.1363559
 H    -1.8275191   -6.3362935   -3.0917220
 H    -0.0651430   -6.4539974   -2.8344056
 H    -0.8353822   -7.3266090   -4.1812671
 C    -2.3222265   -9.1371545   -2.6540485
 H    -3.2823868   -8.6039384   -2.6205892
 H    -2.1716564   -9.4896181   -3.6839823
 H    -2.3824387  -10.0154618   -1.9981466
 C     0.1489513   -7.7116719    2.5555761
 C     1.0779849   -6.4953571    2.6273799
 H     1.8440397   -6.5586925    1.8414765
 H     0.5211678   -5.5560682    2.5007972
 H     1.5771638   -6.4672980    3.6060167
 C     0.8825660   -9.0259410    2.8025751
 H    -0.6282790   -7.6143138    3.3293176
 H     1.7192370   -9.1589926    2.1004387
 H     1.2874427   -9.0132239    3.8245275
 H     0.2160167   -9.8905247    2.6950119
 C    -0.2371344   -8.2224042    0.0762614
 H    -0.2239256   -8.8512275   -2.3097784
Pd     1.3961046   -9.3222966   -0.4453367
Br     2.6493322   -7.2264864   -0.9486924
Br     0.1035635  -11.4255539   -0.0572257
 C     3.0038890  -10.4198154   -1.0248770
 N     3.1283496  -11.7669247   -1.0595453
 N     4.1976017   -9.9773867   -1.4846333
 C     4.3718271  -12.1746604   -1.5346710
 H     2.3391118  -12.3525357   -0.7707360
 C     5.0625166  -11.0188958   -1.8093524
 H     4.3654996   -8.9701619   -1.5628087
 C     6.4333659  -10.7863470   -2.3438204
 H     6.9339521  -11.7405056   -2.5486913
 H     7.0587412  -10.2270797   -1.6308533
 H     6.4086273  -10.2125619   -3.2829846
 C     4.7516729  -13.6091255   -1.6628852
 H     4.0417286  -14.1602363   -2.2982539
 H     4.7785777  -14.1119219   -0.6837561
 H     5.7470744  -13.7039167   -2.1140757
```

HEP complex R_1=F R_2=H

```
45
 Energy =   -6317.8030514800
 H    -2.6643294   -5.7122209    2.9908203
 C    -2.9177318   -6.0272511    1.9791763
 C    -4.1827479   -5.7735237    1.4475383
 H    -4.9218760   -5.2501694    2.0545244
 C    -4.5211652   -6.1835283    0.1467871
 H    -5.5183472   -5.9712109   -0.2393444
 C    -3.6088425   -6.8597546   -0.6643828
 H    -3.8876267   -7.1705177   -1.6690860
 C    -2.3391082   -7.1176207   -0.1367784
 C    -2.0028066   -6.7012805    1.1667701
 N    -1.2039075   -7.7534221   -0.6402475
 N    -0.6823839   -7.0982640    1.3869452
 C    -1.0564643   -8.3750258   -1.9771428
 C    -1.1620957   -7.3308499   -3.0902739
 H    -2.1625394   -6.8807439   -3.1486717
 H    -0.4230998   -6.5333952   -2.9370913
 H    -0.9541203   -7.8110766   -4.0564501
 C    -2.0050026   -9.5651349   -2.1395346
 H    -3.0610456   -9.2615072   -2.1287282
 H    -1.8076394  -10.0571722   -3.1021617
 H    -1.8412373  -10.2984736   -1.3386834
 C    -0.0278365   -6.9116004    2.7070415
 C     1.4664496   -6.6254488    2.6041734
 H     2.0216046   -7.5150355    2.2728673
 H     1.6815282   -5.8127609    1.8995414
 H     1.8352088   -6.3418284    3.6003756
 C    -0.3385016   -8.1005583    3.6234656
 H    -0.5108912   -6.0102199    3.1138746
 H     0.1176979   -9.0184484    3.2268145
 H     0.0645923   -7.9087593    4.6280715
 H    -1.4214286   -8.2644161    3.7143089
 C    -0.2005832   -7.7457155    0.2868226
 H    -0.0237358   -8.7579787   -1.9622328
Pd     1.6009364   -8.5911714   -0.0382167
Br     2.4193840   -6.4890734   -1.0863702
Br     0.7499408  -10.7387127    0.8703344
 C     3.3894445   -9.4679633   -0.4037210
 N     3.8392304  -10.1171073   -1.5014409
 N     4.4919228   -9.5955166    0.3687885
 C     5.1200988  -10.6190990   -1.4368940
 F     3.0682331  -10.2735619   -2.6154263
 C     5.5566945  -10.2700767   -0.1858795
 H     5.5926761  -11.1572452   -2.2477539
 H     6.4924134  -10.4376907    0.3305691
 F     4.5524482   -9.0875689    1.6336117
```

HEP complex R_1=Cl R_2=H

```
45
 Energy =   -7038.6258530280
 H    -2.7513530   -5.9172072    3.0954309
 C    -2.9781147   -6.1674718    2.0595587
 C    -4.2046929   -5.8172837    1.4936138
 H    -4.9413636   -5.2906309    2.1007581
 C    -4.5048674   -6.1279357    0.1564643
 H    -5.4720209   -5.8398149   -0.2562388
 C    -3.5900948   -6.7964313   -0.6580200
 H    -3.8365768   -7.0277884   -1.6921669
 C    -2.3586579   -7.1497848   -0.0961481
 C    -2.0629160   -6.8410778    1.2467486
 N    -1.2326212   -7.8026807   -0.5962306
 N    -0.7789522   -7.3305732    1.4948057
 C    -1.0551379   -8.3296672   -1.9688152
 C    -1.0662758   -7.2000962   -3.0013225
 H    -2.0451323   -6.7066868   -3.0733082
 H    -0.3088215   -6.4453236   -2.7521751
 H    -0.8265945   -7.6126510   -3.9911950
 C    -2.0437581   -9.4612068   -2.2583915
 H    -3.0875664   -9.1186506   -2.2452134
 H    -1.8394182   -9.8760987   -3.2554020
 H    -1.9254025  -10.2658023   -1.5200984
 C    -0.0965817   -7.1224409    2.7969064
 C     0.7761693   -5.8650901    2.7505015
 H     1.5814212   -5.9800557    2.0115259
 H     0.1845518   -4.9803438    2.4766481
 H     1.2220067   -5.6871619    3.7395221
 C     0.6633158   -8.3591278    3.2663867
 H    -0.9231365   -6.9551902    3.5036286
 H     1.5310979   -8.5630981    2.6238441
 H     1.0197888   -8.1853539    4.2918774
 H     0.0277818   -9.2535790    3.2578087
 C    -0.2697692   -7.9090767    0.3672339
 H    -0.0415034   -8.7601687   -1.9414064
Pd     1.5255894   -8.7897222    0.0261993
Br     2.5048760   -6.6111606   -0.6588047
Br     0.5414723  -11.0278738    0.4935792
 C     3.2939321   -9.6833387   -0.3623189
 N     3.7267098  -10.2694509   -1.5167175
 N     4.3753724   -9.8788554    0.4479734
 C     5.0066101  -10.8040846   -1.4335912
Cl     2.7928914  -10.3433711   -2.9302806
 C     5.4258424  -10.5520066   -0.1643527
 H     5.4877949  -11.3014893   -2.2651520
 H     6.3501133  -10.7832895    0.3483190
Cl     4.4419017   -9.3486966    2.0577352
```

HEP complex R_1=CHO R_2=H

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49
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```
 Energy =   -6346.1607376510
 H   -2.5328429   -6.2556251    3.0494801
 C   -2.7124360   -6.4198154    1.9875565
 C   -3.8740823   -5.9439726    1.3792277
 H   -4.6084379   -5.4059918    1.9790427
 C   -4.1119494   -6.1421619    0.0084378
 H   -5.0300323   -5.7578346   -0.4366339
 C   -3.1973238   -6.8194865   -0.7984307
 H   -3.3960691   -6.9623393   -1.8585725
 C   -2.0298787   -7.2980851   -0.1936279
 C   -1.7981488   -7.1029497    1.1818065
 N   -0.9207906   -7.9956555   -0.6735146
 N   -0.5679535   -7.6998507    1.4687701
 C   -0.6884697   -8.4188958   -2.0739589
 C   -0.5508235   -7.2096160   -3.0023217
 H   -1.4851396   -6.6379627   -3.0856451
 H    0.2411608   -6.5388216   -2.6431820
 H   -0.2786758   -7.5551866   -4.0090794
 C   -1.7305006   -9.4444972   -2.5263575
 H   -2.7413699   -9.0178177   -2.5752205
 H   -1.4719622   -9.8055891   -3.5313824
 H   -1.7443342  -10.3044896   -1.8437736
 C    0.0396040   -7.6159187    2.8215077
 C    0.9330713   -6.3758995    2.9302182
 H    1.7826073   -6.4486682    2.2370761
 H    0.3747409   -5.4606202    2.6889480
 H    1.3160725   -6.2837595    3.9562180
 C    0.7448546   -8.9016950    3.2385071
 H   -0.8253379   -7.4881352    3.4897161
 H    1.6434353   -9.0855129    2.6317313
 H    1.0497491   -8.8120401    4.2905461
 H    0.0920198   -9.7767549    3.1302796
 C   -0.0305963   -8.2353744    0.3343488
 H    0.2912269   -8.9196599   -2.0227883
Pd    1.7350142   -9.2189488    0.0415546
Br    2.8404767   -7.0422095   -0.4102074
Br    0.5543741  -11.3826819    0.3742592
 C    3.4780063  -10.1882362   -0.2984013
 N    3.7692818  -11.1123956   -1.2716452
 N    4.6672491  -10.0717130    0.3797952
 C    5.0995933  -11.5541670   -1.1962203
 C    2.8443639  -11.5670011   -2.2617159
 C    5.6629024  -10.9021042   -0.1581609
 H    5.4855654  -12.2831442   -1.8972045
 H    6.6576548  -10.9285030    0.2679911
 C    4.8779055   -9.2134226    1.5016910
 O    3.1690456  -12.3595123   -3.1116465
 O    5.9392275   -9.1669927    2.0732001
 H    3.9700372   -8.6311737    1.7411434
 H    1.8481745  -11.1108112   -2.1249918
```

HEP complex R_1=H R_2=Cl

```
45
 Energy =   -7038.7343369400
 H    -2.2385298   -6.0487307    3.0230852
 C    -2.5283829   -6.1888970    1.9823597
 C    -3.6874175   -5.5983615    1.4776495
 H    -4.3092444   -4.9931083    2.1378435
 C    -4.0651682   -5.7676625    0.1348150
 H    -4.9747944   -5.2895125   -0.2293926
 C    -3.3001565   -6.5336776   -0.7459368
 H    -3.6063893   -6.6534524   -1.7831410
 C    -2.1380172   -7.1299312   -0.2446217
 C    -1.7627330   -6.9574086    1.1025597
 N    -1.1550198   -7.9380946   -0.8162687
 N    -0.5772995   -7.6752169    1.2813535
 C    -1.0913733   -8.3883189   -2.2270969
 C    -0.9055417   -7.2007999   -3.1747036
 H    -1.7714454   -6.5244878   -3.1739509
 H    -0.0118632   -6.6264039   -2.8970941
 H    -0.7708360   -7.5710200   -4.2001195
 C    -2.2732035   -9.2944307   -2.5786134
 H    -3.2336534   -8.7612351   -2.5489011
 H    -2.1373485   -9.6843726   -3.5969494
 H    -2.3214267  -10.1481403   -1.8893136
 C     0.1663645   -7.6508403    2.5672578
 C     1.1643752   -6.4885004    2.5826414
 H     1.9365581   -6.6338956    1.8146962
 H     0.6658916   -5.5276645    2.3927214
 H     1.6509419   -6.4332635    3.5665151
 C     0.8154384   -8.9886594    2.9068422
 H    -0.6146277   -7.4606369    3.3188151
 H     1.6467933   -9.2181875    2.2240509
 H     1.2159814   -8.9332069    3.9291511
 H     0.0983812   -9.8173285    2.8511076
 C    -0.2040780   -8.2647482    0.1086794
 H    -0.1725060   -8.9958700   -2.2551000
Pd     1.4142737   -9.4144003   -0.3341195
Br     2.7242605   -7.3825092   -0.9195748
Br     0.0930688  -11.4782982    0.1268952
 C     3.0112426  -10.5638469   -0.8318798
 N     3.0977825  -11.9175883   -0.8296349
 N     4.2320897  -10.1519990   -1.2560178
 C     4.3439107  -12.3524384   -1.2454528
 H     2.2856830  -12.4811407   -0.5492034
 C     5.0709096  -11.2207373   -1.5188608
 H     4.4257030   -9.1479811   -1.3590245
Cl     6.6725101  -11.0483586   -2.0694550
Cl     4.7818057  -13.9925471   -1.3600428
```

HEP complex R_1=H R_2=(C(=O)OH)

```
51
 Energy =   -6496.7629607610
 H    -1.5762948   -6.1478090    2.8600711
```

C	-1.9425228	-6.2589432	1.8401030
C	-3.0333649	-5.5169637	1.3867716
H	-3.5262821	-4.8212337	2.0661654
C	-3.5064228	-5.6488989	0.0702754
H	-4.3616119	-5.0547322	-0.2530602
C	-2.9046586	-6.5217719	-0.8368270
H	-3.2834980	-6.6110258	-1.8527568
C	-1.8081091	-7.2660325	-0.3891778
C	-1.3435697	-7.1379953	0.9349469
N	-0.9759396	-8.2064447	-0.9980461
N	-0.2647555	-8.0159284	1.0669276
C	-1.0464861	-8.6740120	-2.4027251
C	-0.7781925	-7.5288876	-3.3817147
H	-1.5641153	-6.7613123	-3.3546973
H	0.1861069	-7.0514057	-3.1624059
H	-0.7376180	-7.9297592	-4.4037182
C	-2.3455897	-9.4373230	-2.6700002
H	-3.2339646	-8.7988923	-2.5684515
H	-2.3301015	-9.8297091	-3.6960749
H	-2.4394482	-10.2860181	-1.9798795
C	0.5249238	-8.0990609	2.3224073
C	1.6605018	-7.0700295	2.3083798
H	2.3901419	-7.3134777	1.5240266
H	1.2803997	-6.0557060	2.1229770
H	2.1725106	-7.0710953	3.2809765
C	1.0128111	-9.5117683	2.6268606
H	-0.1972375	-7.8216765	3.1051895
H	1.7845720	-9.8329565	1.9109910
H	1.4542286	-9.5215527	3.6334766
H	0.1948276	-10.2427956	2.5919099
C	-0.0381173	-8.6580894	-0.1148263
H	-0.2091425	-9.3869418	-2.4720834
Pd	1.3717234	-10.0369123	-0.6125165
Br	2.9429530	-8.2113098	-1.2246875
Br	-0.2556998	-11.8707056	-0.1536746
C	2.7591827	-11.4107539	-1.1409195
N	2.6454518	-12.7596371	-1.1140850
N	4.0221482	-11.2076392	-1.6012207
C	3.7954712	-13.3940639	-1.5439505
H	1.7703703	-13.2074832	-0.8086533
C	4.6947753	-12.3773847	-1.8621727
H	4.4034774	-10.2619318	-1.7348580
C	6.0940517	-12.2624944	-2.3767531
C	3.8219048	-14.8556980	-1.5672707
O	6.5826652	-11.1624523	-2.5386051
O	2.8978986	-15.5657154	-1.2312254
O	6.7743057	-13.3888475	-2.6482528
H	6.2292026	-14.1915940	-2.4568026
O	5.0195140	-15.3683939	-2.0158007
H	4.9411729	-16.3450143	-1.9971120

(NHC-1) $Ni(CO)_3$ complex R_1=H R_2=H

16
Energy = -2075.200647802

Ni	-5.5054077	1.9588268	-0.3608720
C	-6.4398316	3.4222845	0.1141820
C	-3.7282748	2.2756738	-0.3372353
C	-5.9476551	0.5547042	0.6785103
O	-7.0426706	4.3552605	0.4408594
O	-2.5905616	2.4797859	-0.3094740
O	-6.2474596	-0.3435733	1.3427334
N	-6.7833196	2.1706084	-3.0914737
C	-6.0204633	1.4786546	-2.1950262
C	-6.9592852	1.4959883	-4.2931939
N	-5.7247853	0.3422582	-2.8924444
C	-6.2805590	0.3230881	-4.1653705
H	-5.1599047	-0.3969199	-2.4907034
H	-7.1723073	3.0796564	-2.8697648
H	-7.5373574	1.8938120	-5.1175637
H	-6.1531574	-0.5010486	-4.8556332

(NHC-1) $Ni(CO)_3$ complex $R_1=NH_2$ $R_2=H$

20
Energy = -2185.893637670

O	-6.4200715	-0.5094037	1.2148652
C	-6.2611481	0.3769256	-4.3668928
C	-6.8336486	1.6020653	-4.5087824
N	-5.8221344	0.3101229	-3.0544979
C	-6.1033049	0.3793216	0.5427862
N	-6.7092346	2.2342086	-3.2705831
C	-6.0816525	1.4497746	-2.3368641
Ni	-5.5964808	1.7871849	-0.4577058
C	-6.4677124	3.2800651	0.0809405
O	-7.0036816	4.2203128	0.4837378
C	-3.8173671	2.0447398	-0.3543720
O	-2.6780318	2.2234493	-0.2573191
H	-6.1188517	-0.4432378	-5.0590531
H	-7.3055692	2.0779193	-5.3597447
N	-5.1490810	-0.8295948	-2.5702390
H	-5.7712926	-1.2897942	-1.8962434
H	-4.3556591	-0.4822710	-2.0199447
N	-7.1531532	3.5330869	-2.9788176
H	-8.1591221	3.5914323	-3.1544074
H	-6.6690029	4.1980226	-3.5870426

(NHC-1) $Ni(CO)_3$ complex $R_1=H$ $R_2=OH$

18
Energy = -2225.715898949

Ni	-5.5397875	1.9132470	-0.3897736
C	-6.4654936	3.3671702	0.1296959
C	-3.7605004	2.2177848	-0.3723690

C	-5.9643114	0.4729719	0.6055053
O	-7.0615472	4.2984914	0.4729763
O	-2.6205006	2.4095992	-0.3547633
O	-6.2366517	-0.4506664	1.2471468
N	-6.7626308	2.2970806	-3.1246841
C	-6.0555332	1.5163835	-2.2450535
C	-6.9476427	1.6881793	-4.3535796
N	-5.8052173	0.3988694	-2.9816893
C	-6.3490450	0.4645024	-4.2715656
H	-5.2637740	-0.3807211	-2.6251050
H	-7.1056480	3.2210214	-2.8855895
O	-7.6189977	2.3281752	-5.3404347
H	-7.5307707	1.8090138	-6.1609911
O	-6.1622830	-0.4800397	-5.2401487
H	-6.7978253	-1.2120928	-5.1248675

(NHC-1) $Ni(CO)_3$ complex R_1=H R_2= NH_2

20
Energy = -2185.967803575

Ni	-5.4867623	1.9417288	-0.3924088
C	-6.4161836	3.3978655	0.1114157
C	-3.7161910	2.2847668	-0.4447362
C	-5.8687192	0.5218013	0.6460103
O	-7.0141541	4.3337487	0.4395571
O	-2.5823260	2.5122713	-0.4714595
O	-6.1243225	-0.3902992	1.3118555
N	-6.7773840	2.2223871	-3.1073697
C	-6.0675080	1.4879688	-2.2176811
C	-7.0323869	1.5506906	-4.3152633
N	-5.8592139	0.3200387	-2.9078220
C	-6.4304580	0.3249237	-4.1751837
H	-5.3090206	-0.4417689	-2.5269639
H	-7.1073700	3.1621979	-2.9156266
N	-6.2617819	-0.7387620	-5.0638588
H	-6.6411864	-0.5287129	-5.9861546
H	-6.6495190	-1.6230051	-4.7309693
N	-7.7826277	2.1509419	-5.3371401
H	-7.2487732	2.4414445	-6.1553794
H	-8.6128417	1.6318723	-5.6189418

(NHC-1) $Ni(CO)_3$ complex R_1=H R_2= CH_3

22
Energy = -2153.869627763

Ni	-5.5340918	1.9435904	-0.3787452
C	-6.4550484	3.4128386	0.1014767
C	-3.7581297	2.2585187	-0.3553386
C	-5.9678696	0.5412324	0.6661051
O	-7.0395505	4.3564792	0.4324333
O	-2.6203265	2.4652377	-0.3259520
O	-6.2507715	-0.3525720	1.3445496

N	-6.8133943	2.1718527	-3.1091972
C	-6.0437271	1.4790497	-2.2231192
C	-6.9695678	1.5259057	-4.3389102
N	-5.7189369	0.3685830	-2.9437865
C	-6.2616798	0.3593025	-4.2318361
C	-6.0399679	-0.7587081	-5.1902442
H	-6.5587571	-0.5625689	-6.1364974
H	-6.4191348	-1.7139160	-4.7952971
H	-4.9714337	-0.8945493	-5.4188198
C	-7.7733465	2.1030920	-5.4516212
H	-8.8257226	2.2463617	-5.1610057
H	-7.7577858	1.4391482	-6.3242015
H	-7.3813150	3.0810766	-5.7711010
H	-5.1377381	-0.3666653	-2.5575546
H	-7.2241146	3.0680307	-2.8728370

(NHC-1) $Ni(CO)_3$ complex R_1=F R_2= H

16
Energy = -2273.609084243

O	-6.1699608	-0.3811133	1.3593080
C	-6.3305194	0.3644652	-4.2197823
C	-6.9609074	1.5741651	-4.3498966
N	-5.8182908	0.3903417	-2.9414272
C	-5.9268791	0.5108787	0.6681956
N	-6.7574221	2.1911594	-3.1354113
C	-6.0499234	1.5048911	-2.2028535
Ni	-5.5249815	1.9381814	-0.3668725
C	-6.4353043	3.4064387	0.1738600
O	-6.9870902	4.3352291	0.5803715
C	-3.7431209	2.2424021	-0.3358605
O	-2.6069744	2.4380435	-0.2784219
H	-6.2124971	-0.4697115	-4.8989314
H	-7.5095841	2.0241087	-5.1669539
F	-5.1083082	-0.6701675	-2.4439158
F	-7.2563363	3.4431275	-2.8931281

(NHC-1) $Ni(CO)_3$ complex R_1=Cl R_2= H

16
Energy = -2994.429574073

O	-6.2304872	-0.3242503	1.2940568
C	-6.3318164	0.3508820	-4.2781821
C	-7.0778813	1.4809183	-4.3948774
N	-5.7685351	0.4085199	-3.0092225
C	-5.9789405	0.5624094	0.5979399
N	-6.9225628	2.1557871	-3.1888574
C	-6.1090062	1.5228565	-2.2767000
Ni	-5.5749321	1.9782279	-0.4492293
C	-6.4358484	3.4435788	0.1692137
O	-6.9365716	4.3655344	0.6532109
C	-3.7939740	2.2802136	-0.4287451

O	-2.6574819	2.4785415	-0.3767442
H	-6.1579527	-0.4695879	-4.9616556
H	-7.6915503	1.8554174	-5.2037084
Cl	-7.6799565	3.6474180	-2.9009926
Cl	-4.7338630	-0.8080165	-2.4317767

(NHC-1) $Ni(CO)_3$ complex R_1=CHO R_2= H

20
Energy = -2301.937413669

O	-5.5841783	-0.4409322	1.3866854
C	-6.5096073	0.2840335	-4.1574104
C	-5.0706487	-0.8425438	-2.5324334
C	-7.0635440	1.4983920	-4.3066451
N	-5.8535729	0.2845253	-2.9119593
C	-5.5569341	0.4392203	0.6427681
N	-6.7442455	2.2381888	-3.1521128
C	-6.0073515	1.4936176	-2.2255634
C	-7.1012875	3.6146799	-3.0815557
Ni	-5.5360351	1.9293526	-0.4049412
C	-6.7359852	3.0961313	0.3160584
O	-7.4648354	3.7984593	0.8677046
C	-3.8940366	2.6713014	-0.2750773
O	-2.8458974	3.1448073	-0.1914966
O	-4.3490107	-0.9157682	-1.5739590
H	-5.2069961	-1.6630113	-3.2718143
O	-6.7634378	4.3932516	-2.2301657
H	-7.7379630	3.8848051	-3.9531061
H	-6.5000861	-0.5783610	-4.8137380
H	-7.6402066	1.9211507	-5.1211780

(NHC-1) $Ni(CO)_3$ complex R_1=H R_2= Cl

16
Energy = -2994.521311480

Ni	-5.5087148	1.9580134	-0.3479457
C	-6.4296566	3.4315083	0.1317628
C	-3.7303836	2.2780369	-0.3269145
C	-5.9262234	0.5504806	0.7013175
O	-7.0134599	4.3771624	0.4528786
O	-2.5946741	2.4868968	-0.2951433
O	-6.1948639	-0.3494449	1.3749307
N	-6.7940880	2.2054769	-3.0626018
C	-6.0377851	1.4908700	-2.1758281
C	-6.9816499	1.5437649	-4.2705360
N	-5.7567676	0.3540023	-2.8820094
C	-6.3163448	0.3550239	-4.1543557
H	-5.2024263	-0.4061817	-2.5026483
H	-7.1755022	3.1205883	-2.8470867
Cl	-7.8833489	2.1827632	-5.5627250
Cl	-6.1429908	-0.9257313	-5.2594051

(NHC-1) $Ni(CO)_3$ complex R_1=H R_2= COOH

```
22
Energy = -2452.535879252
Ni    -5.5540205    1.9527903   -0.4094673
C     -6.5406536    3.3979205    0.0400561
C     -3.7995535    2.3857410   -0.4692930
C     -5.8195549    0.6110495    0.7725279
O     -7.1592248    4.3217545    0.3546243
O     -2.6807277    2.6673029   -0.4950546
O     -5.9837323   -0.2281695    1.5482052
N     -6.8504023    2.0226848   -3.1170170
C     -6.1064155    1.3598462   -2.1781256
C     -7.0582386    1.2948584   -4.2750094
N     -5.8458954    0.1781407   -2.8182815
C     -6.3896959    0.0948515   -4.0855454
H     -7.2132388    2.9637283   -2.9852814
H     -5.2928662   -0.5793182   -2.4225482
C     -7.8117874    1.8966973   -5.3896751
C     -6.0973356   -1.1230386   -4.8842567
O     -7.9253738    3.0910847   -5.5313446
O     -5.5989243   -2.0948869   -4.3567034
O     -8.3641562    1.0215956   -6.3022293
H     -8.5666431    0.1658737   -5.8711903
O     -6.3862890   -1.1195023   -6.2095718
H     -6.6893405   -0.2379344   -6.5182191
```

(NHC-1) R_2=H R_1=H

```
9
Energy = -226.0168640933
C     -5.3903825    0.9058243    0.0000000
C     -4.0203917    0.9772736   -0.0000000
N     -3.5825313   -0.3476368    0.0000000
N     -5.6881349   -0.4572446    0.0000000
C     -4.5894703   -1.2849257   -0.0000000
H     -3.3476241    1.8429933    0.0000000
H     -6.1494378    1.6970061   -0.0000000
H     -2.5982499   -0.6206636   -0.0000000
H     -6.6387775   -0.8309665    0.0000000
```

(NHC-1) R_2=NH_2 R_1=H

```
13
Energy = -337.0267915719
C     -4.0328824    1.2881369   -0.0000000
C     -4.5765005   -0.9844150    0.0000000
C     -5.3990674    1.2024662   -0.0000000
N     -3.5834094   -0.0400309    0.0000000
N     -5.6792593   -0.1711537    0.0000000
```

```
H    -2.6056595   -0.3012606   -0.0000000
H    -6.6168154   -0.5525165    0.0000000
N    -6.3915204    2.1781627   -0.0000000
H    -6.1645313    3.1590573    0.0000000
H    -7.3663899    1.9257858   -0.0000000
N    -3.1699030    2.3800224    0.0000000
H    -2.1711691    2.2510484   -0.0000000
H    -3.5173623    3.3248970    0.0000000
```

(NHC-1) R_2=H R_1=OH

```
11
Energy = -376.6784763955
C    -3.9338590    0.7924341    0.0000000
C    -4.5672424   -1.4386336   -0.0000000
C    -5.3072557    0.7592653    0.0000000
N    -3.5591505   -0.5381254    0.0000000
N    -5.6175508   -0.5877041   -0.0000000
H    -6.0340023    1.5648318   -0.0000000
H    -3.2466571    1.6319105    0.0000000
O    -6.9217861   -1.1016887    0.0000000
H    -7.4992785   -0.3134539    0.0000000
O    -2.2317502   -0.9889497    0.0000000
H    -1.6926274   -0.1739963   -0.0000000
```

(NHC-1) R_2=H R_1=NH_2

```
13
Energy = -336.9832255856
C    -4.0506882    0.9038931    0.0004888
C    -4.8116020   -1.2824456    0.0312469
C    -5.4128912    0.9531341    0.0168281
N    -3.7302432   -0.4485642    0.0029604
N    -5.8302902   -0.3723201    0.0419319
H    -6.1089011    1.7827737    0.0110560
H    -3.2963395    1.6806461   -0.0101627
N    -7.2086246   -0.7013394    0.0597981
H    -7.4020307   -1.1340419    0.9690720
H    -7.3334756   -1.4425311   -0.6363492
N    -2.3793101   -0.8760669   -0.0073830
H    -2.2189858   -1.3410606   -0.9070581
H    -2.3075479   -1.6100472    0.7037107
```

(NHC-1) R_2=H R_1=CH_3

```
15
Energy = -304.9255260297
C    -5.4846405    0.8167670    0.0000020
C    -4.1234729    0.8845498   -0.0000015
N    -3.6750430   -0.4328800   -0.0000020
N    -5.7995189   -0.5388414    0.0000034
```

C	-4.6942888	-1.3491540	0.0000010
H	-6.2308673	1.6035884	0.0000039
H	-3.4592197	1.7415327	-0.0000040
C	-2.2704884	-0.8221794	-0.0000058
H	-1.6436558	0.0778795	-0.0000065
H	-2.0430146	-1.4199886	-0.8914672
H	-2.0430104	-1.4199900	0.8914535
C	-7.1582196	-1.0666146	0.0000075
H	-7.8722734	-0.2338428	0.0000084
H	-7.3242310	-1.6842473	0.8914510
H	-7.3242357	-1.6842494	-0.8914336

(NHC-1) R_2=F R_1=H

9
Energy = -424.8362714725

C	-5.4545629	0.9573938	-0.0000000
C	-4.1010472	1.0776831	0.0000000
N	-3.6024578	-0.2134386	0.0000000
N	-5.7165478	-0.4018036	0.0000000
C	-4.5819354	-1.1792507	-0.0000000
H	-2.6140720	-0.4388415	-0.0000000
H	-6.6493778	-0.7988326	0.0000000
F	-6.4100450	1.8903056	-0.0000000
F	-3.3258940	2.1642044	0.0000000

(NHC-1) R_2=Cl R_1=H

9
Energy = -1145.607235801

C	-4.0875907	1.0010623	0.0000000
C	-4.5847696	-1.2591073	0.0000000
C	-5.4505810	0.8867594	-0.0000000
N	-3.6035704	-0.3023018	-0.0000000
N	-5.7110081	-0.4785841	0.0000000
H	-2.6158091	-0.5315172	0.0000000
H	-6.6467728	-0.8691415	-0.0000000
Cl	-6.6553103	2.0963408	0.0000000
Cl	-3.1005378	2.3941795	-0.0000000

(NHC-1) R_2=CHO R_1=H

13
Energy = -453.0495984467

C	-5.6444890	1.1812996	0.0000000
C	-4.2783065	1.4421812	-0.0000000
N	-3.6738653	0.1996180	-0.0000000
N	-5.7482311	-0.1967940	-0.0000000
C	-4.5461125	-0.8618228	-0.0000000
H	-2.6628778	0.0911682	0.0000000
H	-6.6478782	-0.6707852	-0.0000000

```
C    -3.5300944    2.6940414   -0.0000000
C    -6.8008911    2.0698279    0.0000000
O    -7.9510927    1.6514117   -0.0000000
H    -6.5763904    3.1617261    0.0000000
O    -2.3066841    2.7280712   -0.0000000
H    -4.1404768    3.6266966   -0.0000000
```

(NHC-1) R_2=H R_1=Cl

```
9
Energy = -1145.520841177
C    -3.9914838    0.8786771    0.0000000
C    -4.6403659   -1.3629274    0.0000000
C    -5.3538392    0.8591609    0.0000000
N    -3.6193687   -0.4642103   -0.0000000
N    -5.6868967   -0.4942311    0.0000000
H    -6.0846745    1.6581778   -0.0000000
H    -3.2841128    1.6986733    0.0000000
Cl   -7.3168020   -1.0205026    0.0000000
Cl   -1.9747664   -0.9430477   -0.0000000
```

(NHC-1) R_2=H R_1=COOH

```
15
Energy = -603.6398998313
C    -4.0042393    0.5823930   -0.0056233
C    -4.5189700   -1.6638545   -0.0000800
C    -5.3562201    0.4835123   -0.0075028
N    -3.5230097   -0.7337075   -0.0011269
N    -5.6396125   -0.8889938   -0.0040736
C    -6.9692378   -1.4638256   -0.0046140
C    -2.1233198   -1.1063307    0.0021717
O    -1.2462773   -0.2831960    0.0012722
O    -7.9578303   -0.7789165   -0.0082164
O    -6.9283964   -2.7965224   -0.0006894
H    -5.9612067   -3.0489637    0.0016585
O    -1.9668529   -2.4308826    0.0061473
H    -2.8855272   -2.8249414    0.0057405
H    -6.1412586    1.2292087   -0.0108681
H    -3.3361714    1.4344507   -0.0069656
```

carbene-phosphinidene adduct R_2=H R_1=H

```
21
Energy = -799.4558273320
C    -2.6026514    1.3070047    0.4904400
C    -3.7088463    1.9726227   -0.0470148
C    -3.6336637    2.6212041   -1.2965807
C    -2.4019106    2.5904344   -1.9787112
H    -2.3214044    3.0923166   -2.9451348
C    -1.2915241    1.9330932   -1.4394945
```

H	-0.3474747	1.9241072	-1.9877345
C	-1.3892798	1.2862884	-0.2045108
H	-0.5225583	0.7758481	0.2185461
P	-5.0610259	3.5891175	-1.9840142
C	-7.6599885	1.0072466	-3.5759103
C	-6.7183324	0.1222772	-3.1599738
N	-5.7112971	0.8625166	-2.5471404
N	-7.2145608	2.2731707	-3.2076874
C	-5.9888783	2.2143805	-2.5666105
H	-6.6786583	-0.9559099	-3.2453997
H	-8.5976786	0.8486361	-4.0927611
H	-4.8597303	0.5012136	-2.1323532
H	-7.6955058	3.1449846	-3.3880015
H	-2.6846575	0.8154423	1.4618469
H	-4.6456730	2.0111848	0.5133602

carbene-phosphinidene adduct R_2=NH_2 R_1=H

25
Energy = -910.2229750647

C	-2.7764081	1.2426315	0.3253673
C	-3.7760601	1.8508365	-0.4377241
C	-3.4787961	2.5094746	-1.6530053
C	-2.1215749	2.5663751	-2.0372175
H	-1.8581897	3.0718968	-2.9692153
C	-1.1181772	1.9839007	-1.2601369
H	-0.0780039	2.0485263	-1.5861280
C	-1.4392911	1.3050684	-0.0805486
H	-0.6568623	0.8403446	0.5209434
P	-4.7055811	3.4088836	-2.6853073
C	-7.9507329	1.1721001	-3.4023663
C	-7.1924595	0.2380057	-2.7500251
N	-6.0048564	0.8644731	-2.3800865
N	-7.2003517	2.3640344	-3.3777433
C	-5.9765133	2.1877498	-2.7786569
H	-5.2423057	0.4407838	-1.8605116
H	-7.4927547	3.2235644	-3.8272817
H	-3.0412712	0.7403557	1.2583160
H	-4.8031354	1.8521567	-0.0638897
N	-7.4661778	-1.0747899	-2.3538300
H	-6.8390642	-1.7693530	-2.7652122
H	-8.4313098	-1.3338229	-2.5526464
N	-9.2123588	1.1362875	-4.0147993
H	-9.3286035	0.3946644	-4.7025678
H	-10.0077606	1.1585720	-3.3768571

carbene-phosphinidene adduct R_2=H R_1=OH

23
Energy = -949.8672611161

C	-3.0305690	1.1480513	0.1740048
C	-3.9601031	1.6101672	-0.7667362
C	-3.5489268	2.3358123	-1.9120985
C	-2.1670278	2.6022925	-2.0444222
H	-1.8151776	3.1545191	-2.9187485
C	-1.2490373	2.1625952	-1.0929480
H	-0.1892116	2.3880979	-1.2260373
C	-1.6704285	1.4189100	0.0172134
H	-0.9475435	1.0639147	0.7522903
P	-4.6548586	3.0084760	-3.2063062
C	-8.1520295	1.1113347	-3.1732687
C	-7.3697496	0.0156776	-2.9099047
N	-6.0646150	0.4629784	-2.8947803
N	-7.2844725	2.1686987	-3.3128045
C	-5.9719583	1.8152174	-3.1287188
H	-7.6164178	-1.0299682	-2.7847113
H	-9.2213701	1.2145971	-3.2992093
H	-3.3815042	0.5915007	1.0452189
H	-5.0262225	1.4731982	-0.5660446
O	-7.6641822	3.4900348	-3.3682767
H	-6.8161724	3.9470639	-3.0537742
O	-4.9885629	-0.3798229	-2.7578650
H	-4.4176193	0.0534532	-2.0633824

carbene-phosphinidene adduct R_2=H R_1=NH_2

25
Energy = -910.1567149584

C	-2.0701340	2.0078381	0.7322889
C	-3.3704274	2.3819997	0.3893374
C	-3.8369487	2.2818150	-0.9391710
C	-2.9276031	1.8062782	-1.9117982
H	-3.2290899	1.7815578	-2.9622504
C	-1.6333294	1.4116310	-1.5634020
H	-0.9561596	1.0442353	-2.3372730
C	-1.1953403	1.5087185	-0.2385427
H	-0.1823470	1.2080004	0.0313443
P	-5.5113595	2.9300843	-1.3106036
C	-7.3749789	1.0681870	-4.2943467
C	-6.6501790	0.0050966	-3.8555929
N	-5.8659934	0.4499132	-2.7958671
N	-7.0343869	2.1454778	-3.4898906
C	-6.0833931	1.7959490	-2.5458756
H	-6.6126825	-1.0266705	-4.1788357
H	-8.0928754	1.1716320	-5.0970163
H	-1.7409032	2.0959616	1.7694301
H	-4.0472775	2.7511152	1.1632943
N	-7.5177990	3.4448840	-3.6932160
H	-6.7049482	4.0710052	-3.5732244
H	-8.1495724	3.6720792	-2.9162452
N	-5.1596856	-0.4401252	-1.9768408
H	-5.4896813	-0.2851963	-1.0148451
H	-4.1716747	-0.1514571	-1.9744178

carbene-phosphinidene adduct R_2=H R_1=CH_3

```
27
Energy = -878.0991643687
C    -2.1751099    2.4846559    0.7030457
C    -3.3966564    2.8836829    0.1581841
C    -3.7914431    2.4817692   -1.1368849
C    -2.8934483    1.6697944   -1.8644945
H    -3.1404894    1.3836013   -2.8894048
C    -1.6803251    1.2548472   -1.3116631
H    -1.0081692    0.6258890   -1.8996107
C    -1.3111679    1.6590534   -0.0239874
H    -0.3585398    1.3421315    0.4025863
P    -5.3290801    3.2023796   -1.8266215
C    -7.2938382    0.8552611   -4.3598816
C    -6.8152125   -0.1219903   -3.5444334
N    -6.0362669    0.4884724   -2.5703136
N    -6.7854228    2.0598884   -3.9012047
C    -6.0000381    1.8593877   -2.7753215
H    -6.9615311   -1.1946830   -3.5718997
H    -7.9375797    0.7953334   -5.2285888
H    -1.8999551    2.8135161    1.7072791
H    -4.0679997    3.5151754    0.7449789
C    -5.5340867   -0.1793481   -1.3834247
H    -6.0666113   -1.1305555   -1.2645320
H    -5.7205760    0.4651407   -0.5126111
H    -4.4524943   -0.3626917   -1.4452699
C    -7.0268670    3.3611990   -4.4931498
H    -7.8429450    3.8916834   -3.9804755
H    -7.2837131    3.2344056   -5.5520062
H    -6.1106033    3.9616413   -4.3873446
```

carbene-phosphinidene adduct R_2=F R_1=H

```
21
Energy = -998.0071389540
C    -2.6368002    1.3268188    0.4907086
C    -3.7301719    1.9981359   -0.0636863
C    -3.6387892    2.6163638   -1.3272112
C    -2.4077581    2.5505052   -2.0075177
H    -2.3150073    3.0298159   -2.9841883
C    -1.3104170    1.8867853   -1.4499834
H    -0.3653052    1.8505648   -1.9947596
C    -1.4225217    1.2707782   -0.2007710
H    -0.5658339    0.7551062    0.2358998
P    -5.0432833    3.5939127   -2.0384851
C    -7.6784137    1.0502828   -3.5643489
C    -6.7560010    0.1597115   -3.1363473
N    -5.7798542    0.8685436   -2.4417980
N    -7.2804566    2.3119975   -3.1284136
C    -6.0353369    2.2309904   -2.5074361
```

```
H    -4.8610314    0.5137983   -2.1912756
H    -7.6381395    3.1806420   -3.5121507
H    -2.7292031    0.8593272    1.4728802
H    -4.6678178    2.0610649    0.4925411
F    -6.7464533   -1.1710051   -3.1720216
F    -8.8602543    0.8705400   -4.1501654
```

carbene-phosphinidene adduct R_2=Cl R_1=H

```
21
Energy = -1718.777682076
C    -2.6336941    1.3443183    0.4954697
C    -3.6986575    2.0450103   -0.0782008
C    -3.5717452    2.6540601   -1.3433390
C    -2.3314869    2.5528089   -2.0019963
H    -2.2116163    3.0234476   -2.9798955
C    -1.2615780    1.8623207   -1.4243711
H    -0.3093332    1.7977744   -1.9541684
C    -1.4106240    1.2522464   -0.1760251
H    -0.5762207    0.7137224    0.2759031
P    -4.9413730    3.6564154   -2.0899927
C    -7.7013475    1.1316279   -3.4780387
C    -6.8067208    0.2225060   -3.0009746
N    -5.7545829    0.9430503   -2.4408028
N    -7.1859424    2.3951687   -3.1982154
C    -5.9557862    2.3069023   -2.5605855
H    -4.9217873    0.5489917   -2.0146712
H    -7.6219993    3.2695753   -3.4646630
H    -2.7550719    0.8825068    1.4772031
H    -4.6416415    2.1400276    0.4648224
Cl   -6.8519263   -1.4783021   -3.0062821
Cl   -9.1937351    0.9077411   -4.2624161
```

carbene-phosphinidene adduct R_2=CHO R_1=H

```
25
Energy = -1026.223941844
C    -2.7691901    1.3118357    0.4383359
C    -3.7987933    1.9762747   -0.2343778
C    -3.5660634    2.6106352   -1.4717384
C    -2.2601335    2.5816945   -1.9953316
H    -2.0574740    3.0742179   -2.9485234
C    -1.2272232    1.9294500   -1.3160884
H    -0.2219246    1.9196403   -1.7409257
C    -1.4793656    1.2875305   -0.1007808
H    -0.6730342    0.7781465    0.4285849
P    -4.8833799    3.5647522   -2.3556261
C    -7.5926468    1.0174436   -3.7637933
C    -6.7290734    0.1009478   -3.1761496
N    -5.7088723    0.8442617   -2.6078834
N    -7.0673896    2.2645246   -3.5287472
C    -5.8770753    2.2093160   -2.8107964
```

```
H    -4.9119537    0.4799478   -2.0916175
H    -7.5120092    3.1160652   -3.8621936
H    -2.9715509    0.8290275    1.3961781
H    -4.7943910    2.0252510    0.2131853
C    -8.8411343    0.8445729   -4.5035462
C    -6.7798789   -1.3574287   -3.1045206
O    -7.6505033   -2.0522353   -3.6103909
H    -5.9332869   -1.8154761   -2.5330247
O    -9.4556306    1.8152414   -4.9386246
H    -9.1821219   -0.2011569   -4.6386540
```

carbene-phosphinidene adduct R_2=H R_1=Cl

```
21
Energy = -1718.783405707
C    -2.8990876    1.5879404    0.5951286
C    -3.7862382    1.8749986   -0.4444444
C    -3.3004763    2.1396805   -1.7372466
C    -1.9146060    2.1184425   -1.9624304
H    -1.5231617    2.3175106   -2.9604934
C    -1.0337016    1.8258382   -0.9201661
H     0.0395874    1.8000712   -1.1142952
C    -1.5220533    1.5624393    0.3618804
H    -0.8323075    1.3332836    1.1753796
P    -4.4199920    2.7967639   -3.0349130
C    -8.0160037    1.0638405   -3.0737723
C    -7.2887670    0.1088738   -2.3950092
N    -5.9830595    0.5035485   -2.2585242
N    -7.1074235    2.0612699   -3.3359376
C    -5.8656643    1.6970842   -2.8357210
H    -7.6376928   -0.8401866   -1.9991853
H    -9.0500378    1.1409090   -3.3868655
H    -3.2913636    1.3721965    1.5900803
H    -4.8585596    1.8718216   -0.2505289
Cl   -7.4924120    3.4915042   -4.1931898
Cl   -3.5786711    1.9819522   -4.7940924
```

carbene-phosphinidene adduct R_2=H R_1=COOH

```
27
Energy = -1176.789455396
C    -1.8051178    2.0338265    0.6482750
C    -3.0703531    2.5288740    0.3221595
C    -3.5990341    2.3695243   -0.9726373
C    -2.8068272    1.7191263   -1.9394299
H    -3.1746892    1.6164157   -2.9621815
C    -1.5468996    1.2180280   -1.6112891
H    -0.9496482    0.7163096   -2.3746310
C    -1.0404900    1.3721663   -0.3155982
H    -0.0510142    0.9876690   -0.0641157
P    -5.1511000    3.2682973   -1.3599279
C    -7.4218508    1.4040817   -4.0535008
```

C	-6.6751507	0.3563384	-3.6795696
N	-5.9004827	0.7457302	-2.5625955
N	-7.1191206	2.4888954	-3.2088021
C	-6.0612399	2.1343328	-2.3156121
H	-1.4149692	2.1690311	1.6586898
H	-3.6604126	3.0476003	1.0812296
H	-8.1641941	1.5184690	-4.8318575
H	-6.6307541	-0.6619015	-4.0419775
C	-7.7744762	3.7062046	-3.3979461
C	-5.4053464	-0.2706999	-1.7260767
O	-5.1947093	-1.3981553	-2.1307950
O	-8.5713445	3.9017849	-4.2979999
O	-5.2631000	0.1335256	-0.4480129
H	-4.8678372	-0.6254825	0.0265498
O	-7.4193937	4.6137051	-2.4607157
H	-7.8999744	5.4357332	-2.6876214

carbene-phosphinidene adduct R_2=H R_1=C(CH_3)$_3$

45

Energy = -1114.0424742960

C	-2.8879702	2.2969828	0.6456225
C	-3.7762425	2.4098549	-0.4229843
C	-3.3166622	2.5966313	-1.7480807
C	-1.9192875	2.6932729	-1.9363873
H	-1.5296157	2.8453872	-2.9460647
C	-1.0303647	2.5992743	-0.8628599
H	0.0436478	2.6792985	-1.0442444
C	-1.5060380	2.3919374	0.4352945
H	-0.8124158	2.3108770	1.2732723
P	-4.4109858	2.9738150	-3.1650658
C	-7.9289639	1.0818220	-2.8574884
C	-7.1245797	0.0079037	-2.6720333
N	-5.8061100	0.4260615	-2.7807669
N	-7.1237213	2.1910248	-3.0413786
C	-5.7780291	1.8160921	-2.9595899
H	-7.4043664	-1.0181769	-2.4872782
H	-9.0075255	1.1248173	-2.8662474
C	-4.6866599	-0.5958895	-2.8847790
C	-7.6779039	3.5852255	-3.2192206
H	-3.2769863	2.1476061	1.6554804
H	-4.8506594	2.3638677	-0.2323960
C	-9.2116283	3.5154273	-3.2908399
C	-7.1650760	4.1735214	-4.5442837
C	-7.2814125	4.4563726	-2.0141816
C	-5.2854856	-1.9291657	-3.3816913

C	-4.0595225	-0.8294772	-1.5027689
C	-3.6321361	-0.1682042	-3.9137162
H	-9.5629298	2.8993693	-4.1310928
H	-9.5845096	4.5353960	-3.4510844
H	-9.6586928	3.1460650	-2.3574745
H	-6.1889271	4.5151994	-1.9232836
H	-7.7018092	4.0433179	-1.0860710
H	-7.6814594	5.4704111	-2.1533754
H	-3.3171296	-1.6375353	-1.5752602
H	-4.8243792	-1.1350319	-0.7741179
H	-3.5568401	0.0668663	-1.1271456
H	-4.0831395	-0.0156426	-4.9037329
H	-2.8911373	-0.9767943	-3.9898460
H	-3.1193932	0.7559701	-3.6333570
H	-5.8523223	-1.8016161	-4.3141696
H	-5.9287875	-2.4131487	-2.6341995
H	-4.4539002	-2.6172252	-3.5800918
H	-7.4550669	3.5347995	-5.3909745
H	-6.0729664	4.2805274	-4.5354872
H	-7.6086791	5.1684424	-4.6940686

carbene-phosphinidene adduct R_2= CH_3 R_1=$C(CH_3)_3$

51

Energy = -1192.6849968550

C	-3.0533990	1.8079865	0.8059486
C	-3.9002527	2.0891209	-0.2644385
C	-3.3918697	2.5120573	-1.5136485
C	-1.9926502	2.6602920	-1.6248256
H	-1.5685431	2.9953864	-2.5746845
C	-1.1430769	2.3950797	-0.5464179
H	-0.0650343	2.5233886	-0.6646265
C	-1.6658609	1.9598923	0.6735418
H	-1.0045470	1.7487141	1.5151903
P	-4.4367167	3.1470726	-2.8847717
C	-7.8702096	1.1269272	-2.6468677
C	-6.9961302	0.1153908	-2.3661485
N	-5.6947784	0.5717922	-2.6657029
N	-7.1268454	2.2342231	-3.0914287
C	-5.7642439	1.9385845	-2.9509818
C	-7.3345833	-1.1829616	-1.6929629
C	-9.3404695	1.0642613	-2.3817314
C	-4.6017404	-0.3865731	-3.1460652
C	-7.6533342	3.5797460	-3.5348212
H	-3.4772582	1.4842488	1.7591276
H	-4.9800136	1.9927608	-0.1346146

C	-9.1039676	3.4866979	-4.0435788
C	-6.8266889	4.0708468	-4.7382856
C	-7.5858714	4.5661765	-2.3551512
C	-5.2746040	-1.5279977	-3.9438734
C	-3.8138630	-0.9595257	-1.9561882
C	-3.6256483	0.2840738	-4.1212199
H	-9.2243507	2.6873509	-4.7880463
H	-9.3366016	4.4382499	-4.5402839
H	-9.8399444	3.3528487	-3.2452578
H	-6.5535843	4.6662025	-1.9946986
H	-8.2234292	4.2230713	-1.5275391
H	-7.9450134	5.5543166	-2.6766353
H	-3.1044972	-1.7161176	-2.3215924
H	-4.4671494	-1.4440771	-1.2189715
H	-3.2479278	-0.1735217	-1.4444219
H	-4.1456984	0.7070728	-4.9906534
H	-2.9361104	-0.4956568	-4.4749975
H	-3.0368894	1.0811100	-3.6596306
H	-5.9336271	-1.1250145	-4.7256155
H	-5.8514213	-2.2151045	-3.3174041
H	-4.4893500	-2.1185167	-4.4338196
H	-6.9087855	3.3613224	-5.5745303
H	-5.7654521	4.2103749	-4.4981730
H	-7.2252893	5.0401595	-5.0678285
H	-9.6942703	1.8922660	-1.7509054
H	-9.5537494	0.1311570	-1.8463029
H	-9.9502661	1.0549218	-3.2950339
H	-8.0722570	-1.0118976	-0.8956579
H	-6.4564455	-1.6302706	-1.2167008
H	-7.7621497	-1.9323689	-2.3764030

carbene-phosphinidene adduct R_2=Br R_1=C$(CH_3)_3$

45

Energy = -6261.7019558980

C	-2.6053018	2.0326876	0.8350522
C	-3.5812646	2.2520981	-0.1360326
C	-3.2424841	2.7752115	-1.4013477
C	-1.8886752	3.0882566	-1.6411305
H	-1.6019906	3.5084383	-2.6081216
C	-0.9119322	2.8785516	-0.6633779
H	0.1284110	3.1327411	-0.8753382
C	-1.2641159	2.3440603	0.5774634
H	-0.5041763	2.1777707	1.3424183
P	-4.4721724	3.3626442	-2.6340805

C	-7.7421600	1.1961778	-2.3193934
C	-6.8248617	0.2617704	-1.9518746
N	-5.5462859	0.7295635	-2.2791048
N	-7.0724618	2.2897748	-2.8850147
C	-5.6928834	2.0843224	-2.6605644
Br	-7.1703610	-1.1950736	-0.7900112
Br	-9.5290716	1.1753017	-1.7205088
C	-4.5123482	-0.2438958	-2.8913044
C	-7.6703850	3.4633535	-3.6350685
H	-2.8937338	1.6277329	1.8071086
H	-4.6240927	2.0254810	0.0900742
C	-9.0273707	3.0894056	-4.2602333
C	-6.7518388	3.8323649	-4.8128030
C	-7.8360877	4.6426049	-2.6607031
C	-5.2822838	-1.2841252	-3.7307114
C	-3.7271527	-0.9206561	-1.7592932
C	-3.5441503	0.4645042	-3.8412489
H	-8.9737368	2.1337227	-4.7999917
H	-9.2828104	3.8711115	-4.9880786
H	-9.8397076	3.0374590	-3.5311378
H	-6.8695441	4.9300408	-2.2259810
H	-8.5255651	4.3767338	-1.8477713
H	-8.2509653	5.5097856	-3.1939956
H	-3.0330013	-1.6577980	-2.1884354
H	-4.3920348	-1.4464328	-1.0633069
H	-3.1436001	-0.1827001	-1.1954272
H	-4.0663880	0.9651063	-4.6659908
H	-2.8916023	-0.3099059	-4.2693553
H	-2.9078632	1.1972992	-3.3364870
H	-5.8668944	-0.7926350	-4.5209253
H	-5.9567661	-1.9029454	-3.1286630
H	-4.5559571	-1.9531659	-4.2124004
H	-6.6505495	2.9852065	-5.5064079
H	-5.7500650	4.1474383	-4.4975331
H	-7.2100478	4.6686426	-5.3579416

carbene-phosphinidene adduct R_2=F R_1=C$(CH_3)_3$

45

Energy = -1312.5877038950

C	-2.7499474	2.2963026	0.7033574
C	-3.6607459	2.3839299	-0.3487642
C	-3.2557636	2.8085981	-1.6327695
C	-1.8979149	3.1593835	-1.8026450
H	-1.5556565	3.4968381	-2.7841059

C	-0.9891456	3.0841509	-0.7444956
H	0.0534915	3.3636643	-0.9089997
C	-1.4062627	2.6449867	0.5145215
H	-0.6978012	2.5807623	1.3414240
P	-4.3870957	3.1953759	-3.0212696
C	-7.7420889	1.0995900	-2.6188524
C	-6.8612231	0.1689028	-2.2047877
N	-5.5672541	0.6294096	-2.4242748
N	-7.0411896	2.2145582	-3.0769713
C	-5.6694663	1.9645472	-2.8687699
F	-7.1358434	-0.9853890	-1.5809027
F	-9.0690257	1.0404310	-2.5039222
C	-4.5005698	-0.4189147	-2.7995771
C	-7.6473651	3.5103744	-3.5782127
H	-3.0940657	1.9673612	1.6862948
H	-4.7080379	2.1342802	-0.1698464
C	-9.1368173	3.3285468	-3.9209507
C	-6.9345785	3.9131159	-4.8801424
C	-7.5098545	4.5837909	-2.4846379
C	-5.1641340	-1.4341555	-3.7561550
C	-4.0300642	-1.0996382	-1.5051220
C	-3.3009675	0.1773592	-3.5364857
H	-9.3016410	2.5014818	-4.6246335
H	-9.4680427	4.2539327	-4.4106820
H	-9.7649132	3.1766381	-3.0369235
H	-6.4570695	4.7399538	-2.2167276
H	-8.0716422	4.2914405	-1.5861572
H	-7.9232607	5.5328472	-2.8534776
H	-3.2713496	-1.8566139	-1.7479863
H	-4.8548513	-1.6007443	-0.9836534
H	-3.5772134	-0.3638866	-0.8278945
H	-3.5993798	0.7420039	-4.4279033
H	-2.6760046	-0.6693125	-3.8554966
H	-2.6923720	0.8279796	-2.9036922
H	-5.5334184	-0.9298990	-4.6604972
H	-5.9908983	-1.9849503	-3.2933491
H	-4.4091652	-2.1690517	-4.0657078
H	-7.0651734	3.1362775	-5.6471962
H	-5.8613484	4.0865812	-4.7326698
H	-7.3811981	4.8451795	-5.2532893

carbene-phosphinidene adduct R_2=Cl R_1=C(CH$_3$)$_3$

45
Energy = -2033.3460608250

C	-2.6814472	2.1349945	0.8299153
C	-3.6304676	2.3194481	-0.1745482
C	-3.2538213	2.7664367	-1.4584358
C	-1.8883697	3.0389765	-1.6821585
H	-1.5715127	3.3987218	-2.6641508
C	-0.9383508	2.8651014	-0.6716727
H	0.1114434	3.0870138	-0.8730336
C	-1.3285059	2.4065622	0.5880456
H	-0.5895655	2.2687342	1.3786724
P	-4.4423236	3.3087321	-2.7506159
C	-7.7508903	1.1841736	-2.3877143
C	-6.8441242	0.2534284	-1.9885114
N	-5.5580997	0.7083882	-2.3069742
N	-7.0670412	2.2693821	-2.9528421
C	-5.6900106	2.0490427	-2.7282229
Cl	-7.1891016	-1.0958927	-0.9755980
Cl	-9.4122533	1.1287144	-1.9720353
C	-4.5161590	-0.2939970	-2.8509643
C	-7.6480017	3.4865317	-3.6447866
H	-3.0004777	1.7900724	1.8154989
H	-4.6827921	2.1264090	0.0396792
C	-9.0569958	3.2069465	-4.1989333
C	-6.7727969	3.8274130	-4.8633014
C	-7.7037513	4.6509623	-2.6401231
C	-5.2667747	-1.3535923	-3.6856798
C	-3.7817806	-0.9411430	-1.6680612
C	-3.5045224	0.3688632	-3.7880488
H	-9.0943688	2.2694133	-4.7702381
H	-9.3042491	4.0269120	-4.8864974
H	-9.8275922	3.1815945	-3.4238442
H	-6.7053415	4.8758908	-2.2428279
H	-8.3730848	4.4049947	-1.8041470
H	-8.0929198	5.5500001	-3.1385434
H	-3.0826856	-1.7013903	-2.0450895
H	-4.4783584	-1.4329396	-0.9782336
H	-3.2087511	-0.1903274	-1.1102674
H	-3.9902804	0.8576952	-4.6417103
H	-2.8559368	-0.4305213	-4.1739279
H	-2.8695089	1.1022602	-3.2832730
H	-5.8135876	-0.8818728	-4.5140538
H	-5.9700914	-1.9474754	-3.0921872
H	-4.5298203	-2.0443566	-4.1172481
H	-6.7675723	2.9944790	-5.5813245
H	-5.7360529	4.0649745	-4.5951579
H	-7.1996344	4.7082552	-5.3618282

carbene-phosphinidene adduct R_2=I R_1=C(CH_3)$_3$

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45
 Energy =   -1708.5244725380
 C    -2.6440102    2.0023660    0.8762738
 C    -3.6087492    2.2651872   -0.0951089
 C    -3.2451249    2.7598593   -1.3650404
 C    -1.8788872    3.0034391   -1.6100120
 H    -1.5727371    3.4038365   -2.5792920
 C    -0.9122757    2.7493139   -0.6322200
 H     0.1392727    2.9499217   -0.8460369
 C    -1.2894577    2.2420194    0.6128453
 H    -0.5371012    2.0419588    1.3772043
 P    -4.4656130    3.3904497   -2.5863852
 C    -7.7374398    1.2330110   -2.2823662
 C    -6.8163212    0.2844509   -1.9383280
 N    -5.5426908    0.7531443   -2.2871974
 N    -7.0646540    2.3210878   -2.8584190
 C    -5.6863979    2.1152049   -2.6410157
 I    -7.1698019   -1.2973820   -0.5835496
 I    -9.6817043    1.2675075   -1.4905913
 C    -4.5034902   -0.2000194   -2.9201795
 C    -7.6612026    3.4661742   -3.6526243
 H    -2.9509984    1.6200257    1.8516315
 H    -4.6619535    2.0944563    0.1324063
 C    -8.9715894    3.0275043   -4.3325494
 C    -6.7061066    3.8576088   -4.7933808
 C    -7.9058158    4.6565043   -2.7089605
 C    -5.2714972   -1.2807402   -3.7073022
 C    -3.6468747   -0.8330026   -1.8152609
 C    -3.6019585    0.5244439   -3.9233523
 H    -8.8472012    2.0712065   -4.8598647
 H    -9.2367782    3.7905201   -5.0765455
 H    -9.8109888    2.9382887   -3.6376737
 H    -6.9651061    4.9868703   -2.2485442
 H    -8.6125669    4.3843346   -1.9134139
 H    -8.3316584    5.4977820   -3.2743739
 H    -2.9695043   -1.5758814   -2.2612538
 H    -4.2652510   -1.3449234   -1.0674107
 H    -3.0410738   -0.0742771   -1.3063572
 H    -4.1769682    0.9828486   -4.7381732
 H    -2.9316432   -0.2299595   -4.3594053
 H    -2.9805798    1.2974261   -3.4610497
 H    -5.9219739   -0.8256502   -4.4673106
 H    -5.8830627   -1.9225143   -3.0629747
 H    -4.5430995   -1.9218834   -4.2226750
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H	-6.5198322	3.0034076	-5.4596214
H	-5.7421101	4.2394384	-4.4378172
H	-7.1837814	4.6526750	-5.3817241

carbene-phosphinidene adduct R_2=NH_2 R_1=$C(CH_3)_3$

49

Energy = -1224.7893897710

C	-2.9530873	2.3215145	0.6697380
C	-3.8071365	2.3583482	-0.4318834
C	-3.3433569	2.7368600	-1.7132559
C	-1.9755149	3.0843597	-1.8213808
H	-1.5816604	3.3816311	-2.7969615
C	-1.1245972	3.0629711	-0.7144906
H	-0.0760409	3.3434912	-0.8369419
C	-1.6032193	2.6753831	0.5407695
H	-0.9396689	2.6534985	1.4061899
P	-4.3952758	3.0563803	-3.1751366
C	-7.8140292	1.0342004	-2.5893366
C	-6.9059518	0.0941875	-2.1948327
N	-5.6242145	0.5282971	-2.5404766
N	-7.0884573	2.1290068	-3.1148196
C	-5.7246466	1.8600552	-2.9834538
N	-7.2346979	-1.1436859	-1.6129390
N	-9.1992318	0.8385235	-2.6490557
C	-4.5265591	-0.4865449	-2.8707018
C	-7.6476666	3.4873050	-3.4866233
H	-3.3481917	2.0313624	1.6462185
H	-4.8619351	2.1112100	-0.2960877
C	-9.1698651	3.4538803	-3.7080271
C	-7.0233042	3.9194694	-4.8263569
C	-7.3541715	4.4902618	-2.3544473
C	-5.1559625	-1.5958513	-3.7456665
C	-3.9385029	-1.0569759	-1.5662517
C	-3.3729414	0.0985241	-3.6955280
H	-9.4759827	2.6937375	-4.4346894
H	-9.4507368	4.4424705	-4.0976568
H	-9.7341704	3.3038521	-2.7797854
H	-6.2756989	4.5671288	-2.1650539
H	-7.8642840	4.1826241	-1.4298057
H	-7.7333177	5.4815680	-2.6409323
H	-3.1152111	-1.7418104	-1.8121559
H	-4.6598994	-1.6351308	-0.9704879
H	-3.5406366	-0.2501498	-0.9375949
H	-3.7286533	0.6084780	-4.5977140

H	-2.7458080	-0.7527233	-3.9999507
H	-2.7508429	0.7963733	-3.1294409
H	-5.5191651	-1.1669528	-4.6903147
H	-5.9876847	-2.1178351	-3.2601634
H	-4.3814609	-2.3358621	-3.9860698
H	-7.2756994	3.1955837	-5.6144221
H	-5.9319438	4.0135458	-4.7661210
H	-7.4329153	4.8988268	-5.1116719
H	-8.0678404	-1.0452222	-1.0297684
H	-6.4821807	-1.5250898	-1.0425315
H	-9.7597851	1.2886476	-1.9262795
H	-9.4513854	-0.1436433	-2.7434506

carbene-phosphinidene adduct R_2=NO_2 R_1=$C(CH_3)_3$

49

Energy = -1523.2580807770

C	-2.6013122	2.0898130	0.8793201
C	-3.6085262	2.2724138	-0.0661785
C	-3.2964215	2.6683139	-1.3819449
C	-1.9469199	2.9042687	-1.7067189
H	-1.6864729	3.2352831	-2.7147250
C	-0.9381996	2.7234880	-0.7563108
H	0.1021818	2.9074628	-1.0297084
C	-1.2612958	2.3110979	0.5379215
H	-0.4758189	2.1705028	1.2817894
P	-4.5684068	3.1792419	-2.5996946
C	-7.7785047	0.9537032	-2.3194438
C	-6.8570884	0.0386648	-1.8731474
N	-5.5758419	0.5386817	-2.1589092
N	-7.1459388	2.0629579	-2.8032784
C	-5.7438642	1.8745091	-2.5592168
N	-7.1676358	-1.0370733	-0.9948297
N	-9.2369045	0.8283122	-2.1402091
C	-4.4888176	-0.4083544	-2.7610834
C	-7.7743562	3.3224807	-3.4021096
H	-2.8626803	1.7782368	1.8920258
H	-4.6485632	2.1054411	0.2169108
C	-9.2205928	3.0724768	-3.8572082
C	-6.9787650	3.7071834	-4.6601102
C	-7.7652820	4.4329590	-2.3367327
C	-5.2071432	-1.6484814	-3.3273363
C	-3.4824774	-0.8225007	-1.6807244
C	-3.7641927	0.2691778	-3.9271219
H	-9.3026501	2.2144767	-4.5356402

H	-9.5344834	3.9649402	-4.4137312
H	-9.9246463	2.9575164	-3.0260759
H	-6.7473966	4.6653459	-2.0024686
H	-8.3687290	4.1362878	-1.4681286
H	-8.2063577	5.3421698	-2.7676255
H	-2.7961371	-1.5679818	-2.1088854
H	-3.9924777	-1.2703702	-0.8225243
H	-2.8871730	0.0308682	-1.3400213
H	-4.4541027	0.5562663	-4.7321439
H	-3.0507320	-0.4622123	-4.3311525
H	-3.1961336	1.1561267	-3.6261502
H	-5.9794419	-1.3724377	-4.0584802
H	-5.6515563	-2.2720371	-2.5445848
H	-4.4598548	-2.2632928	-3.8464436
H	-7.0304645	2.9062344	-5.4113049
H	-5.9254246	3.9279845	-4.4514306
H	-7.4316206	4.6100081	-5.0908537
O	-6.2428535	-1.5553915	-0.3422057
O	-8.3622198	-1.3893048	-0.9375068
O	-9.8531810	0.2219214	-3.0080856
O	-9.7017833	1.3661713	-1.1368719

carbene-phosphinidene adduct R_2=H R_1=C$(CH_3)_3$

carbene-phosphinidene adduct R_2=OH R_1=C$(CH_3)_3$

47

Energy = -1264.5462800350

C	-2.8492300	2.4076042	0.6027618
C	-3.7389995	2.3820225	-0.4708896
C	-3.3346206	2.7592467	-1.7720947
C	-1.9912917	3.1767981	-1.9298870
H	-1.6421520	3.4728767	-2.9225560
C	-1.1066312	3.2172981	-0.8511924
H	-0.0777356	3.5466785	-1.0120768
C	-1.5247306	2.8264074	0.4247486
H	-0.8328606	2.8504189	1.2675921
P	-4.4336185	2.9621908	-3.2183702
C	-7.7947980	0.9175555	-2.4585602
C	-6.8774978	-0.0213881	-2.1176025
N	-5.6102469	0.4273791	-2.4613039
N	-7.1063612	2.0205329	-2.9928494
C	-5.7297615	1.7530059	-2.9119826
O	-7.1191492	-1.2406061	-1.5621241
O	-9.1368984	0.6416342	-2.4658013
C	-4.4995816	-0.5995222	-2.7162987

C	-7.7077651	3.3757426	-3.2996702
H	-3.1975631	2.1107441	1.5946802
H	-4.7728868	2.0785644	-0.2949973
C	-9.2436008	3.3040036	-3.3824954
C	-7.2098750	3.8318530	-4.6823316
C	-7.3373132	4.3747882	-2.1882716
C	-5.0855762	-1.6934799	-3.6392102
C	-4.0571055	-1.1810639	-1.3635428
C	-3.2809743	-0.0239469	-3.4427994
H	-9.6002747	2.5331087	-4.0758090
H	-9.5912154	4.2788058	-3.7490788
H	-9.7169398	3.1701853	-2.3960379
H	-6.2473676	4.4743180	-2.1013281
H	-7.7490994	4.0457596	-1.2228596
H	-7.7656775	5.3586564	-2.4275278
H	-3.2772977	-1.9359904	-1.5371750
H	-4.8857241	-1.6619747	-0.8308838
H	-3.6321170	-0.3918351	-0.7292880
H	-3.5524909	0.4704391	-4.3825667
H	-2.6278947	-0.8785673	-3.6737824
H	-2.7125242	0.6829044	-2.8331451
H	-5.4199721	-1.2513390	-4.5885232
H	-5.9190639	-2.2362943	-3.1829754
H	-4.2935562	-2.4191171	-3.8664726
H	-7.5142296	3.1133394	-5.4568127
H	-6.1180557	3.9395313	-4.7036217
H	-7.6547418	4.8091567	-4.9191571
H	-8.0910612	-1.3152759	-1.4872245
H	-9.6304317	1.3187108	-1.9678750

carbene-phosphinidene adduct R_2=SH R_1=C$(CH_3)_3$

47

Energy = -1910.5303934520

C	-2.7082624	2.1039727	0.7904098
C	-3.6638119	2.2423690	-0.2154542
C	-3.3105165	2.7094802	-1.4996625
C	-1.9581162	3.0492485	-1.7185941
H	-1.6569661	3.4225375	-2.7005766
C	-1.0029161	2.9237495	-0.7062742
H	0.0348987	3.1977045	-0.9062097
C	-1.3700250	2.4440970	0.5528231
H	-0.6260930	2.3423052	1.3442431
P	-4.5100348	3.1904695	-2.8049773
C	-7.7869216	1.0199794	-2.2374884

C	-6.8233133	0.1148836	-1.8600719
N	-5.5793645	0.5858688	-2.2847769
N	-7.1334395	2.1045305	-2.8778713
C	-5.7533134	1.9151713	-2.7261230
S	-7.0457393	-1.3086262	-0.8453990
S	-9.4815636	0.7969686	-1.8708889
C	-4.5208668	-0.4023078	-2.8101025
C	-7.7546078	3.3399861	-3.4930562
H	-3.0118826	1.7411498	1.7747091
H	-4.7050247	1.9971939	-0.0000467
C	-9.1917654	3.0843786	-3.9810733
C	-6.9525797	3.7220335	-4.7504560
C	-7.7546113	4.4747097	-2.4524333
C	-5.2495186	-1.4491922	-3.6814485
C	-3.8114965	-1.0621447	-1.6189381
C	-3.4797899	0.2657151	-3.7120148
H	-9.2611041	2.1753995	-4.5939011
H	-9.4755538	3.9381038	-4.6120284
H	-9.9209407	3.0123797	-3.1696616
H	-6.7367274	4.6770706	-2.0939042
H	-8.3904947	4.2113204	-1.5950352
H	-8.1557581	5.3928948	-2.9041514
H	-3.0747841	-1.7874082	-1.9925267
H	-4.5062026	-1.6059790	-0.9651332
H	-3.2858338	-0.3105322	-1.0168472
H	-3.9403505	0.7947291	-4.5546577
H	-2.8492125	-0.5398947	-4.1149479
H	-2.8329634	0.9643191	-3.1747976
H	-5.7476018	-0.9611623	-4.5308546
H	-5.9930048	-2.0291200	-3.1232150
H	-4.5078038	-2.1528085	-4.0829978
H	-6.9848633	2.9081152	-5.4893019
H	-5.9034187	3.9596431	-4.5363042
H	-7.4122424	4.6128441	-5.1995624
H	-8.3845927	-1.0638378	-0.7476963
H	-9.6020549	1.6813915	-0.8396433

carbene-phosphinidene adduct R_2=OCH_3 R_1=$C(CH_3)_3$

53

Energy = -1343.1641890680

C	-2.8723698	1.4655885	0.7367798
C	-3.7740885	1.7332123	-0.2922039
C	-3.3852908	2.4586140	-1.4401162
C	-2.0508044	2.9190879	-1.4905511

H	-1.7197660	3.4888088	-2.3625145
C	-1.1510315	2.6655781	-0.4516883
H	-0.1274676	3.0394126	-0.5223035
C	-1.5518518	1.9301895	0.6663359
H	-0.8501601	1.7261061	1.4761908
P	-4.5279297	3.0861066	-2.7309988
C	-7.7151597	0.6900337	-2.8580353
C	-6.7493811	-0.2305518	-2.5931301
N	-5.4877837	0.3796795	-2.7421279
N	-7.0842315	1.9225576	-3.1339991
C	-5.7043727	1.7541365	-2.9291097
O	-6.9226681	-1.5394392	-2.2674907
O	-9.0517060	0.4744248	-2.8866681
C	-4.3555803	-0.4527182	-3.3748187
C	-7.7479359	3.2297159	-3.5017949
H	-3.2053800	0.9047748	1.6130261
H	-4.8067266	1.3910786	-0.2019568
C	-9.1836124	3.0160366	-4.0163453
C	-6.9661792	3.8662230	-4.6658052
C	-7.7790710	4.1538190	-2.2701890
C	-4.9735438	-1.2926184	-4.5148826
C	-3.7367996	-1.3562540	-2.2987288
C	-3.2548792	0.4066585	-3.9992456
H	-9.2276097	2.2697320	-4.8199839
H	-9.5216673	3.9780965	-4.4255314
H	-9.8887774	2.7281385	-3.2306668
H	-6.7650162	4.3360350	-1.8904859
H	-8.3850975	3.7108259	-1.4666021
H	-8.2321349	5.1168300	-2.5456328
H	-2.8973924	-1.9155659	-2.7362436
H	-4.4581400	-2.0876765	-1.9161026
H	-3.3495806	-0.7566566	-1.4647537
H	-3.6460649	1.1073217	-4.7461047
H	-2.5633611	-0.2847154	-4.5025403
H	-2.6857935	0.9749993	-3.2582297
H	-5.4114742	-0.6380994	-5.2817606
H	-5.7415543	-1.9872404	-4.1578953
H	-4.1772620	-1.8825608	-4.9898745
H	-6.9786735	3.2026864	-5.5421896
H	-5.9230756	4.0862699	-4.4061250
H	-7.4519606	4.8122874	-4.9426168
C	-6.9208305	-1.8259595	-0.8503070
C	-9.7528199	0.6755765	-1.6423398
H	-6.0045277	-1.4526789	-0.3704748
H	-6.9692564	-2.9176441	-0.7610023
H	-7.7989896	-1.3769377	-0.3615840

H	-9.5396322	1.6678642	-1.2158808
H	-9.4786595	-0.1014149	-0.9131773
H	-10.8207375	0.5943455	-1.8769630

carbene-phosphinidene adduct R_2=COH R_1=C(CH_3)$_3$

49

Energy = -1340.7813571560

C	-2.9683868	1.9373449	0.7844345
C	-3.8421116	2.1454281	-0.2819747
C	-3.3622667	2.5178954	-1.5558479
C	-1.9720612	2.6973729	-1.7052951
H	-1.5738951	3.0040642	-2.6756743
C	-1.0966828	2.4983919	-0.6337086
H	-0.0246354	2.6453066	-0.7780074
C	-1.5889304	2.1118129	0.6148222
H	-0.9076140	1.9570750	1.4524846
P	-4.4560703	3.0700254	-2.9244269
C	-7.8518287	1.0182023	-2.8445652
C	-6.9815238	0.0270672	-2.4249280
N	-5.6697984	0.4912382	-2.6245074
N	-7.1170977	2.1280494	-3.1852875
C	-5.7381762	1.8494442	-2.9442154
C	-7.4306189	-1.1862386	-1.7786281
C	-9.3254945	0.7220730	-2.9550245
C	-4.5651457	-0.4898469	-3.0440187
C	-7.6634103	3.5175407	-3.4863726
H	-3.3663245	1.6502235	1.7596597
H	-4.9163852	2.0280789	-0.1277131
C	-9.1650761	3.4750873	-3.7840932
C	-6.9574579	4.0580915	-4.7410808
C	-7.4574863	4.4226717	-2.2546554
C	-5.2209784	-1.6619303	-3.8074743
C	-3.8306129	-1.0148721	-1.8010142
C	-3.5706269	0.1500395	-4.0169296
H	-9.4112324	2.8378176	-4.6405149
H	-9.4741393	4.5037082	-4.0138921
H	-9.7582599	3.1507230	-2.9177131
H	-6.3997766	4.5193353	-1.9863886
H	-8.0130093	4.0259480	-1.3927294
H	-7.8534980	5.4216522	-2.4844469
H	-3.1070037	-1.7844794	-2.1039420
H	-4.5246702	-1.4722166	-1.0825189
H	-3.2882450	-0.2110739	-1.2910226
H	-4.0712951	0.5379499	-4.9136222

H	-2.8698840	-0.6370803	-4.3281472
H	-2.9893526	0.9610433	-3.5686579
H	-5.8225647	-1.3016526	-4.6529469
H	-5.8553888	-2.2935689	-3.1745578
H	-4.4219933	-2.3020085	-4.2038026
H	-7.1478887	3.4013221	-5.6011824
H	-5.8737496	4.1594902	-4.6031599
H	-7.3613369	5.0535547	-4.9719256
O	-8.6096389	-1.5547738	-1.7943107
H	-6.6658563	-1.7633313	-1.2129035
O	-9.8910360	0.5993416	-4.0250473
H	-9.8497636	0.5829023	-1.9856557

carbene-phosphinidene adduct R_2=$COOCH_3$ R_1=$C(CH_3)_3$

57

Energy = -1569.9889924660

C	-2.5330510	2.1308912	0.7337108
C	-3.5323165	2.3275575	-0.2171076
C	-3.2181716	2.7701100	-1.5189507
C	-1.8671441	3.0355844	-1.8174323
H	-1.6000229	3.3978698	-2.8130526
C	-0.8657383	2.8482055	-0.8598853
H	0.1741788	3.0597788	-1.1162475
C	-1.1929104	2.3892881	0.4177271
H	-0.4131141	2.2405097	1.1662626
P	-4.4940819	3.3012795	-2.7277990
C	-7.6898962	0.9871530	-2.3929221
C	-6.7199734	0.0503042	-2.1073028
N	-5.4677578	0.6191076	-2.4262616
N	-7.0756482	2.1496646	-2.8142136
C	-5.6684375	1.9747362	-2.7006271
C	-6.9070901	-1.1508656	-1.2919291
C	-9.1428049	0.8580056	-1.9999165
C	-4.3363893	-0.2480561	-3.0193618
C	-7.7533820	3.4594900	-3.1859490
H	-2.8007405	1.7834960	1.7334103
H	-4.5732280	2.1371469	0.0488452
C	-9.2335602	3.2472121	-3.5378431
C	-7.0839075	4.0189169	-4.4539046
C	-7.6608444	4.4299334	-1.9940089
C	-4.9772245	-1.4981337	-3.6593829
C	-3.3420858	-0.6754912	-1.9299148
C	-3.6063451	0.4903477	-4.1469000
H	-9.3700385	2.4860782	-4.3185260

H	-9.6048973	4.1963206	-3.9464441
H	-9.8577053	3.0080783	-2.6711816
H	-6.6171706	4.6320725	-1.7247988
H	-8.1848519	4.0126230	-1.1234626
H	-8.1422788	5.3799620	-2.2662782
H	-2.6146491	-1.3736886	-2.3703106
H	-3.8603924	-1.1820288	-1.1087491
H	-2.7919342	0.1832517	-1.5328177
H	-4.2907537	0.7800864	-4.9562881
H	-2.8589044	-0.2027930	-4.5577402
H	-3.0835335	1.3897086	-3.8062795
H	-5.7448568	-1.2239877	-4.3962175
H	-5.4097656	-2.1781566	-2.9181272
H	-4.1872295	-2.0507693	-4.1849674
H	-7.2188976	3.3281313	-5.2988446
H	-6.0117601	4.2090005	-4.3236390
H	-7.5642677	4.9730588	-4.7107301
C	-8.5409314	-2.6629251	-0.4654149
C	-9.5114396	-0.3792731	-4.0563556
O	-6.0645387	-1.6871228	-0.5882243
O	-8.1951587	-1.6072509	-1.3887225
H	-9.5945936	-2.8853043	-0.6614694
H	-8.4054754	-2.3252631	0.5702748
H	-7.9155072	-3.5475113	-0.6412003
O	-9.5440295	1.2915085	-0.9415446
O	-9.9982016	0.2443626	-2.8484400
H	-10.4069703	-0.5994124	-4.6467936
H	-8.9800433	-1.3071214	-3.8106127
H	-8.8522961	0.2926633	-4.6226776

carbene-phosphinidene adduct $R_2=C_6H_5$ $R_1=C(CH_3)_3$

65

Energy = -1576.2863340590

C	3.0404112	-9.1246408	-0.6934301
N	3.0944389	-10.1563019	-1.6223509
N	3.7974028	-9.5422172	0.3945274
C	3.8393256	-11.2190087	-1.0911405
C	2.4668113	-10.2379536	-3.0287977
C	4.2724763	-10.8393159	0.1559261
C	4.1218582	-12.5713733	-1.6495425
C	5.0552728	-11.7558500	1.0331445
C	4.1260396	-8.7930353	1.7013966
C	5.6599764	-8.7477089	1.8477151
C	3.4595060	-9.5506153	2.8644772

C	3.6484604	-7.3358759	1.7871006
C	3.5987265	-10.5250520	-4.0345616
C	1.7601914	-8.9702353	-3.5305446
C	1.4106725	-11.3577021	-3.0141595
H	0.9122976	-11.3800576	-3.9928828
H	0.6472017	-11.1483665	-2.2524377
H	1.8374867	-12.3489130	-2.8360189
H	3.1749325	-10.4962196	-5.0473113
H	4.0646427	-11.5046682	-3.8989228
H	4.3729690	-9.7466498	-3.9740592
H	1.4237129	-9.2173380	-4.5519938
H	2.4198093	-8.0992327	-3.5819801
H	0.8884427	-8.6986715	-2.9298931
H	4.0625154	-6.6997434	0.9993504
H	4.0147330	-6.9725756	2.7620330
H	2.5603343	-7.2389320	1.7613707
H	3.8637830	-10.5570544	3.0064995
H	2.3743612	-9.6127493	2.7046031
H	3.6322516	-8.9879321	3.7922351
H	6.1149367	-8.2657818	0.9711024
H	6.1138979	-9.7311531	1.9919446
H	5.9037161	-8.1379040	2.7282198
C	3.2596177	-13.6453054	-1.3710030
C	5.3196328	-12.8394932	-2.3332422
C	3.5646557	-14.9394167	-1.7971813
H	2.3431633	-13.4622839	-0.8082102
C	4.7464651	-15.1864914	-2.4991149
H	2.8783923	-15.7571703	-1.5725185
C	5.6264068	-14.1331315	-2.7598212
H	4.9856853	-16.1970883	-2.8324275
H	6.5599813	-14.3184631	-3.2929168
H	6.0168788	-12.0240251	-2.5305848
C	4.3979508	-12.6448668	1.9002339
C	6.4509110	-11.8569494	0.9076122
C	5.1174079	-13.5783687	2.6494006
C	7.1717536	-12.7896708	1.6554767
C	6.5076858	-13.6496787	2.5343319
H	3.3111167	-12.6068611	1.9811207
H	7.0700368	-14.3788207	3.1190356
H	4.5867476	-14.2569194	3.3185665
H	8.2556635	-12.8482905	1.5461574
H	6.9743812	-11.1951879	0.2163803
C	-2.0387186	-8.4625195	0.9299418
C	-1.6844287	-7.2026610	0.4228665
C	-1.0830344	-9.4826095	0.8949458
C	0.1909382	-9.2585527	0.3690863

C	0.5747799	-7.9928925	-0.1508002
C	-0.4172985	-6.9723274	-0.1013999
H	-0.1732410	-5.9791108	-0.4889975
H	-2.4109206	-6.3865860	0.4370377
H	-1.3314771	-10.4737826	1.2834023
H	-3.0330893	-8.6407610	1.3402694
H	0.9044137	-10.0865715	0.3626087
P	2.1660080	-7.5268538	-0.8759051

Selenourea R_2=H R_1=H

10
Energy = -2628.184125121

C	-5.3822171	0.8837357	-0.0000000
C	-4.0238814	0.9651177	-0.0000000
N	-3.5483368	-0.3395759	0.0000000
N	-5.6984594	-0.4684189	-0.0000000
C	-4.5723760	-1.2563953	-0.0000000
H	-3.3698535	1.8275589	0.0000000
H	-6.1346029	1.6617322	0.0000000
H	-2.5788440	-0.6344606	-0.0000000
H	-6.6258428	-0.8768569	0.0000000
Se	-4.4631461	-3.0796667	0.0000000

Selenourea R_2=NH_2 R_1=H

14
Energy = -2738.935470429

C	-4.0309069	1.2791820	0.0000000
C	-4.5763116	-0.9537233	0.0000000
C	-5.3985907	1.1926062	0.0000000
N	-3.5573629	-0.0375515	0.0000000
N	-5.7023205	-0.1730374	-0.0000000
H	-2.5883158	-0.3324397	0.0000000
H	-6.6266368	-0.5879288	-0.0000000
N	-6.3871501	2.1647653	-0.0000000
H	-6.1578208	3.1455150	0.0000000
H	-7.3636566	1.9155811	0.0000000
N	-3.1726884	2.3679996	0.0000000
H	-2.1725464	2.2434408	-0.0000000
H	-3.5235881	3.3119970	-0.0000000
Se	-4.4601943	-2.7843062	-0.0000000

Selenourea R_2=H R_1=OH

12
Energy = -2778.564213131

C	-3.9248779	0.7308751	0.0000000
C	-4.5295509	-1.4999896	0.0000000
C	-5.2952248	0.6809837	-0.0000000

N	-3.4984909	-0.5781062	-0.0000000
N	-5.6249234	-0.6557341	0.0000000
H	-6.0273638	1.4788841	-0.0000000
H	-3.2528170	1.5801247	-0.0000000
O	-6.9022128	-1.1903308	-0.0000000
H	-7.4940135	-0.4118393	0.0000000
O	-2.1856117	-1.0182351	-0.0000000
H	-1.6520194	-0.1987308	-0.0000000
Se	-4.4634140	-3.3149016	-0.0000000

Selenourea R_2=H R_1=NH_2

14
Energy = -2738.889132896

C	-4.0563560	0.8585228	0.0003608
C	-4.8268803	-1.2908740	0.0269744
C	-5.4169517	0.9149804	0.0240483
N	-3.7097114	-0.4849464	-0.0035094
N	-5.8734651	-0.3950446	0.0457799
H	-6.1048535	1.7498007	0.0282554
H	-3.3019749	1.6338384	-0.0155838
N	-7.2323417	-0.7383940	0.0688690
H	-7.3985373	-1.2466852	0.9470222
H	-7.3654579	-1.4427785	-0.6688192
N	-2.3837476	-0.9395315	-0.0239437
H	-2.2623470	-1.4719578	-0.8950684
H	-2.3063862	-1.6417138	0.7237572
Se	-4.9031595	-3.1184565	0.0391671

Selenourea R_2=H R_1=CH_3

16
Energy = -2706.832547867

C	-5.4761523	0.7713350	0.0000000
C	-4.1160999	0.8466059	-0.0000000
N	-3.6326911	-0.4534121	-0.0000000
N	-5.8129967	-0.5740203	0.0000000
C	-4.6764131	-1.3530356	-0.0000000
H	-6.2246601	1.5538074	0.0000000
H	-3.4585363	1.7068468	-0.0000000
C	-2.2361124	-0.8510725	-0.0000000
H	-1.6148506	0.0517440	-0.0000000
H	-2.0181806	-1.4591952	-0.8883080
H	-2.0181806	-1.4591952	0.8883080
C	-7.1571479	-1.1236848	-0.0000000
H	-7.8743638	-0.2949520	-0.0000000
H	-7.3065112	-1.7521181	0.8881681
H	-7.3065112	-1.7521181	-0.8881681
Se	-4.5752023	-3.1827853	0.0000000

Selenourea R_2=F R_1=H

```
10
Energy = -2826.733951801
C    -5.4456060    0.8952040    0.0000000
C    -4.0952008    1.0225688   -0.0000000
N    -3.5659388   -0.2617890   -0.0000000
N    -5.7245379   -0.4655934   -0.0000000
C    -4.5651083   -1.2127051    0.0000000
H    -2.5810136   -0.5050042    0.0000000
H    -6.6464873   -0.8886969   -0.0000000
F    -6.4113060    1.8071808   -0.0000000
F    -3.3179396    2.0990909    0.0000000
Se   -4.3932517   -3.0248159   -0.0000000
```

Selenourea R_2=Cl R_1=H

```
10
Energy = -3547.504626047
C    -4.0759100    1.0326135   -0.0000000
C    -4.4885213   -1.2209367    0.0000000
C    -5.4314926    0.8668423    0.0000000
N    -3.5185619   -0.2425482   -0.0000000
N    -5.6654941   -0.5048681   -0.0000000
H    -2.5276129   -0.4599776    0.0000000
H    -6.5750279   -0.9543765    0.0000000
Cl   -6.6815958    2.0191048   -0.0000000
Cl   -3.1402884    2.4521402    0.0000000
Se   -4.2672350   -3.0267338   -0.0000000
```

Selenourea R_2=CHO R_1=H

```
14
Energy = -2854.951281781
C    -5.6279272    1.1489054   -0.0000000
C    -4.2633451    1.4207499   -0.0000000
N    -3.6259296    0.2035496   -0.0000000
N    -5.7499521   -0.2196241    0.0000000
C    -4.5193779   -0.8545234    0.0000000
H    -2.6155438    0.0845630   -0.0000000
H    -6.6376512   -0.7166325    0.0000000
C    -3.5374648    2.6865157    0.0000000
C    -6.7838107    2.0394822   -0.0000000
O    -7.9320297    1.6137299    0.0000000
H    -6.5566673    3.1289240   -0.0000000
O    -2.3138464    2.7335122    0.0000000
H    -4.1649372    3.6056123    0.0000000
Se   -4.1665970   -2.6257544   -0.0000000
```

Selenourea R_2=H R_1=Cl

```
10
Energy = -3547.413316995
C    -3.9859005    0.7722487   -0.0000000
C    -4.6132890   -1.4642204   -0.0000000
C    -5.3446307    0.7404112    0.0000000
N    -3.5609491   -0.5513537    0.0000000
N    -5.7070774   -0.6015832   -0.0000000
H    -6.0758591    1.5374950    0.0000000
H    -3.2928894    1.6026865    0.0000000
Cl   -7.3042842   -1.1457197   -0.0000000
Cl   -1.9400474   -1.0200436   -0.0000000
Se   -4.5711231   -3.2683008    0.0000000
```

Selenourea R_2=H R_1=COOH

```
16
Energy = -3005.535902971
C    -4.0001561    0.4348956   -0.0050214
C    -4.5208747   -1.7842215   -0.0019132
C    -5.3447172    0.3413354   -0.0068491
N    -3.4856024   -0.8687776   -0.0019485
N    -5.6730864   -1.0210275   -0.0049270
C    -7.0813752   -1.4195916   -0.0055270
C    -2.0352840   -1.0658250    0.0014874
O    -1.3228100   -0.0934121   -0.0001603
O    -7.9238510   -0.5573712   -0.0095023
O    -7.3196197   -2.7185654   -0.0012403
H    -6.4623297   -3.2619532    0.0009604
O    -1.6158093   -2.3178557    0.0065702
H    -2.3871398   -2.9769812    0.0064514
H    -6.1276816    1.0874347   -0.0090522
H    -3.3284224    1.2826283   -0.0052563
Se   -4.3903706   -3.6282820    0.0011482
```

Selenourea R_1=CH_3 R_2=SH

```
18
 Energy =   -3503.3417192240
 C    0.4924239    8.6211550   24.1264502
 N    0.6856703    7.6697980   25.1232145
 C    0.1184534    6.4643095   24.7556156
 C   -0.4452970    6.6301670   23.5109593
 N   -0.2086157    7.9689308   23.1442523
 C    1.3916121    7.9167604   26.3698912
 C   -0.6437855    8.5838461   21.9019870
 H    1.6894061    8.9733030   26.3635747
 H    2.2846143    7.2798751   26.4367118
 H    0.7319886    7.7197799   27.2260993
 H   -1.7371779    8.5342767   21.8142117
 H   -0.1896397    8.0755480   21.0408380
 H   -0.3150142    9.6301477   21.9331369
 S    0.1931254    5.0594614   25.7939777
```

```
 S   -1.3892937    5.4864999   22.5993845
 H   -0.5222341    4.3075909   24.9159924
 H   -0.4136496    5.0080402   21.7754026
Se    1.0646431   10.3645305   24.1496803
```

Selenourea R_1=CH_3 R_2=COH

```
20
 Energy =   -2933.5799080590
 C   -0.1945083   -0.5981639    0.0695999
 N    0.2463815   -1.5742279    0.9488366
 C   -0.3666509   -2.7926903    0.6894644
 C   -0.0861856   -3.9779195    1.5171311
 C   -1.2200454   -2.5888664   -0.3935282
 C   -2.0840149   -3.5046422   -1.1587312
 N   -1.1060222   -1.2508255   -0.7442315
 C    1.2089776   -1.3067668    2.0122231
 C   -1.8112481   -0.5866893   -1.8356285
 H   -2.8961335   -0.6273017   -1.6737138
 H   -1.5595504   -1.0513287   -2.7975348
 H   -1.4781813    0.4589843   -1.8332068
 H    1.4571075   -0.2395104    1.9480131
 H    2.1190638   -1.9039024    1.8684860
 H    0.7691933   -1.5267307    2.9936592
 O   -2.0870346   -4.7183239   -1.0693766
 O   -0.7160042   -5.0193240    1.4998686
 H   -2.7609840   -2.9819959   -1.8774314
 H    0.7811544   -3.8437638    2.2082162
Se    0.3171054    1.1527889   -0.0035555
```

Selenourea R_1=CH_3 R_2=C_6H_5

```
36
 Energy =   -3169.1206996230
 C   -0.2005518   -1.0496581    0.1928219
 N    0.0360941   -1.9478537    1.2087898
 C   -0.6676732   -3.1363954    0.9893212
 C   -0.6442011   -4.2825777    1.9094796
 C   -1.3672799   -2.9733683   -0.1885873
 C   -2.2512865   -3.9170825   -0.8877741
 N   -1.0655344   -1.6927357   -0.6636269
 C    0.8244881   -1.6106140    2.3835362
 C   -1.4851723   -1.1149405   -1.9308639
 H   -2.3407382   -0.4385152   -1.7921160
 H   -1.7586618   -1.9195173   -2.6212356
 H   -0.6497092   -0.5255935   -2.3295380
 H    0.6612354   -0.5493220    2.6098056
 H    1.8978650   -1.7552791    2.1939894
 H    0.5093943   -2.2408713    3.2218603
 C   -1.8186279   -5.2289742   -1.1586615
 C   -1.8486033   -4.8533516    2.3620621
 C   -3.5487836   -3.5416557   -1.2863662
```

```
 C    0.5708081   -4.8449374    2.3464964
 C   -4.3845345   -4.4497692   -1.9374359
 C   -3.9439155   -5.7509622   -2.1973185
 C   -2.6596704   -6.1370407   -1.8025359
 H   -0.8121653   -5.5286129   -0.8646161
 H   -2.3061522   -7.1490454   -2.0053418
 H   -4.5980606   -6.4597392   -2.7068578
 H   -5.3879524   -4.1418083   -2.2348217
 H   -3.9104780   -2.5361102   -1.0663724
 C   -1.8370056   -5.9550908    3.2174582
 H   -2.7965532   -4.4199764    2.0422444
 C    0.5785690   -5.9422044    3.2081032
 C   -0.6246554   -6.5019865    3.6469796
 H    1.5300972   -6.3667504    3.5315341
 H    1.5153047   -4.4305693    1.9909536
 H   -0.6170110   -7.3590132    4.3216806
 H   -2.7811145   -6.3819935    3.5591116
Se    0.4894561    0.6420059    0.0178421
```

Selenourea R_1=CH_3 R_2=Br

```
16
 Energy =   -7854.5114028830
 C    0.5609315    8.4959987   24.0856505
 N    0.7360257    7.6100567   25.1343992
 C    0.1556548    6.3873001   24.8190788
 C   -0.3873068    6.4973252   23.5705619
 N   -0.1371125    7.7925963   23.1237537
 C    1.4248674    7.9323783   26.3732981
 C   -0.5252497    8.3750079   21.8490126
 H    1.7551247    8.9750116   26.2842632
 H    2.2922066    7.2735462   26.5112330
 H    0.7440195    7.8255843   27.2279650
 H   -1.0688516    7.6222821   21.2692766
 H    0.3711223    8.7018855   21.3060297
 H   -1.1591900    9.2537270   22.0248099
Br    0.1711114    4.9181393   25.9699481
Br   -1.3049981    5.2049728   22.5855705
Se    1.1206849   10.2343679   23.9646791
```

Selenourea R_1=CH_3 R_2=CH_3

```
22
 Energy =   -2785.4961363050
 C    0.5625034    8.4770202   24.1071636
 N    0.7392737    7.5976469   25.1505208
 C    0.1623665    6.3623507   24.8527790
 C   -0.3873534    6.4619348   23.6029532
 N   -0.1347863    7.7675594   23.1571172
 C    1.4285253    7.9318672   26.3827668
 C   -0.5149610    8.3675178   21.8892918
 C   -1.1264278    5.4208813   22.8235502
```

C	0.1932695	5.2094715	25.7946950
H	1.7640119	8.9733426	26.2882908
H	2.2983913	7.2770882	26.5324909
H	0.7518928	7.8410212	27.2442230
H	-1.0814496	7.6447509	21.2943012
H	0.3829335	8.6816248	21.3396180
H	-1.1258748	9.2621075	22.0707725
H	-0.3198118	4.3480500	25.3502864
H	-0.3075207	5.4409751	26.7483903
H	1.2224279	4.8980108	26.0341758
H	-1.4390579	5.7903594	21.8403996
H	-2.0365067	5.0936509	23.3480537
H	-0.5042152	4.5307996	22.6484006
Se	1.1246293	10.2246594	23.9805594

Selenourea R_1=CH_3 R_2=Cl

16
Energy = -3626.1536605630

C	0.5573906	8.4847755	24.0864022
N	0.7319723	7.5991702	25.1348361
C	0.1515821	6.3757274	24.8204805
C	-0.3914576	6.4857108	23.5719920
N	-0.1402799	7.7813400	23.1253184
C	1.4196073	7.9136708	26.3758202
C	-0.5320462	8.3559450	21.8484594
H	1.7524386	8.9560617	26.2936753
H	2.2858017	7.2526223	26.5108246
H	0.7371742	7.8040884	27.2289106
H	-1.0735392	7.5980671	21.2731519
H	0.3623996	8.6842333	21.3029163
H	-1.1687366	9.2336149	22.0203911
Cl	0.1695753	5.0393582	25.8755528
Cl	-1.2300669	5.3128669	22.6657154
Se	1.1172448	10.2229075	23.9650535

Selenourea R_1=CH_3 R_2=$COOCH_3$

28
Energy = -3162.8003079040

C	0.5580781	8.3658975	24.0762089
N	0.4695978	7.6312043	25.2449004
C	-0.1662862	6.4178877	25.0055059
C	-0.4843522	6.3859630	23.6646648
N	-0.0400395	7.5744739	23.1088929
C	1.0570549	8.0717746	26.5054265
C	-0.2262276	8.0045151	21.7280392
H	1.5864783	9.0086906	26.2917891
H	1.7593487	7.3158146	26.8789859
H	0.2744279	8.2411583	27.2533472
H	-1.2883104	7.9535339	21.4572157
H	0.3543166	7.3695396	21.0498549

H	0.1285266	9.0408616	21.6719772
C	-0.3760639	5.3308093	25.9866880
C	-1.2460647	5.3386880	22.9371728
O	-0.5854184	5.8159671	27.2403616
O	-0.7041109	5.0981758	21.7144238
C	-1.3996977	4.0983753	20.9299971
O	-2.2303556	4.7801243	23.3746370
O	-0.3640929	4.1487098	25.7051995
C	-0.7844428	4.8019895	28.2545225
H	-1.7021497	4.2364740	28.0490482
H	-0.8685744	5.3493925	29.1982745
H	0.0670983	4.1101503	28.2762545
H	-0.8809804	4.0737455	19.9670637
H	-2.4531753	4.3771051	20.8016480
H	-1.3428612	3.1223984	21.4279996
Se	1.3049667	10.0227904	23.8491807

Selenourea R_1=CH_3 R_2=F

16
Energy = -2905.3843741360

C	0.5512369	8.4592453	24.0917975
N	0.7241802	7.5691384	25.1386969
C	0.1418220	6.3529329	24.8159060
C	-0.3968700	6.4673904	23.5767962
N	-0.1472328	7.7578714	23.1295849
C	1.4081280	7.8674836	26.3868489
C	-0.5506797	8.3077491	21.8447630
H	1.7434002	8.9102837	26.3116163
H	2.2728528	7.2043915	26.5203621
H	0.7232759	7.7548168	27.2375573
H	-1.0893480	7.5345947	21.2872245
H	0.3373580	8.6304043	21.2859724
H	-1.1960451	9.1812876	22.0034433
F	0.1713125	5.3218449	25.6577044
F	-1.0586253	5.5829513	22.8341318
Se	1.1142946	10.1977941	23.9771245

Selenourea R_1=CH_3 R_2=H

16
Energy = -2706.8324856230

C	0.5418087	8.4314056	24.0943732
N	0.7103703	7.5391229	25.1350736
C	0.1308301	6.3186857	24.8204417
C	-0.4079868	6.4348990	23.5759533
N	-0.1544396	7.7261483	23.1378099
C	1.3981443	7.8526807	26.3753369
C	-0.5504576	8.2897691	21.8589069
H	1.7340990	8.8956760	26.3017319
H	2.2664586	7.1934591	26.5106104
H	0.7170410	7.7436275	27.2303668
H	-1.0900896	7.5234371	21.2907388

H	0.3374284	8.6177672	21.3017407
H	-1.1941061	9.1654031	22.0175156
H	0.1500942	5.4777776	25.5025105
H	-0.9455992	5.7164729	22.9698075
Se	1.1054643	10.1738482	23.9766223

Selenourea R_1=CH_3 R_2=I

16
Energy = -3301.3364258470

C	0.5664568	8.5117306	24.0846186
N	0.7406473	7.6259495	25.1329782
C	0.1593955	6.4006400	24.8201689
C	-0.3851468	6.5113422	23.5678326
N	-0.1316964	7.8088886	23.1229643
C	1.4315681	7.9553846	26.3690500
C	-0.5159481	8.3987256	21.8501281
H	1.7583836	8.9987790	26.2782752
H	2.3016065	7.3004968	26.5076139
H	0.7540684	7.8478578	27.2261234
H	-1.0582169	7.6486807	21.2651746
H	0.3809875	8.7277629	21.3092270
H	-1.1513907	9.2764187	22.0262172
I	0.1734732	4.7681636	26.0931938
I	-1.4015203	5.0690681	22.4837295
Se	1.1263722	10.2503214	23.9622145

Selenourea R_1=CH_3 R_2=$COCH_3$

26
Energy = -3012.2563495190

C	0.3615583	8.5830820	24.2683101
N	0.4304257	7.6456857	25.2818776
C	-0.1352346	6.4348147	24.8635567
C	-0.5555004	6.6285721	23.5561291
N	-0.2615493	7.9284897	23.2150229
C	0.9210931	7.9850910	26.6106961
C	-0.5260977	8.5516449	21.9211087
H	1.2216092	9.0404136	26.5699304
H	1.7884621	7.3706015	26.8798715
H	0.1279156	7.8590233	27.3590042
H	-1.6050982	8.5790374	21.7360945
H	-0.0347730	7.9831961	21.1212286
H	-0.1125199	9.5655356	21.9691348
C	-0.3398555	5.1874507	25.6208417
C	-1.2702163	5.7062005	22.6087937
C	0.4421464	4.8952586	26.8846067
H	0.2773744	3.8445687	27.1470991
H	0.0940827	5.5228880	27.7180282
H	1.5172151	5.0838758	26.7554162
C	-0.6543841	4.3668038	22.2845652
H	0.0621064	4.0248724	23.0369498

H	-0.1312403	4.4759661	21.3194707
H	-1.4474974	3.6213606	22.1530830
O	-2.2736761	6.1165192	22.0415630
O	-1.1408203	4.3598817	25.1802032
Se	0.9579941	10.3122361	24.2939642

Selenourea R_1=CH_3 R_2=NH_2

20
Energy = -2817.5986682590

C	-0.2980874	-0.5991373	0.0756339
N	0.1852233	-1.5772198	0.9272867
C	-0.3562821	-2.8153616	0.5991538
N	-0.0976121	-3.9505629	1.3746489
C	-1.1952336	-2.6289725	-0.4694638
N	-1.9559231	-3.5241344	-1.2356979
N	-1.1480263	-1.2533566	-0.7753691
C	1.1035614	-1.3275678	2.0223291
C	-1.8922087	-0.6087341	-1.8413397
H	-2.8540523	-0.2207562	-1.4734765
H	-2.0732874	-1.3429908	-2.6344989
H	-1.2967531	0.2365851	-2.2079455
H	0.9985738	-0.2728322	2.3066437
H	2.1474230	-1.5001844	1.7191839
H	0.8472144	-1.9868577	2.8610065
H	-1.4479541	-4.3506494	-1.5455464
H	-2.8562564	-3.7883129	-0.8361033
H	-0.7009695	-4.7282578	1.1107288
H	0.8770641	-4.2562096	1.3563754
Se	0.1177363	1.1927429	0.0998804

Selenourea R_1=CH_3 R_2=NO_2

20
Energy = -3116.0557007120

C	-0.2516430	-0.5920733	0.0933544
N	0.2081648	-1.5693046	0.9735693
C	-0.3716072	-2.7795361	0.6692824
N	-0.1198552	-3.9901139	1.4192286
C	-1.2131577	-2.5816398	-0.4029101
N	-2.0260606	-3.5450772	-1.1111196
N	-1.1367410	-1.2536419	-0.7549360
C	1.1050085	-1.2888285	2.0943882
C	-1.8069974	-0.6093734	-1.8841212
H	-2.8858228	-0.5606343	-1.7022446
H	-1.6177117	-1.1731547	-2.8052509
H	-1.3821321	0.3987104	-1.9576839
H	1.2324948	-0.2003317	2.1189701
H	2.0676091	-1.7870124	1.9396462
H	0.6572433	-1.6429359	3.0305333
O	-3.1148626	-3.1380940	-1.5390873
O	-1.5688790	-4.6810355	-1.2383799
O	1.0350268	-4.1482805	1.8378182

```
 O   -1.0698815   -4.7544197    1.5880881
Se    0.2054647    1.1671071    0.0584148
```

Selenourea R_1=CH_3 R_2=OH

```
18
 Energy =   -2857.3477796950
 C    0.5666131    8.4518718   24.0780331
 N    0.7149826    7.5487031   25.1201119
 C    0.1320508    6.3396613   24.7841236
 C   -0.3970315    6.4617711   23.5346448
 N   -0.1015266    7.7645598   23.0967981
 C    1.3719346    7.8334086   26.3846337
 C   -0.4611661    8.3223719   21.8063660
 H    1.7166181    8.8739923   26.3302456
 H    2.2268345    7.1605357   26.5318220
 H    0.6680753    7.7145376   27.2190700
 H   -0.7313152    7.4987802   21.1351602
 H    0.3983441    8.8742499   21.4053205
 H   -1.3024094    9.0244956   21.9025082
 O    0.1822432    5.3044431   25.6612949
 O   -0.9587712    5.4977545   22.7429762
 H   -0.1519102    4.5092514   25.2069106
 H   -1.9291155    5.6036338   22.7223128
Se    1.1250796   10.2006484   24.0132977
```

Selenourea R_1=CH_3 R_2=OCH_3G

```
24
 Energy =   -2935.9713770060
 C    0.5125733    8.5861851   24.1043358
 N    0.6825534    7.6244046   25.0832455
 C    0.1196344    6.4185191   24.6833370
 C   -0.4163537    6.6068433   23.4359736
 N   -0.1737543    7.9550251   23.1000494
 C    1.3571172    7.8358553   26.3523122
 C   -0.6143928    8.5984635   21.8761950
 H    1.6526773    8.8925647   26.3762134
 H    2.2459332    7.1950268   26.4277478
 H    0.6788591    7.6123810   27.1862390
 H   -1.5392584    8.1197268   21.5338990
 H    0.1541415    8.5305941   21.0908142
 H   -0.7859248    9.6597725   22.0958638
 O    0.2028120    5.3824260   25.5463690
 O   -1.1389516    5.7844398   22.6315061
 C   -0.5612512    4.2120093   25.2135845
 C   -0.3896328    5.1699989   21.5553466
Se    1.0783055   10.3359806   24.1406043
 H   -1.1054615    4.5520941   21.0014780
 H    0.4191840    4.5415811   21.9596002
 H    0.0399955    5.9295406   20.8850586
 H   -0.4367427    3.5293295   26.0603855
 H   -0.1768946    3.7379775   24.2978507
```

```
 H   -1.6231581    4.4629506   25.0799809
```

Selenourea R_1=C(CH$_3$)$_3$ R_2=H

```
34
 Energy =   -2942.7801711410
 C   -0.3273007   -0.6754150    0.2732272
 N    0.2008160   -1.6054411    1.1652670
 C   -0.0459784   -2.8883255    0.6903042
 C   -0.7104721   -2.7836840   -0.4826664
 N   -0.8853985   -1.4354839   -0.7541293
 C    0.9438819   -1.4654635    2.4775634
 C   -1.5726509   -0.9331706   -2.0037096
 C   -2.8343296   -0.1438372   -1.6173951
 C   -2.0008745   -2.1346864   -2.8616326
 C   -0.5852006   -0.0871462   -2.8247862
 C    1.2076896   -0.0235787    2.9214426
 C    2.3059147   -2.1696707    2.3106234
 C    0.0978393   -2.1613450    3.5621167
 H   -2.4842471   -1.7400565   -3.7645011
 H   -2.7323706   -2.7772541   -2.3509585
 H   -1.1452400   -2.7438294   -3.1862351
 H   -1.0790453    0.2508037   -3.7469177
 H    0.2934866   -0.6869313   -3.1041480
 H   -0.2520062    0.7897684   -2.2568220
 H    1.8109000    0.5321459    2.1966786
 H    1.7607855   -0.0835952    3.8716486
 H    0.2837154    0.5393640    3.0841544
 H    2.8894613   -1.6908218    1.5127950
 H    2.2045720   -3.2366902    2.0730962
 H    2.8732235   -2.0878943    3.2474947
 H   -0.0615952   -3.2275235    3.3522849
 H   -0.8832099   -1.6760491    3.6547714
 H    0.6121246   -2.0836521    4.5297811
 H   -3.3397345    0.1965429   -2.5324646
 H   -2.5800152    0.7293874   -1.0048580
 H   -3.5317435   -0.7829202   -1.0564716
 H    0.2657227   -3.7774631    1.2195107
 H   -1.0664297   -3.5671641   -1.1343591
Se   -0.3339106    1.1745604    0.3841948
```

Selenourea R_1=C(CH$_3$)$_3$ R_2=COH

```
38
 Energy =   -3169.5190993670
 C   -0.7789004   -0.8897607    0.5388458
 N   -0.1256101   -1.8530374    1.3030782
 C   -0.4158909   -3.1141023    0.7782508
 C   -0.5324508   -4.3999010    1.4961153
 C   -1.0797502   -2.9119130   -0.4328515
 C   -1.8317912   -3.9459634   -1.1764002
 N   -1.2182486   -1.5455925   -0.6199743
 C    0.8957349   -1.5673066    2.4060825
```

C	-1.5965812	-0.8638365	-1.9302311
C	-3.0675440	-0.4252610	-1.8688065
C	-1.3653457	-1.8346698	-3.1027092
C	-0.6637165	0.3333316	-2.1831224
C	1.6742084	-0.2771091	2.0904892
C	1.9354531	-2.7027986	2.4158248
C	0.1677931	-1.4584650	3.7525434
H	-1.4702215	-1.2615171	-4.0332420
H	-2.0954625	-2.6503546	-3.1551453
H	-0.3524420	-2.2597649	-3.0850632
H	-0.9266214	0.7672601	-3.1575719
H	0.3850580	0.0064726	-2.2266293
H	-0.7621513	1.1103556	-1.4187132
H	2.1407323	-0.3283871	1.0961427
H	2.4767282	-0.1918169	2.8356313
H	1.0551852	0.6222488	2.1427655
H	2.3739489	-2.8464545	1.4175329
H	1.5237679	-3.6468383	2.7776762
H	2.7467681	-2.4068033	3.0935085
H	-0.3451799	-2.3980577	3.9922779
H	-0.5595083	-0.6360206	3.7278806
H	0.9011446	-1.2509754	4.5443741
H	-3.3391052	0.0775821	-2.8077167
H	-3.2251054	0.2715202	-1.0360995
H	-3.7355771	-1.2890982	-1.7398011
Se	-1.2749175	0.7923218	1.0724278
O	-1.4679752	-5.1041197	-1.3126995
H	-2.8181552	-3.6084135	-1.5691239
O	-0.3855249	-4.5788582	2.6981130
H	-0.8391255	-5.2251860	0.8230504

Selenourea R_1=C(CH$_3$)$_3$ R_2=Br

34

Energy = -8090.4363539730

C	-0.7319061	-0.9959685	0.5136484
N	0.0257940	-1.9063179	1.2570607
C	-0.0351215	-3.1417304	0.6072913
Br	0.2829882	-4.8459965	1.3515618
C	-0.7136060	-2.9767050	-0.5693770
Br	-1.3892863	-4.4390032	-1.5515934
N	-1.0904835	-1.6358848	-0.6766036
C	0.9380539	-1.5029477	2.4250395
C	-1.5918346	-0.8955205	-1.9259327
C	-3.0577484	-0.4920890	-1.7047943
C	-1.5069164	-1.7709412	-3.1861020
C	-0.6739462	0.3124524	-2.1891362
C	1.7799638	-0.2844817	2.0012308
C	1.9456790	-2.6101557	2.7743274
C	0.0702694	-1.2246186	3.6619059
H	-1.6823197	-1.1036040	-4.0404759
H	-2.2687948	-2.5550415	-3.2180093
H	-0.5158932	-2.2246249	-3.3186185

H	-1.0527781	0.8447483	-3.0724617
H	0.3489773	-0.0268626	-2.4086922
H	-0.6491781	1.0141665	-1.3496543
H	2.4474246	-0.5543399	1.1701151
H	2.4028520	0.0165152	2.8542247
H	1.1647531	0.5713277	1.7064967
H	2.4945061	-2.9741218	1.8959173
H	1.4887850	-3.4592545	3.2899608
H	2.6776676	-2.1608322	3.4589539
H	-0.4980558	-2.1237577	3.9394200
H	-0.6281650	-0.4000500	3.4828620
H	0.7248163	-0.9613305	4.5049708
H	-3.4214944	0.0402167	-2.5954637
H	-3.1619035	0.1635042	-0.8326054
H	-3.6820480	-1.3855259	-1.5613341
Se	-1.3068206	0.6645553	1.0815471

Selenourea R_1=C(CH$_3$)$_3$ R_2=Cl

34

Energy = -3862.0821264590

C	-0.6501341	-0.9810665	0.4662766
N	0.0997970	-1.8924673	1.2167921
C	0.0803765	-3.1154300	0.5429907
Cl	0.5153729	-4.6622292	1.1420916
C	-0.5891257	-2.9502518	-0.6358951
Cl	-1.0468200	-4.2737881	-1.6253556
N	-1.0059261	-1.6203190	-0.7258346
C	0.9289476	-1.5163140	2.4530545
C	-1.5978318	-0.9008962	-1.9461138
C	-3.0486081	-0.5044879	-1.6295051
C	-1.6096441	-1.7899780	-3.1993915
C	-0.7056420	0.3061281	-2.2881876
C	1.8192187	-0.3095181	2.1016083
C	1.8863671	-2.6427007	2.8755478
C	-0.0258520	-1.2364110	3.6246168
H	-1.8980109	-1.1364390	-4.0338658
H	-2.3434144	-2.6004604	-3.1463187
H	-0.6226785	-2.2080419	-3.4343373
H	-1.1679313	0.8510458	-3.1228433
H	0.2888947	-0.0343970	-2.6111360
H	-0.5969309	0.9970926	-1.4458880
H	2.5357174	-0.5831715	1.3138466
H	2.3885753	-0.0284769	2.9981260
H	1.2379497	0.5587462	1.7751017
H	2.5347045	-2.9798654	2.0571135
H	1.3710036	-3.5058027	3.3079734
H	2.5329233	-2.2183388	3.6556546
H	-0.6152184	-2.1343839	3.8589637
H	-0.7062688	-0.4084215	3.3994993
H	0.5693730	-0.9774837	4.5120324
H	-3.4781652	0.0001292	-2.5066834
H	-3.0994659	0.1733945	-0.7700769

```
 H   -3.6516345   -1.3995941   -1.4197921
Se   -1.1956787    0.6999686    1.0155954
```

Selenourea R_1=C(CH$_3$)$_3$ R_2=CH$_3$

```
40
 Energy =   -3021.4192214990
 C   -0.6406778   -0.7912605    0.4317615
 N   -0.1547430   -1.7112990    1.3542023
 C   -0.5748421   -3.0000614    0.9713094
 C   -0.5657035   -4.2212001    1.8408635
 C   -1.2030687   -2.8932670   -0.2392625
 C   -1.9760863   -3.9900081   -0.9061257
 N   -1.1702858   -1.5381663   -0.6179130
 C    0.8878377   -1.4936777    2.4419087
 C   -1.5732289   -0.9503369   -1.9628623
 C   -2.9348331   -0.2487909   -1.8268838
 C   -1.6793638   -2.0351621   -3.0499014
 C   -0.4711689    0.0095685   -2.4540271
 C    1.4195107   -0.0557810    2.5453930
 C    2.1196518   -2.3563389    2.0827497
 C    0.2826485   -1.8570231    3.8108854
 H   -1.7741130   -1.5142719   -4.0117204
 H   -2.5590273   -2.6772992   -2.9450865
 H   -0.7746868   -2.6563434   -3.1015411
 H   -0.7826597    0.4280038   -3.4212888
 H    0.4699437   -0.5395356   -2.6059905
 H   -0.2972548    0.8346524   -1.7558708
 H    1.7881215    0.3243960    1.5862803
 H    2.2626344   -0.0907021    3.2530745
 H    0.6707966    0.6476238    2.9178524
 H    2.5744983   -1.9842837    1.1541124
 H    1.9024996   -3.4200929    1.9473640
 H    2.8655320   -2.2661082    2.8846754
 H    0.0073536   -2.9126190    3.9035647
 H   -0.6106135   -1.2447781    3.9959307
 H    1.0162711   -1.6332797    4.5979602
 H   -3.2250820    0.1798188   -2.7971947
 H   -2.8830331    0.5551105   -1.0819928
 H   -3.7110302   -0.9669593   -1.5244178
 H   -0.7790964   -5.1084146    1.2344760
 H   -1.3370027   -4.1609519    2.6265225
 H    0.3895367   -4.4091817    2.3424786
 H   -3.0047057   -3.6804624   -1.1383141
 H   -2.0502052   -4.8399121   -0.2187659
 H   -1.5200785   -4.3587725   -1.8336708
Se   -0.8688456    1.0349175    0.6920446
```

Selenourea R_1=C(CH$_3$)$_3$ R_2=COOCH$_3$

```
46
 Energy =   -3398.7240277000
```

C	0.3115075	-1.2259281	-0.1636258
N	0.2221462	-2.0068440	0.9965548
C	-0.8513652	-2.8792743	0.8667317
C	-1.0272539	-4.1747422	1.6253130
C	-1.4717854	-2.6120111	-0.3318178
C	-2.3489125	-3.6221197	-0.9665920
N	-0.8037669	-1.5407086	-0.9304079
C	1.1362443	-1.8808347	2.2124744
C	-1.3873825	-0.6559236	-2.0318194
C	-2.8679543	-1.0075072	-2.2616610
C	-0.5886814	-0.8639645	-3.3263924
C	-1.3690520	0.8145037	-1.5729230
C	1.2059114	-0.4036484	2.6415899
C	2.5144829	-2.4620554	1.8589617
C	0.5614512	-2.6549313	3.4085917
H	-1.0112791	-0.2308330	-4.1197437
H	-0.6444988	-1.9121072	-3.6485035
H	0.4631830	-0.5898651	-3.1791234
H	-1.8285082	1.4232642	-2.3635252
H	-0.3554433	1.1857481	-1.3929161
H	-1.9633708	0.9402842	-0.6563121
H	1.6098251	0.2397025	1.8535825
H	1.8585877	-0.3309159	3.5221082
H	0.2080307	-0.0388601	2.9262687
H	2.9793674	-1.9063987	1.0367425
H	2.4179115	-3.5183828	1.5734750
H	3.1666129	-2.4009376	2.7417164
H	0.6211221	-3.7415741	3.2922031
H	-0.4723236	-2.3594708	3.6356336
H	1.1686237	-2.3893223	4.2837449
H	-3.2873292	-0.2364783	-2.9210826
H	-3.4441702	-0.9882683	-1.3263568
H	-3.0093381	-1.9710771	-2.7581614
Se	1.7167711	-0.1493986	-0.6793829
O	-3.2582565	-4.1956906	-0.3893810
C	-2.7170907	-4.9718418	-2.8732981
O	-0.2495084	-5.0927945	1.4647086
O	-2.0681668	-4.3096235	2.4691808
O	-1.9515698	-3.9243359	-2.2297275
H	-2.2721945	-5.0839854	-3.8666221
H	-3.7742581	-4.6852968	-2.9494895
H	-2.6367042	-5.9050885	-2.3025652
C	-3.0513015	-3.2605430	2.6201513
H	-3.5789099	-3.4940663	3.5508326
H	-3.7399118	-3.2841417	1.7669223
H	-2.5766512	-2.2728520	2.6988628

Selenourea R_1=C(CH$_3$)$_3$ R_2=F

34

Energy = -3141.3286640760

C	-0.4502524	-0.8747477	0.3641309
N	0.3116571	-1.7792104	1.1112885

C	0.3965560	-2.9604830	0.3841862
F	1.0343383	-4.0677639	0.7667369
C	-0.2789526	-2.8089751	-0.7747983
F	-0.4217530	-3.7442574	-1.7141262
N	-0.8126910	-1.5269879	-0.8188416
C	0.9411920	-1.5183883	2.4775811
C	-1.6293644	-0.9330858	-1.9639166
C	-3.0285956	-0.5722034	-1.4394211
C	-1.8049224	-1.9480498	-3.1062275
C	-0.8759548	0.2813556	-2.5314845
C	1.9375298	-0.3551739	2.3484851
C	1.7197554	-2.7483848	2.9730723
C	-0.1785043	-1.2304712	3.4908209
H	-2.3932078	-1.4410342	-3.8825016
H	-2.3602269	-2.8425989	-2.7994878
H	-0.8519383	-2.2512448	-3.5567589
H	-1.4697598	0.7109779	-3.3504607
H	0.0969536	-0.0280228	-2.9395221
H	-0.7185581	1.0516568	-1.7682343
H	2.7470273	-0.6184044	1.6527601
H	2.3827851	-0.1624940	3.3347091
H	1.4452614	0.5592996	1.9989691
H	2.5516266	-3.0196366	2.3118344
H	1.0796314	-3.6258735	3.1255463
H	2.1455228	-2.4740932	3.9474345
H	-0.8507362	-2.0964821	3.5760855
H	-0.7631105	-0.3489202	3.2035347
H	0.2749523	-1.0500297	4.4755825
H	-3.6118370	-0.1390250	-2.2642398
H	-2.9767549	0.1570082	-0.6225326
H	-3.5504857	-1.4736725	-1.0872341
Se	-0.9029433	0.8551963	0.8526997

Selenourea R_1=$C(CH_3)_3$ R_2=C_6H_5

54

Energy = -3405.0462421510

C	-0.6873547	-1.1260042	0.7748788
N	-0.1721490	-2.0426526	1.6865279
C	-0.2685679	-3.3314859	1.1361144
C	-0.2082039	-4.6207678	1.8691197
C	-0.7554682	-3.2058425	-0.1418058
C	-1.3027439	-4.3351539	-0.9319655
N	-0.9582497	-1.8374311	-0.3892257
C	0.5551667	-1.6538730	2.9729311
C	-1.2095698	-1.1909886	-1.7503570
C	-2.6288381	-0.6009598	-1.7834257
C	-1.0711859	-2.2089651	-2.8931549
C	-0.1309778	-0.1197431	-2.0061236
C	1.6097770	-0.5780630	2.6455107
C	1.3294181	-2.8403140	3.5671931
C	-0.4690356	-1.1666239	4.0106343
H	-1.1122491	-1.6372695	-3.8303492

H	-1.8781105	-2.9472489	-2.9201717
H	-0.1082269	-2.7355432	-2.8670132
H	-0.3221363	0.3360727	-2.9874718
H	0.8662662	-0.5826333	-2.0327725
H	-0.1404944	0.6704942	-1.2479054
H	2.3500205	-0.9761780	1.9356582
H	2.1343950	-0.3130065	3.5740815
H	1.1617697	0.3287547	2.2265587
H	2.0231616	-3.2886478	2.8434526
H	0.6827769	-3.6244665	3.9719753
H	1.9278073	-2.4412293	4.3977174
H	-1.1600019	-1.9781460	4.2803781
H	-1.0438656	-0.3153624	3.6266398
H	0.0623468	-0.8541834	4.9215221
H	-2.7968740	-0.1208896	-2.7583463
H	-2.7619732	0.1467996	-0.9924037
H	-3.3792766	-1.3949205	-1.6614816
Se	-1.1234160	0.6481242	1.1115916
C	-2.6958583	-4.5118289	-1.0162838
C	-0.4682976	-5.2905634	-1.5307697
C	-3.2364404	-5.6028565	-1.6970143
C	-1.0091301	-6.3858194	-2.2083096
C	-2.3938402	-6.5434697	-2.2978724
H	0.6133955	-5.1631937	-1.4770995
H	-0.3444712	-7.1175143	-2.6701508
H	-2.8160488	-7.3977796	-2.8287565
H	-4.3194140	-5.7246588	-1.7505713
H	-3.3558651	-3.7886576	-0.5346878
C	-1.2230637	-4.9497207	2.7854840
C	-1.2256707	-6.1855329	3.4336601
C	0.7920984	-5.5689346	1.6070110
C	0.7894624	-6.8072763	2.2540054
C	-0.2169983	-7.1181577	3.1715111
H	-2.0234105	-6.4250513	4.1384043
H	-0.2201154	-8.0853143	3.6761924
H	-2.0182753	-4.2288417	2.9819980
H	1.5863592	-5.3237991	0.9009751
H	1.5774870	-7.5310415	2.0404623

Selenourea R_1=C(CH$_3$)$_3$ R_2=OH

36

Energy = -3093.2877169530

C	-0.4036268	-0.8584204	0.3249619
N	0.2540746	-1.8055124	1.1247757
C	0.1946109	-3.0287323	0.4734115
O	0.8296657	-4.1636333	0.8714914
C	-0.4916162	-2.8793196	-0.6883462
O	-0.4563001	-3.8470711	-1.6637865
N	-0.8562547	-1.5255200	-0.8063316
C	0.8377910	-1.5431932	2.5102197

C	-1.7183580	-0.9250149	-1.9036485
C	-3.0173066	-0.3691459	-1.2943883
C	-2.1257278	-1.9910217	-2.9360208
C	-0.9055693	0.1530756	-2.6400061
C	1.9796911	-0.5212883	2.3849143
C	1.4265248	-2.8239265	3.1252767
C	-0.2895566	-1.0652802	3.4417015
H	-2.7510835	-1.4859497	-3.6842180
H	-2.7528650	-2.7815585	-2.4927045
H	-1.2698099	-2.4350023	-3.4561695
H	-1.5287109	0.5978703	-3.4291326
H	-0.0173073	-0.2918564	-3.1108369
H	-0.5882185	0.9444243	-1.9508377
H	2.7786075	-0.9209147	1.7435969
H	2.4018317	-0.3392964	3.3835463
H	1.6275670	0.4295747	1.9702143
H	2.2718934	-3.2200268	2.5516769
H	0.6789336	-3.6164577	3.2489468
H	1.7925899	-2.5478115	4.1232612
H	-1.0503031	-1.8522040	3.5516722
H	-0.7668514	-0.1525521	3.0665091
H	0.1345984	-0.8586314	4.4343938
H	-3.6301502	0.0605569	-2.0995776
H	-2.8134996	0.4091376	-0.5508941
H	-3.5925781	-1.1768213	-0.8183291
Se	-0.6164430	0.9490562	0.7033412
H	-1.3579414	-4.1513998	-1.8744374
H	0.7160382	-4.7914532	0.1292237

Selenourea R_1=C(CH$_3$)$_3$ R_2=SH

36

Energy = -3739.2689767830

C	-0.5843223	-0.8682795	0.4169023
N	0.0907828	-1.8187180	1.2013575
C	-0.0419504	-3.0639949	0.5998858
S	0.3968466	-4.6324892	1.2782479
C	-0.7079660	-2.8948365	-0.5999161
S	-1.1672078	-4.2428660	-1.6208140
N	-1.0011631	-1.5167271	-0.7336055
C	0.9017978	-1.4690685	2.4539931
C	-1.5966826	-0.7920523	-1.9462745
C	-3.0088809	-0.3010486	-1.5843516
C	-1.7194085	-1.6914703	-3.1855179
C	-0.6472467	0.3497386	-2.3589679

C	1.9134900	-0.3637890	2.0954623
C	1.7310723	-2.6620836	2.9489333
C	-0.0591983	-1.0661159	3.5851256
H	-2.0249767	-1.0302124	-4.0084210
H	-2.4819594	-2.4701484	-3.0865046
H	-0.7686791	-2.1585603	-3.4709313
H	-1.1065256	0.8958924	-3.1946591
H	0.3113814	-0.0622514	-2.7058603
H	-0.4635316	1.0579776	-1.5453385
H	2.6188427	-0.7278993	1.3342687
H	2.4859588	-0.1114457	2.9987988
H	1.4238250	0.5441992	1.7293137
H	2.4002711	-3.0667502	2.1788498
H	1.1150947	-3.4680797	3.3665482
H	2.3613638	-2.2875436	3.7667857
H	-0.7364761	-1.8985044	3.8235989
H	-0.6522845	-0.1858262	3.3150080
H	0.5300035	-0.8363781	4.4847845
H	-3.4342157	0.2316913	-2.4469876
H	-2.9900992	0.3782650	-0.7246198
H	-3.6621173	-1.1557483	-1.3556254
Se	-0.9780091	0.8740223	0.9229653
H	-2.4413322	-4.4284296	-1.1703193
H	-0.2090875	-5.2521595	0.2188650

Selenourea R_1=C(CH$_3$)$_3$ R_2=I

34

Energy = -3537.2573616940

C	-0.7998861	-0.9693446	0.5550203
N	-0.0489861	-1.8823308	1.2961319
C	-0.2155021	-3.1471079	0.7178013
I	-0.0960373	-4.9916127	1.7190137
C	-0.9111972	-2.9889520	-0.4567808
I	-1.9169291	-4.5788883	-1.3939634
N	-1.1870789	-1.6257646	-0.6162970
C	0.9527156	-1.4863242	2.3872383
C	-1.5695801	-0.8918862	-1.9083638
C	-3.0381207	-0.4517736	-1.8167663
C	-1.3774074	-1.7947000	-3.1377802
C	-0.6184172	0.3026983	-2.1114655
C	1.6872214	-0.1936941	1.9836930
C	2.0499246	-2.5559508	2.5310833
C	0.1963997	-1.3213179	3.7131334
H	-1.4224990	-1.1457667	-4.0226072

H	-2.1603864	-2.5505710	-3.2441180
H	-0.3979435	-2.2918500	-3.1385328
H	-0.9040154	0.8110802	-3.0424911
H	0.4185920	-0.0473873	-2.2197658
H	-0.6684468	1.0287436	-1.2943945
H	2.2342569	-0.3380519	1.0405343
H	2.4195664	0.0337705	2.7699760
H	1.0162276	0.6633801	1.8784755
H	2.4647927	-2.8491615	1.5565731
H	1.7148762	-3.4533002	3.0576547
H	2.8632657	-2.1117919	3.1198098
H	-0.2998408	-2.2603998	3.9962452
H	-0.5575448	-0.5280156	3.6326814
H	0.9068124	-1.0553411	4.5086727
H	-3.3185739	0.0687127	-2.7439874
H	-3.1907994	0.2262759	-0.9685422
H	-3.6959650	-1.3248341	-1.7014809
Se	-1.3952741	0.6772474	1.1292691

Selenourea R_1=C(CH_3)$_3$ R_2=NH_2

38

Energy = -3053.5342665690

C	0.2146881	-1.1754325	0.0205619
N	0.1955861	-1.9192731	1.1871118
C	-0.8944595	-2.8271836	1.1200643
N	-1.3530157	-3.8015615	2.0254944
C	-1.5452763	-2.6022938	-0.0619550
N	-2.7642911	-3.2112760	-0.3768458
N	-0.8798156	-1.5918961	-0.7525572
C	1.1899884	-1.7603936	2.3269238
C	-1.2363520	-1.0205803	-2.1216659
C	-2.4800936	-1.6961846	-2.7247981
C	-0.0766245	-1.2749772	-3.1016510
C	-1.5695777	0.4734415	-1.9635822
C	1.1049305	-0.3232138	2.8736324
C	2.5984632	-2.1193424	1.8210533
C	0.8879113	-2.6948919	3.5113161
H	-0.3629065	-0.8933965	-4.0924794
H	0.1129381	-2.3549399	-3.1940783
H	0.8449790	-0.7775352	-2.7807227
H	-1.7956522	0.8962809	-2.9529655
H	-0.7294289	1.0269306	-1.5288619
H	-2.4561158	0.5986070	-1.3253427
H	1.3083841	0.4164730	2.0914508

H	1.8457300	-0.2014846	3.6768416
H	0.1067037	-0.1345344	3.2957821
H	2.9004749	-1.4721576	0.9894329
H	2.6286832	-3.1681904	1.4898441
H	3.3171655	-1.9990883	2.6445561
H	0.9767327	-3.7592107	3.2587629
H	-0.0890657	-2.5026914	3.9731228
H	1.6505872	-2.4816487	4.2730096
H	-2.6809991	-1.1851644	-3.6758342
H	-3.3693735	-1.6039438	-2.0923216
H	-2.3037080	-2.7538453	-2.9727596
Se	1.4617291	0.1282639	-0.4536560
H	-2.7962728	-3.6617068	-1.2897318
H	-2.9377062	-3.9029410	0.3596045
H	-1.6855624	-3.4340506	2.9169117
H	-0.6887183	-4.5525668	2.2108517

Selenourea R_1=C(CH$_3$)$_3$ R_2=NO$_2$

38

Energy = -3351.9879372020

C	0.3942582	-1.3391145	-0.1409652
N	0.3152512	-1.9928627	1.1144624
C	-0.7170009	-2.8959261	1.0440080
N	-0.9306375	-4.0259992	1.9732635
C	-1.3266717	-2.7950035	-0.1811186
N	-2.0251507	-3.9154323	-0.7754614
N	-0.6995033	-1.7704159	-0.8839278
C	1.1712576	-1.6543198	2.3454547
C	-1.3327492	-1.0052068	-2.0641109
C	-2.8111612	-1.4099311	-2.2069184
C	-0.5537105	-1.3354840	-3.3424765
C	-1.3261160	0.5025571	-1.7568828
C	1.1078060	-0.1355881	2.5859641
C	2.6018290	-2.1603752	2.1070992
C	0.6071554	-2.3264993	3.6054969
H	-1.0124452	-0.8040600	-4.1883823
H	-0.5875487	-2.4125071	-3.5471104
H	0.4917718	-1.0156976	-3.2546677
H	-1.8120686	1.0133363	-2.5989124
H	-0.3184633	0.9129164	-1.6447417
H	-1.9057553	0.7190796	-0.8480681
H	1.5093323	0.4394224	1.7458576
H	1.7051952	0.0914013	3.4793309
H	0.0727983	0.1809432	2.7795623

H	3.0614200	-1.6738182	1.2401945
H	2.6046261	-3.2482574	1.9539011
H	3.2061832	-1.9379399	2.9974549
H	0.7399849	-3.4142112	3.6132850
H	-0.4469492	-2.0752328	3.7797331
H	1.1809424	-1.9324834	4.4537862
H	-3.2745692	-0.7011203	-2.9050311
H	-3.3511753	-1.3248851	-1.2531943
H	-2.9467686	-2.4128555	-2.6185445
Se	1.7635403	-0.2837712	-0.7354012
O	-2.7766424	-4.5591038	-0.0325066
O	-0.1295108	-4.9559294	1.8730935
O	-1.8716370	-3.9431321	2.7516472
O	-1.7857072	-4.1786331	-1.9610731

Selenourea R_1=C(CH_3)$_3$ R_2=OCH_3

42

Energy = -3171.8994369900

C	-0.6791149	-0.7962069	0.3808553
N	-0.0290828	-1.7254671	1.1877326
C	-0.2867579	-3.0080930	0.6776588
O	0.0753202	-4.1316446	1.3479616
C	-0.9544774	-2.8713080	-0.5034124
O	-1.4177264	-3.8830937	-1.2830074
N	-1.1421352	-1.4917189	-0.7347847
C	0.8619938	-1.4884231	2.3987413
C	-1.5105387	-0.8466710	-2.0653093
C	-2.9231571	-0.2457302	-1.9779394
C	-1.4629902	-1.8715379	-3.2130672
C	-0.4611430	0.2273510	-2.4118041
C	1.4369469	-0.0635858	2.4440255
C	2.0872383	-2.4278070	2.3097946
C	0.0322837	-1.7621097	3.6626038
H	-1.5753574	-1.3043349	-4.1469776
H	-2.2742398	-2.6055054	-3.1798501
H	-0.5051817	-2.4048541	-3.2552932
H	-0.7359427	0.6819347	-3.3737901
H	0.5330530	-0.2295113	-2.5198155
H	-0.4138004	1.0172462	-1.6539475
H	1.9402715	0.1984482	1.5035821
H	2.1865744	-0.0481568	3.2492996
H	0.6777205	0.6954314	2.6427364
H	2.6105953	-2.2865621	1.3535509

H	1.8344992	-3.4844705	2.4182740
H	2.7820540	-2.1536551	3.1142805
H	-0.3260370	-2.7998943	3.6871291
H	-0.8295395	-1.0824235	3.7047529
H	0.6507999	-1.5927331	4.5555867
H	-3.1744305	0.2308086	-2.9367373
H	-2.9744204	0.5051174	-1.1792539
H	-3.6721500	-1.0265109	-1.7803166
Se	-1.1430255	0.9476746	0.8210042
C	-2.8383032	-4.1404554	-1.1788172
C	-0.9486603	-5.1238176	1.5518807
H	-3.0387142	-5.0035169	-1.8240209
H	-3.4272959	-3.2775786	-1.5230955
H	-3.1153027	-4.3738732	-0.1399722
H	-0.5225039	-5.8495023	2.2544872
H	-1.2005167	-5.6300788	0.6098941
H	-1.8492253	-4.6666306	1.9906003

Selenourea R_1=C(CH_3)$_3$ R_2=$COCH_3$

44

Energy = -3248.1857920420

C	0.2412087	-1.2787044	-0.2597382
N	0.2013838	-2.0056819	0.9309909
C	-0.9124738	-2.8439615	0.9145256
C	-1.0658490	-4.1248697	1.7202553
C	-1.6055859	-2.6024816	-0.2520202
C	-2.5504538	-3.6087165	-0.8403475
N	-0.9218576	-1.6024104	-0.9522771
C	1.1442221	-1.7963773	2.1138042
C	-1.5475902	-0.7368869	-2.0461935
C	-3.0108967	-1.1494123	-2.2644315
C	-0.7669644	-0.8928637	-3.3602688
C	-1.5701111	0.7288295	-1.5737847
C	1.2120832	-0.2936664	2.4488985
C	2.5207848	-2.3842462	1.7681533
C	0.6004304	-2.4891624	3.3734552
H	-1.2246619	-0.2509147	-4.1265784
H	-0.8015460	-1.9293459	-3.7244446
H	0.2809418	-0.5985342	-3.2295823
H	-2.0516673	1.3373015	-2.3516583
H	-0.5621049	1.1205950	-1.3991209
H	-2.1587904	0.8248334	-0.6502758
H	1.6044668	0.3016266	1.6188297
H	1.8742252	-0.1645637	3.3159152

H	0.2153975	0.0832053	2.7213056
H	2.9545980	-1.8836520	0.8949077
H	2.4340683	-3.4599087	1.5634821
H	3.1955686	-2.2469495	2.6249096
H	0.6737687	-3.5793998	3.3349325
H	-0.4344797	-2.1892620	3.5907523
H	1.2151713	-2.1514033	4.2179431
H	-3.4518883	-0.4301845	-2.9674681
H	-3.5962597	-1.1103440	-1.3364825
H	-3.1207443	-2.1405932	-2.7190746
Se	1.6225640	-0.2291148	-0.8858044
O	-3.5725676	-3.9479886	-0.2563663
C	-2.0889612	-4.3336067	-2.0922226
O	-0.2040843	-4.9857151	1.6190610
C	-2.3040248	-4.2885423	2.5562390
H	-1.3908281	-3.7509352	-2.7033961
H	-2.9545062	-4.6578295	-2.6831064
H	-1.5534171	-5.2362724	-1.7540214
H	-2.4026938	-3.4489113	3.2603192
H	-2.2684739	-5.2405400	3.0975427
H	-3.1869712	-4.2461688	1.8997216

NHC R_2=H R_1=SH

11
Energy = -1022.7433313120

C	0.6796012	8.4964604	23.8696488
N	1.1389401	7.5517051	24.7602875
C	0.6173040	6.2642704	24.5496051
H	0.8744702	5.4187461	25.1760808
C	-0.2035255	6.3714763	23.4772684
H	-0.8167017	5.6392838	22.9655947
N	-0.1430415	7.7192113	23.0849986
S	2.1966451	7.9352063	26.0635815
S	-1.0719673	8.3624455	21.7857930
H	3.3610636	7.7345045	25.3938388
H	-0.1362582	8.1934404	20.8158630

NHC R_2=H R_1=Br

9
Energy = -5373.8944113760

C	0.9013224	8.4422957	23.7648874
N	1.2870143	7.4523381	24.6106861
C	0.6852681	6.2127492	24.4005922
H	0.8941514	5.3322740	24.9956388
C	-0.1515222	6.4089449	23.3426641
H	-0.8233973	5.7351721	22.8251876

N	0.0156166	7.7501885	23.0028073
Br	2.5376502	7.7251289	25.9794060
Br	-0.9296237	8.5366585	21.5886604

NHC R_2=H R_1=CCH

13

Energy = -378.5861342800

C	0.8690647	8.1269328	23.8220202
N	1.1881973	7.1124954	24.7119359
C	0.5120077	5.8977536	24.4619128
H	0.6580205	5.0162936	25.0736009
C	-0.2681796	6.1217676	23.3835162
H	-0.9521659	5.4783311	22.8444197
N	-0.0416949	7.4656304	23.0118443
C	2.0682142	7.2751917	25.7291054
C	-0.6561504	8.0578767	21.9596295
C	2.8456636	7.3811034	26.6479685
C	-1.2222268	8.5526713	21.0137532
H	-1.7122676	9.0088055	20.1798770
H	3.5353870	7.4983869	27.4566565

NHC R_2=H R_1=COOCH$_3$

21

Energy = -682.2424168926

C	0.6773145	8.1929302	23.6443299
N	1.0965035	7.0733646	24.3306947
C	0.3356411	5.9161271	24.0512578
H	0.5345753	4.9545220	24.5046712
C	-0.6037986	6.2977634	23.1626377
H	-1.3940202	5.7379078	22.6810696
N	-0.3796308	7.6729380	22.9288525
C	2.2043018	7.1238578	25.2301109
C	-1.1532483	8.4872134	22.0470822
O	2.4349200	5.8776856	25.7125410
O	-2.1618310	7.7403829	21.5327488
C	-3.0208350	8.4594310	20.6166327
H	-3.7921291	7.7412605	20.3231152
H	-2.4487814	8.7956467	19.7426536
H	-3.4665350	9.3288816	21.1152198
C	3.5429366	5.8030362	26.6405377
H	3.6152624	4.7472558	26.9174324
H	3.3433741	6.4250669	27.5221121
H	4.4665416	6.1448171	26.1573258
O	2.8264902	8.1150430	25.5088831
O	-0.9387318	9.6460983	21.8061914

NHC R_2=H R_1=CHCH$_2$

17

Energy = -381.1274762042

C	0.8725864	8.4223617	23.7642398

N	1.3589521	7.3704961	24.5124173
C	0.6819082	6.1708759	24.2644037
H	0.9170046	5.2353681	24.7569362
C	-0.2623314	6.4521181	23.3337197
H	-0.9972344	5.8054315	22.8700720
N	-0.1339923	7.8151441	23.0426225
C	2.4272001	7.5566767	25.4103662
C	-0.9069387	8.5500974	22.1236124
C	-1.8793678	8.0643220	21.3456863
C	2.9732066	6.6181772	26.1899842
H	2.7718292	8.5902223	25.3978273
H	2.6351498	5.5826900	26.2092863
H	3.7988962	6.8835770	26.8463506
H	-0.6101930	9.5984390	22.1148010
H	-2.1798729	7.0170537	21.3436041
H	-2.4093826	8.7350792	20.6731003

NHC R_2=C_6H_5 R_1=H

29

Energy = -688.5764019568

C	0.6248836	8.1816823	24.0439304
N	1.2120946	7.3665464	24.9699920
C	0.4209951	6.2952609	25.4058705
C	-0.7700676	6.4351013	24.7211360
N	-0.5905958	7.5698408	23.9186859
H	2.1751247	7.4924349	25.2613504
H	-1.3282259	7.9553225	23.3397332
H	0.8680121	1.9333601	26.9689844
C	1.1114131	2.9884795	27.1045435
H	2.3262664	2.6471821	28.8630857
C	1.9329500	3.3867842	28.1645281
H	-0.0083480	3.6087943	25.3687716
C	0.6118786	3.9297972	26.2060395
C	2.2498559	4.7388052	28.3186603
C	0.9146842	5.2973815	26.3556547
C	1.7443930	5.6854433	27.4265291
H	2.8866458	5.0615584	29.1436140
H	1.9736903	6.7424562	27.5760568
H	-4.1671783	4.1483599	26.9309233
C	-3.7725361	4.5166211	25.9825033
H	-5.4437746	3.7830982	24.8188931
C	-4.4919716	4.3155586	24.7995814
H	-2.0155091	5.3772390	26.8911328
C	-2.5588602	5.2015909	25.9624107
C	-3.9842942	4.8057341	23.5937061
C	-2.0303012	5.6910700	24.7522971
C	-2.7652286	5.4847407	23.5680946
H	-4.5349749	4.6513945	22.6646449
H	-2.3638912	5.8366920	22.6156166

NHC R_2=Br R_1=H

9

```
 Energy =   -5373.9659470950
 C    1.0356301    8.8496208   23.7341571
 N    1.6266388    7.8049941   24.3955171
 C    0.9513454    6.5991028   24.2565992
Br    1.4964344    4.9877212   25.0354293
 C   -0.1312311    6.8720665   23.4662184
Br   -1.4877286    5.7392478   22.8520532
 N   -0.0485214    8.2269778   23.1728842
 H    2.4786303    7.9121538   24.9346242
 H   -0.7234879    8.7191351   22.5981775
```

NHC R_2=CCH R_1=H

```
13
 Energy =    -378.6403671320
 C    0.9638789    8.5868512   23.7693967
 N    1.4718402    7.5688493   24.5238730
 C    0.8235207    6.3360578   24.3577321
 C    1.1755574    5.1560609   25.0292762
 C   -0.1748476    6.5821861   23.4282552
 C   -1.1381431    5.7250255   22.8760046
 N   -0.0439626    7.9424309   23.1115819
 H    2.2559317    7.6945756   25.1546303
 H   -0.6487990    8.4107431   22.4456384
 C    1.5008427    4.1484488   25.6256519
 C   -1.9805609    4.9996424   22.3847533
 H   -2.7169790    4.3500300   21.9593692
 H    1.7772907    3.2536083   26.1437970
```

NHC R_2=$COOCH_3$ R_1=H

```
21
 Energy =    -682.2503370271
 C    0.9611350    8.4186177   23.7138408
 N    1.4136809    7.3840022   24.4730785
 C    0.8840239    6.1388712   24.1398563
 C    0.0229072    6.3808869   23.0889791
 N    0.1120929    7.7496270   22.8654115
 H    2.1093308    7.4831893   25.2075371
 H   -0.3919823    8.2151405   22.1169500
 C    1.3928888    4.9390952   24.8101132
 C   -0.7742950    5.5296707   22.1597571
 O   -1.7265987    4.7025808   22.6511162
 O    0.8952102    3.7938966   24.2801471
 C    1.4056785    2.5723268   24.8682372
 H    2.4943427    2.5177960   24.7435613
 H    0.9118420    1.7632001   24.3222340
 H    1.1619973    2.5300316   25.9374936
 C   -2.1563249    4.7808774   24.0293164
 H   -3.1680747    4.3615619   24.0378931
 H   -2.1842084    5.8200284   24.3820594
 H   -1.4986389    4.1807649   24.6688356
 O   -0.6078641    5.6130299   20.9591414
```

```
 O    2.1971970    4.9833649   25.7279811
```

NHC R_2=CH_2CH_3 R_1=H

```
21
 Energy =    -383.5986467489
 C    0.9437373    8.7429040   23.7543326
 N    1.0756278    7.7885402   24.7229421
 C    0.4207401    6.5742925   24.4599424
 C    0.5053828    5.4327941   25.4256897
 C   -0.1725820    6.7526896   23.2353447
 C   -1.0133083    5.9118368   22.3202551
 N    0.1709922    8.0596588   22.8571137
 H    1.5989906    7.9640637   25.5727243
 H   -0.1355356    8.4852143   21.9896251
 C   -1.5005968    4.5675129   22.8653526
 H   -0.4505901    5.7344431   21.3856633
 H   -1.8930085    6.5095122   22.0205472
 H   -0.6644041    3.8976306   23.1078345
 H   -2.1200591    4.0608015   22.1125171
 H   -2.1133157    4.6955786   23.7685869
 C    1.8696047    4.7178724   25.4298736
 H   -0.2870776    4.7076499   25.2068411
 H    0.2941261    5.8108125   26.4413508
 H    2.0873337    4.2782292   24.4464970
 H    1.8832066    3.9114856   26.1774387
 H    2.6884458    5.4109075   25.6693676
```

NHC R_2=I R_1=H

```
9
 Energy =    -820.7920343634
 C    1.0300194    8.8563058   23.7370918
 N    1.6067102    7.8160982   24.4148828
 C    0.9346655    6.6072640   24.2682812
 I    1.5210872    4.8247131   25.1508398
 C   -0.1340281    6.8780492   23.4523545
 I   -1.6246813    5.6215087   22.7457707
 N   -0.0418660    8.2337723   23.1560838
 H    2.4474375    7.9294902   24.9700778
 H   -0.7014745    8.7272085   22.5650974
```

NHC R_2=$COCH_3$(carbonyl) R_1=H

```
19
 Energy =    -531.7189743587
 C    1.0213690    8.5750784   23.8110208
 N    1.5540940    7.5545183   24.5471033
 C    0.9274827    6.3236906   24.4097039
 C   -0.1105997    6.5605438   23.5005785
 N    0.0033019    7.9085890   23.1888103
 H    2.3557827    7.6467594   25.1671194
 H   -0.6507794    8.3328827   22.5341145
```

C	1.5087875	5.2181012	25.2142025
C	-1.2187793	5.8394998	22.8235133
C	-1.4839386	4.3733410	23.0491867
H	-0.6062701	3.7657039	22.7899119
H	-2.3318767	4.0752550	22.4231161
H	-1.7244972	4.1759698	24.1032507
C	0.9563840	3.8162653	25.1777922
H	1.0215346	3.3945077	24.1649209
H	-0.1004434	3.7972488	25.4767449
H	1.5412464	3.1967400	25.8657369
O	2.4779066	5.4888875	25.9236686
O	-1.9288349	6.4916979	22.0574547

NHC R_2=OCH_3 R_1=H

17

Energy = -455.4213229514

C	1.0719183	8.8046197	23.7569203
N	1.4298001	7.8567598	24.6850072
C	0.8536102	6.6063958	24.4819107
O	1.0916644	5.5844222	25.3424987
C	0.0720232	6.7394527	23.3635259
O	-0.6906612	5.8355159	22.6885391
N	0.2386837	8.0698326	22.9568093
H	2.0588857	8.0538376	25.4549293
H	-0.1838010	8.4530389	22.1183629
C	-2.0831763	5.8167594	23.0840593
H	-2.5691281	5.0624273	22.4544986
H	-2.5531603	6.7978863	22.9147313
H	-2.1824074	5.5419291	24.1451208
C	1.4428899	4.3281164	24.7229512
H	1.6430929	3.6340132	25.5466033
H	2.3449309	4.4456307	24.1032004
H	0.6193848	3.9466227	24.1030315

NHC R_2=SH R_1=H

11

Energy = -1022.7936330280

C	1.0830668	8.8438659	23.7601316
N	1.6710517	7.8001890	24.4012247
C	0.9936214	6.5747594	24.2682615
S	1.5327975	5.0356555	24.8878703
C	-0.0956596	6.8607336	23.4764071
S	-1.3847554	5.8351989	22.8857986
N	-0.0098957	8.2177458	23.1970522
H	2.5311344	7.8979823	24.9292986
H	-0.6788200	8.7245216	22.6285410
H	0.9838292	5.1070533	26.1320986
H	-0.8554202	4.7192145	23.4513657

NHC R_2= H R_1= OCH_3

17

```
 Energy =    -455.3266059842
 C     0.6932719    7.9255645   23.7609782
 N     0.7242137    7.0217362   24.7693377
 C     0.1964010    5.7763410   24.4797917
 H     0.1560180    4.9654671   25.1961245
 C    -0.2208601    5.8742328   23.1786950
 H    -0.6920576    5.1632685   22.5116070
 N     0.1037333    7.1664269   22.8067912
 O     1.1624020    7.3034648   26.0682721
 O    -0.1022646    7.5775011   21.4847002
 C    -0.7373660    8.8700735   21.4408050
 H    -0.8230444    9.0895717   20.3702374
 H    -0.1173304    9.6244440   21.9426950
 H    -1.7353546    8.8300210   21.9050224
 C     2.4607253    7.9286538   26.0476550
 H     2.6831253    8.1210032   27.1036421
 H     2.4292336    8.8689402   25.4818739
 H     3.2130435    7.2504597   25.6149717
```

NHC R_2= H R_1= $COCH_3$

```
19
 Energy =    -531.7026730103
 C     0.9333151    8.5202346   23.7544356
 N     1.4720538    7.4396068   24.4225984
 C     0.7301010    6.2516285   24.2459877
 H     0.9914483    5.2991858   24.6901023
 C    -0.3114235    6.5737863   23.4509392
 H    -1.1147356    5.9501698   23.0789410
 N    -0.1724350    7.9480560   23.1595852
 C     2.6805525    7.5514346   25.2155359
 C    -1.0835756    8.7171434   22.3343547
 C    -2.3121632    7.9671456   21.8680796
 H    -2.0391108    7.1121322   21.2323777
 H    -2.9325774    8.6587362   21.2909635
 H    -2.8893409    7.5802296   22.7204880
 C     3.1837614    6.2508018   25.8020987
 H     2.4544541    5.8282692   26.5092962
 H     4.1180518    6.4577777   26.3319415
 H     3.3645769    5.5009523   25.0184767
 O    -0.8554981    9.8685930   22.0599129
 O     3.2232051    8.6155864   25.3782550
```

HEP complex R_1=Br R_2=H

```
45
 Energy =  -11267.0006294200
 H    -2.4890804   -5.3228989    2.9243477
 C    -2.8258497   -5.7699663    1.9896764
 C    -4.1202246   -5.5470794    1.5188359
 H    -4.7990018   -4.9219717    2.0995210
 C    -4.5618640   -6.1109142    0.3100269
 H    -5.5790968   -5.9170583   -0.0311996
```

C	-3.7259801	-6.9149097	-0.4660879
H	-4.0834418	-7.3420731	-1.4005932
C	-2.4282544	-7.1458153	0.0035405
C	-1.9894851	-6.5790432	1.2166831
N	-1.3494976	-7.8818880	-0.4866124
N	-0.6733412	-7.0053540	1.4039050
C	-1.3141677	-8.6563334	-1.7481801
C	-1.4270702	-7.7307443	-2.9620597
H	-2.3952867	-7.2126557	-3.0019424
H	-0.6264107	-6.9787362	-2.9450635
H	-1.3246224	-8.3214664	-3.8829669
C	-2.3320969	-9.7992813	-1.7302088
H	-3.3696067	-9.4383611	-1.7113535
H	-2.2084690	-10.4083935	-2.6363402
H	-2.1656604	-10.4444830	-0.8575543
C	0.1373937	-6.5448158	2.5588549
C	0.9539253	-5.3051541	2.1794493
H	1.6765604	-5.5463112	1.3877956
H	0.3044111	-4.4961740	1.8166981
H	1.4993488	-4.9369086	3.0600999
C	0.9876836	-7.6571521	3.1623201
H	-0.6139711	-6.2596237	3.3100162
H	1.7904069	-7.9621995	2.4765800
H	1.4445735	-7.2880379	4.0916528
H	0.3896404	-8.5488325	3.3898028
C	-0.2803531	-7.7960865	0.3616991
H	-0.3045686	-9.0977117	-1.7423428
Pd	1.4724710	-8.7649722	0.0147072
Br	2.4322913	-6.7748597	-1.1220085
Br	0.5214963	-10.8326835	1.0194654
C	3.1821036	-9.7703297	-0.3816474
N	4.3879439	-9.7298090	0.2556116
N	3.4310849	-10.6782231	-1.3690674
C	5.3428659	-10.5701115	-0.3034532
Br	4.7396875	-8.6449470	1.7216229
C	4.7257589	-11.1814112	-1.3509710
H	6.3489606	-10.6558985	0.0856206
H	5.0820695	-11.9107281	-2.0664331
Br	2.1707839	-11.1939214	-2.6327071

HEP complex R_1=CCH R_2=H

49

Energy = -6271.6940358700

H	-2.1171206	-5.0568189	2.5860744
C	-2.5031250	-5.6962118	1.7925923
C	-3.8493930	-5.6474096	1.4290581
H	-4.5184371	-4.9618816	1.9498030
C	-4.3557836	-6.4627935	0.4030728
H	-5.4126937	-6.4017733	0.1424009
C	-3.5342546	-7.3500573	-0.2934059
H	-3.9416865	-7.9737522	-1.0862864
C	-2.1833083	-7.4017057	0.0655834

C	-1.6797736	-6.5867522	1.0996199
N	-1.0981237	-8.1435616	-0.4001056
N	-0.3202142	-6.8834660	1.2145659
C	-1.1182079	-9.1459256	-1.4900576
C	-1.4670537	-8.4968656	-2.8314137
H	-2.4971026	-8.1153495	-2.8577128
H	-0.7792345	-7.6686746	-3.0473427
H	-1.3668597	-9.2435216	-3.6313872
C	-1.9936896	-10.3452125	-1.1218020
H	-3.0533096	-10.0741220	-1.0170821
H	-1.9208216	-11.1052175	-1.9124492
H	-1.6473315	-10.7941133	-0.1815572
C	0.5646573	-6.1631535	2.1637833
C	1.2311439	-4.9673963	1.4756310
H	1.8955791	-5.3082173	0.6691565
H	0.4828546	-4.2895051	1.0415923
H	1.8223526	-4.4015500	2.2100167
C	1.5662252	-7.0864930	2.8504051
H	-0.1250343	-5.7899925	2.9360891
H	2.3096008	-7.4715633	2.1374475
H	2.0936246	-6.5162474	3.6284550
H	1.0720341	-7.9488718	3.3153006
C	0.0353697	-7.8271620	0.2940290
H	-0.0716903	-9.4872327	-1.5356709
Pd	1.8357760	-8.6989513	-0.0824906
Br	2.4147896	-6.8931806	-1.6907742
Br	1.2238974	-10.6203481	1.3778704
C	3.5810409	-9.6042138	-0.4703968
N	4.8195648	-9.3708805	0.0881748
N	3.8314747	-10.6395740	-1.3442475
C	5.8016799	-10.2407058	-0.4238680
C	5.0776986	-8.4232967	1.0192714
C	5.1827278	-11.0353387	-1.3211115
C	2.9000329	-11.2199652	-2.1367150
H	5.5472665	-11.8392820	-1.9468110
H	6.8291412	-10.1936989	-0.0883709
C	5.3882132	-7.6034172	1.8497489
C	2.1364414	-11.7878283	-2.8802017
H	1.4363481	-12.2832647	-3.5190398
H	5.6326043	-6.8639136	2.5826680

HEP complex R_1=CHCH$_2$ R_2=H

53

Energy = -6274.2382135470

H	-2.0583782	-5.0205704	2.5462728
C	-2.4616652	-5.6654116	1.7659980
C	-3.8108835	-5.6012541	1.4157479
H	-4.4637688	-4.8984853	1.9339656
C	-4.3410326	-6.4248085	0.4085012
H	-5.3999184	-6.3518096	0.1590348
C	-3.5406557	-7.3355951	-0.2824411
H	-3.9661846	-7.9665931	-1.0598954

C	-2.1870887	-7.4027893	0.0637800
C	-1.6600524	-6.5808510	1.0800838
N	-1.1189085	-8.1710273	-0.3991868
N	-0.3053413	-6.9021138	1.1908492
C	-1.1624418	-9.1786610	-1.4829167
C	-1.5301553	-8.5391196	-2.8238449
H	-2.5657926	-8.1733124	-2.8450941
H	-0.8555346	-7.7025693	-3.0486382
H	-1.4236816	-9.2879719	-3.6210110
C	-2.0360614	-10.3733002	-1.0950226
H	-3.0908624	-10.0938836	-0.9664549
H	-1.9867067	-11.1331241	-1.8879742
H	-1.6741671	-10.8221353	-0.1603158
C	0.6020208	-6.1648993	2.1056217
C	1.2792740	-5.0067251	1.3652998
H	1.9158717	-5.3865140	0.5537272
H	0.5362522	-4.3263802	0.9260813
H	1.8995128	-4.4308754	2.0669639
C	1.5941348	-7.0764280	2.8211578
H	-0.0725225	-5.7497903	2.8696180
H	2.3102922	-7.5213090	2.1144995
H	2.1532781	-6.4814090	3.5570690
H	1.0887991	-7.9015523	3.3381463
C	0.0246660	-7.8704043	0.2858243
H	-0.1165455	-9.5195548	-1.5460360
Pd	1.7918710	-8.8269452	-0.0448494
Br	2.4039308	-7.1275660	-1.7559724
Br	1.0430447	-10.5840454	1.5596703
C	3.5376743	-9.8241483	-0.3716804
N	4.8104385	-9.4142238	-0.0584645
N	3.7152856	-11.0668292	-0.9283217
C	5.7500264	-10.3851448	-0.4061279
C	5.1007609	-8.1638158	0.5320771
C	5.0654690	-11.4164817	-0.9538703
C	2.6510873	-11.8614422	-1.4101336
H	5.4167574	-12.3613529	-1.3458163
H	6.8118074	-10.2526434	-0.2477998
C	6.2685622	-7.8382367	1.0914482
C	2.7943113	-12.9563137	-2.1605029
H	1.6846680	-11.4863053	-1.0761853
H	3.7586251	-13.3359160	-2.4970618
H	1.9093278	-13.5119420	-2.4625024
H	4.2599603	-7.4754417	0.4587275
H	7.1100002	-8.5257629	1.1727150
H	6.4029296	-6.8373952	1.4956403

HEP complex R_1=H R_2=CH_2CH_3

57

Energy = -6276.7324134610

H	-2.5446462	-5.5634673	3.0358155
C	-2.8393003	-5.9023878	2.0431902
C	-4.0903370	-5.5740103	1.5184155

H	-4.7786033	-4.9741724	2.1145406
C	-4.4762670	-5.9997146	0.2361064
H	-5.4601823	-5.7256499	-0.1453816
C	-3.6262431	-6.7657548	-0.5630674
H	-3.9398490	-7.0864858	-1.5544090
C	-2.3709599	-7.0979872	-0.0423927
C	-1.9889581	-6.6721648	1.2459103
N	-1.2906867	-7.8269988	-0.5394727
N	-0.7038054	-7.1714815	1.4667209
C	-1.1957785	-8.4749263	-1.8683685
C	-1.2283299	-7.4377349	-2.9932790
H	-2.1920121	-6.9132183	-3.0512307
H	-0.4320953	-6.6945139	-2.8542406
H	-1.0628763	-7.9417490	-3.9556545
C	-2.2282088	-9.5940080	-2.0191377
H	-3.2598501	-9.2159905	-2.0100452
H	-2.0681136	-10.1076794	-2.9773100
H	-2.1146651	-10.3299552	-1.2120763
C	0.0586118	-6.8472676	2.6987568
C	0.8386833	-5.5416075	2.5125583
H	1.6086407	-5.6625127	1.7377537
H	0.1750269	-4.7180238	2.2146127
H	1.3273249	-5.2633476	3.4572235
C	0.9421349	-7.9965831	3.1740001
H	-0.7217600	-6.6923676	3.4596146
H	1.7832867	-8.1675667	2.4865455
H	1.3500744	-7.7380057	4.1617105
H	0.3806491	-8.9354130	3.2568000
C	-0.2741283	-7.8693136	0.3745661
H	-0.1931490	-8.9322608	-1.8511191
Pd	1.4797974	-8.8395904	0.0158163
Br	2.4580813	-6.7320995	-0.8834222
Br	0.4606528	-10.9778771	0.8137484
C	3.2014989	-9.8285105	-0.4165480
N	4.3512535	-9.3297362	-0.9303026
N	3.4571724	-11.1508020	-0.2883799
C	5.3160194	-10.3122735	-1.1301445
H	4.4132133	-8.3317117	-1.1481088
C	4.7372399	-11.4897993	-0.7153643
C	6.6823704	-10.0366870	-1.6923350
C	5.2665443	-12.8870266	-0.6786101
H	2.7285880	-11.7671833	0.0844697
H	6.2374359	-12.8988370	-1.1951911
H	4.6028597	-13.5465177	-1.2637821
C	5.4269656	-13.4586726	0.7417498
C	6.9168906	-8.5775369	-2.0978116
H	6.8473155	-10.6863849	-2.5675727
H	7.4449276	-10.3323630	-0.9527957
H	6.2091354	-8.2519526	-2.8735191
H	7.9303526	-8.4542589	-2.5015169
H	6.8204815	-7.8965022	-1.2400752
H	6.1170104	-12.8459860	1.3379491
H	5.8208986	-14.4838674	0.7047663
H	4.4654972	-13.4897931	1.2728437

HEP complex R_1=H R_2=C_6H_5

65

Energy = -6581.7065405000

H	-1.8468831	-5.3759143	3.2825873
C	-2.4496293	-5.7510021	2.4563393
C	-3.7911219	-5.3883103	2.3289183
H	-4.2373018	-4.7244811	3.0698032
C	-4.5737227	-5.8586058	1.2610422
H	-5.6180236	-5.5539544	1.1873563
C	-4.0428568	-6.7062360	0.2878166
H	-4.6617764	-7.0599158	-0.5342895
C	-2.6985403	-7.0729284	0.4100464
C	-1.9173648	-6.6007505	1.4838115
N	-1.8517103	-7.8747072	-0.3552100
N	-0.6412723	-7.1440979	1.3186313
C	-2.2016624	-8.5941153	-1.6019197
C	-2.5513521	-7.6139263	-2.7247635
H	-3.4651666	-7.0420904	-2.5115541
H	-1.7255712	-6.9088685	-2.8878633
H	-2.7153905	-8.1729593	-3.6564319
C	-3.2657611	-9.6646092	-1.3489042
H	-4.2319959	-9.2332306	-1.0533216
H	-3.4245405	-10.2404327	-2.2711008
H	-2.9343904	-10.3582971	-0.5651348
C	0.4822610	-6.7812478	2.2183212
C	1.1894121	-5.5222200	1.7053170
H	1.6662443	-5.7194807	0.7348956
H	0.4837997	-4.6891872	1.5806279
H	1.9625562	-5.2130853	2.4228044
C	1.4468605	-7.9365129	2.4677781
H	-0.0109898	-6.5480415	3.1747536
H	2.0092333	-8.1927296	1.5567011
H	2.1647544	-7.6330186	3.2429250
H	0.9230892	-8.8407927	2.8030539
C	-0.5991530	-7.9119566	0.1902833
H	-1.2609096	-9.1025175	-1.8684272
Pd	0.9476847	-8.9308534	-0.6560080
Br	1.5572343	-6.9000964	-1.9623653
Br	0.2536897	-11.0108123	0.5355003
C	2.4836488	-9.9381813	-1.5210164
N	3.4019549	-9.4676705	-2.3960634
N	2.8499107	-11.2271984	-1.3379309
C	4.3428164	-10.4267251	-2.7589775
H	3.3756688	-8.4827692	-2.6780502
C	3.9749182	-11.5796271	-2.0786424
C	5.4603660	-10.1037488	-3.6513339
C	4.5105599	-12.9427125	-2.0627239
H	2.2774407	-11.8340299	-0.7425718
C	4.4483137	-13.7152217	-0.8864249
C	5.0634185	-13.5239725	-3.2198534
C	4.9291946	-15.0248795	-0.8681553
C	5.4860403	-15.5867360	-2.0196454

C	5.5509190	-14.8295684	-3.1939052
H	5.8631405	-16.6099898	-2.0043678
H	4.8732816	-15.6055935	0.0535227
H	5.0968544	-12.9492664	-4.1456369
H	5.9725051	-15.2638495	-4.1016827
H	4.0382602	-13.2810210	0.0273502
C	6.7521938	-10.6098841	-3.4137821
C	7.8112232	-10.2734291	-4.2554184
C	5.2663939	-9.2404277	-4.7466644
H	6.9239457	-11.2580568	-2.5542642
H	4.2699146	-8.8477530	-4.9572648
C	6.3312098	-8.9003585	-5.5817644
C	7.6067166	-9.4174864	-5.3424735
H	8.8066938	-10.6711533	-4.0527222
H	6.1603011	-8.2327625	-6.4274020
H	8.4382822	-9.1518719	-5.9964245

HEP complex R_1=H R_2=Br

45

Energy = -11267.0925200000

H	-2.5972454	-5.5342252	3.0427268
C	-2.8912963	-5.8765184	2.0510807
C	-4.1410194	-5.5497080	1.5232594
H	-4.8299812	-4.9477632	2.1161583
C	-4.5254673	-5.9797915	0.2417694
H	-5.5088567	-5.7067988	-0.1417201
C	-3.6753266	-6.7486230	-0.5540290
H	-3.9883350	-7.0723361	-1.5445449
C	-2.4208956	-7.0793078	-0.0302276
C	-2.0408048	-6.6491427	1.2568190
N	-1.3393732	-7.8095042	-0.5243089
N	-0.7554834	-7.1468877	1.4815199
C	-1.2401539	-8.4580571	-1.8531732
C	-1.2666339	-7.4196004	-2.9768759
H	-2.2308129	-6.8966149	-3.0392364
H	-0.4722258	-6.6755025	-2.8322498
H	-1.0947812	-7.9220633	-3.9387496
C	-2.2742815	-9.5749368	-2.0080244
H	-3.3045495	-9.1932837	-2.0099738
H	-2.1071351	-10.0929195	-2.9625564
H	-2.1713824	-10.3084596	-1.1973058
C	0.0047678	-6.8210873	2.7150873
C	0.7869098	-5.5171627	2.5281643
H	1.5554366	-5.6376148	1.7521214
H	0.1242570	-4.6918979	2.2330847
H	1.2781644	-5.2411886	3.4718651
C	0.8826885	-7.9729047	3.1936459
H	-0.7771328	-6.6631601	3.4735401
H	1.7231207	-8.1504237	2.5067942
H	1.2933205	-7.7144520	4.1799155
H	0.3158905	-8.9082646	3.2796521
C	-0.3261903	-7.8462285	0.3915702
H	-0.2385673	-8.9174343	-1.8328108

Pd	1.4320761	-8.8028811	0.0397510
Br	2.3996467	-6.7010461	-0.8754555
Br	0.4506062	-10.9493864	0.8447576
C	3.1638624	-9.7734992	-0.3810127
N	4.2956539	-9.2611165	-0.9261466
N	3.4452655	-11.0885562	-0.2024315
C	5.2685439	-10.2305012	-1.0919316
H	4.3379332	-8.2652277	-1.1738979
C	4.7235387	-11.4011078	-0.6283292
Br	6.9529308	-9.8879578	-1.8141829
Br	5.4500782	-13.1158603	-0.5390060
H	2.7326205	-11.7125862	0.1964876

HEP complex R_1=H R_2=CCH

49

Energy = -6271.7669974420

H	-2.4671128	-5.7872888	3.1094780
C	-2.7413027	-6.1168084	2.1076287
C	-4.0109720	-5.8539355	1.5913737
H	-4.7350515	-5.3163352	2.2039100
C	-4.3705737	-6.2652652	0.2966713
H	-5.3703556	-6.0433244	-0.0772262
C	-3.4745203	-6.9511282	-0.5241972
H	-3.7670267	-7.2601454	-1.5255034
C	-2.2007171	-7.2185224	-0.0115415
C	-1.8448063	-6.8078144	1.2887287
N	-1.0765959	-7.8616854	-0.5304172
N	-0.5292249	-7.2279979	1.4947345
C	-0.9425500	-8.4560265	-1.8811724
C	-1.0336260	-7.3820740	-2.9677014
H	-2.0258792	-6.9125539	-3.0095897
H	-0.2819735	-6.5995964	-2.7996336
H	-0.8386273	-7.8412184	-3.9467575
C	-1.9097266	-9.6252815	-2.0767001
H	-2.9608473	-9.3056202	-2.0603208
H	-1.7178344	-10.0932999	-3.0522099
H	-1.7592446	-10.3837052	-1.2970842
C	0.2149457	-6.8866784	2.7333112
C	0.9201350	-5.5354544	2.5758847
H	1.6990530	-5.5961368	1.8026580
H	0.2121825	-4.7448454	2.2915133
H	1.3885444	-5.2494474	3.5280922
C	1.1585604	-7.9963965	3.1858081
H	-0.5734245	-6.7911218	3.4958851
H	1.9982376	-8.1205082	2.4862171
H	1.5668696	-7.7295980	4.1706938
H	0.6428785	-8.9611902	3.2669102
C	-0.0595060	-7.8632751	0.3820175
H	0.0842809	-8.8561030	-1.8779642
Pd	1.7567356	-8.6983634	0.0005814
Br	2.5899309	-6.5062133	-0.8362116
Br	0.8976455	-10.9237694	0.7249728
C	3.5471340	-9.5421936	-0.4465643

N	4.6498976	-8.9310661	-0.9391915
N	3.9083998	-10.8426329	-0.3420086
C	5.6993152	-9.8190952	-1.1505278
C	5.2156577	-11.0665597	-0.7624109
C	5.8399631	-12.3234141	-0.7660946
C	6.9575287	-9.4440236	-1.6478634
H	4.6352982	-7.9229773	-1.1311628
H	3.2363367	-11.5323935	0.0118872
C	8.0417007	-9.1031438	-2.0748000
H	8.9999830	-8.8091634	-2.4502120
C	6.3721887	-13.4147926	-0.7683395
H	6.8427559	-14.3758957	-0.7702615

HEP complex R_1=H R_2=$COOCH_3$

57

Energy = -6575.3592682040

H	-2.0636632	-5.3644500	2.8410291
C	-2.4381742	-5.8201288	1.9250369
C	-3.7378104	-5.5701526	1.4832456
H	-4.3838309	-4.9151590	2.0682029
C	-4.2281325	-6.1460270	0.2987445
H	-5.2487723	-5.9308200	-0.0187775
C	-3.4369278	-6.9890459	-0.4824914
H	-3.8322571	-7.4265977	-1.3967670
C	-2.1337539	-7.2458369	-0.0426946
C	-1.6471049	-6.6691437	1.1470646
N	-1.0888207	-8.0216235	-0.5474117
N	-0.3385998	-7.1308386	1.3088030
C	-1.1138818	-8.8369256	-1.7844778
C	-1.2622311	-7.9539373	-3.0263697
H	-2.2313538	-7.4371726	-3.0577151
H	-0.4633799	-7.2011095	-3.0635441
H	-1.1872905	-8.5794028	-3.9265020
C	-2.1503226	-9.9591373	-1.6898434
H	-3.1782130	-9.5756317	-1.6339669
H	-2.0786141	-10.5943097	-2.5833842
H	-1.9585607	-10.5850028	-0.8086590
C	0.5145109	-6.6741925	2.4357341
C	1.2702661	-5.3982983	2.0500729
H	1.9816751	-5.6040989	1.2386543
H	0.5814603	-4.6103981	1.7154106
H	1.8269195	-5.0201453	2.9190941
C	1.4354841	-7.7668158	2.9685291
H	-0.2075358	-6.4345767	3.2309188
H	2.2316533	-8.0086567	2.2497343
H	1.9071779	-7.4079115	3.8942707
H	0.8865590	-8.6913303	3.1874884
C	0.0025465	-7.9501641	0.2715065
H	-0.1124807	-9.2954926	-1.8038774
Pd	1.7304105	-8.9711768	-0.0807202
Br	2.7381067	-7.0026079	-1.2392177
Br	0.7225721	-10.9977695	0.9571885
C	3.4287118	-10.0165488	-0.4358278

N	4.5437382	-9.5907144	-1.0641457
N	3.7214597	-11.2991379	-0.0843384
C	5.5266035	-10.5786038	-1.1306061
H	4.5502597	-8.6347217	-1.4399956
C	4.9766208	-11.6814872	-0.5016748
H	3.0289160	-11.8515486	0.4365006
C	5.1892058	-13.7937711	-2.3537161
C	7.0567812	-8.0888373	-1.4340807
O	5.5979102	-14.0116230	-0.9794845
O	7.4708958	-9.3426380	-2.0198878
H	4.1707807	-13.3855317	-2.4038677
H	5.2074600	-14.7867994	-2.8126857
H	5.9060898	-13.1293802	-2.8510619
H	6.7030976	-8.2182516	-0.4033741
H	6.2873972	-7.6018225	-2.0507483
H	7.9538926	-7.4610867	-1.4323701
C	5.5613489	-13.0067392	-0.0874342
C	6.8647867	-10.5280858	-1.7543010
O	5.9216574	-13.1738830	1.0576866
O	7.4417458	-11.5585998	-2.0555557

HEP complex R_1=H R_2=I

45

Energy = -6713.9181685590

H	-2.6056945	-5.5312907	3.0446284
C	-2.8989239	-5.8731237	2.0525860
C	-4.1482806	-5.5460773	1.5238751
H	-4.8376862	-4.9443115	2.1164439
C	-4.5318592	-5.9756435	0.2419042
H	-5.5148121	-5.7023980	-0.1422836
C	-3.6814226	-6.7446836	-0.5533712
H	-3.9935406	-7.0678313	-1.5442409
C	-2.4274967	-7.0756038	-0.0286304
C	-2.0479780	-6.6456449	1.2586986
N	-1.3456708	-7.8060103	-0.5221020
N	-0.7627633	-7.1433424	1.4837722
C	-1.2451861	-8.4544913	-1.8506563
C	-1.2708017	-7.4159660	-2.9743421
H	-2.2350612	-6.8932395	-3.0377021
H	-0.4765402	-6.6718897	-2.8290218
H	-1.0981657	-7.9183635	-3.9360890
C	-2.2791622	-9.5713664	-2.0062419
H	-3.3093715	-9.1896709	-2.0095071
H	-2.1111903	-10.0895681	-2.9604839
H	-2.1771526	-10.3045243	-1.1951406
C	-0.0020938	-6.8167849	2.7167887
C	0.7806126	-5.5134244	2.5285548
H	1.5481512	-5.6340250	1.7515426
H	0.1177939	-4.6882062	2.2338254
H	1.2724116	-5.2369156	3.4718571
C	0.8753311	-7.9685065	3.1963374
H	-0.7834489	-6.6577370	3.4756288
H	1.7157551	-8.1473604	2.5099208

H	1.2852755	-7.7097311	4.1828696
H	0.3080066	-8.9034702	3.2827634
C	-0.3327498	-7.8427512	0.3941351
H	-0.2435827	-8.9139132	-1.8294891
Pd	1.4261857	-8.8006528	0.0425166
Br	2.3917999	-6.6987279	-0.8733037
Br	0.4431002	-10.9454674	0.8485886
C	3.1590808	-9.7718103	-0.3788425
N	4.2901529	-9.2602323	-0.9253259
N	3.4417579	-11.0861705	-0.2004287
C	5.2664185	-10.2285549	-1.0930259
H	4.3299199	-8.2643878	-1.1724164
C	4.7210824	-11.4020634	-0.6272706
I	7.1326002	-9.8461883	-1.8961629
I	5.5264096	-13.3036101	-0.5291137
H	2.7281496	-11.7077877	0.1995851

HEP complex R_1=H R_2=$COCH_3$

55

Energy = -6424.8387337180

H	-2.4923182	-5.6758721	3.0604816
C	-2.7978680	-6.0002049	2.0662749
C	-4.0601159	-5.6778630	1.5659362
H	-4.7464618	-5.0971033	2.1826715
C	-4.4605439	-6.0852656	0.2817841
H	-5.4531342	-5.8161421	-0.0800898
C	-3.6145253	-6.8269891	-0.5435485
H	-3.9400652	-7.1341747	-1.5351377
C	-2.3474324	-7.1524158	-0.0474543
C	-1.9507226	-6.7447061	1.2417479
N	-1.2649222	-7.8573715	-0.5755346
N	-0.6548536	-7.2297287	1.4332685
C	-1.1789586	-8.4708585	-1.9218824
C	-1.2481238	-7.4060860	-3.0189141
H	-2.2274383	-6.9100484	-3.0586437
H	-0.4740200	-6.6427900	-2.8649755
H	-1.0730081	-7.8798845	-3.9945233
C	-2.1941757	-9.6034627	-2.0859901
H	-3.2312582	-9.2424038	-2.0516810
H	-2.0408156	-10.0888687	-3.0597946
H	-2.0575946	-10.3587623	-1.3007694
C	0.1259573	-6.9086966	2.6550398
C	0.8793529	-5.5877955	2.4690213
H	1.6374157	-5.6867449	1.6796034
H	0.1962414	-4.7733012	2.1919377
H	1.3806090	-5.3105387	3.4069460
C	1.0367633	-8.0488948	3.0991826
H	-0.6421815	-6.7762640	3.4323670
H	1.8677825	-8.1976343	2.3943372
H	1.4610319	-7.7956909	4.0810908
H	0.4920881	-8.9973824	3.1832180
C	-0.2356919	-7.9005909	0.3218679
H	-0.1682896	-8.9102929	-1.9321910

Pd	1.5277533	-8.8387269	-0.0816906
Br	2.4692056	-6.7122984	-0.9708776
Br	0.5782414	-11.0083858	0.7033313
C	3.2503159	-9.7882562	-0.5610588
N	4.3844881	-9.2552866	-1.0758688
N	3.5321444	-11.1103502	-0.4711894
C	5.3621861	-10.2076435	-1.3201212
H	4.4045113	-8.2504010	-1.2881795
C	4.8107158	-11.4177755	-0.9103227
C	6.6546399	-9.8703359	-1.9797821
C	5.3762781	-12.7933007	-0.8191094
H	2.8226034	-11.7382708	-0.0728317
C	4.3758170	-13.9328805	-0.7844517
C	7.1112895	-8.4279701	-1.8686732
H	6.4315702	-7.7587303	-2.4206666
H	8.1135321	-8.3409917	-2.3007193
H	7.1221090	-8.0917313	-0.8212153
H	3.6739671	-13.8731435	-1.6299083
H	3.7768130	-13.9004705	0.1402474
H	4.9199886	-14.8824512	-0.8153362
O	6.5804367	-12.9762481	-0.7524369
O	7.2876909	-10.7125928	-2.5945458

HEP complex R_1=H R_2=OCH_3

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Energy = -6348.5514118910

H	-2.5042465	-5.4730068	3.0039258
C	-2.8099242	-5.8327185	2.0219415
C	-4.0621359	-5.5057803	1.4992661
H	-4.7402019	-4.8856704	2.0862065
C	-4.4625491	-5.9590605	0.2308826
H	-5.4475981	-5.6865219	-0.1487096
C	-3.6261738	-6.7519256	-0.5561881
H	-3.9511255	-7.0941342	-1.5365447
C	-2.3696343	-7.0827365	-0.0376356
C	-1.9730751	-6.6290585	1.2365572
N	-1.3003434	-7.8340991	-0.5254235
N	-0.6906241	-7.1347639	1.4590247
C	-1.2247337	-8.5186750	-1.8368248
C	-1.2579995	-7.5116096	-2.9886459
H	-2.2170869	-6.9791659	-3.0510498
H	-0.4534051	-6.7726708	-2.8769963
H	-1.1069445	-8.0424926	-3.9387161
C	-2.2706161	-9.6301752	-1.9470881
H	-3.2979530	-9.2405616	-1.9403221
H	-2.1244228	-10.1729623	-2.8911659
H	-2.1583754	-10.3440164	-1.1203071
C	0.0860573	-6.7864800	2.6757778
C	0.8930105	-5.5055135	2.4408965
H	1.6571435	-5.6693711	1.6686904
H	0.2455712	-4.6789000	2.1166514
H	1.3917412	-5.2045887	3.3731405
C	0.9466832	-7.9382975	3.1847779

H	-0.6860134	-6.5882954	3.4346187
H	1.7796806	-8.1510926	2.4990369
H	1.3669679	-7.6564839	4.1607727
H	0.3653303	-8.8612978	3.3020378
C	-0.2769929	-7.8637585	0.3811986
H	-0.2268639	-8.9863160	-1.8164606
Pd	1.4601296	-8.8680601	0.0422821
Br	2.4818457	-6.8141967	-0.9439668
Br	0.4217095	-10.9620389	0.9128351
C	3.1633813	-9.9011328	-0.3582686
N	4.2905472	-9.4242705	-0.9581951
N	3.4415646	-11.1995586	-0.1182800
C	5.2620420	-10.4058988	-1.0821001
H	4.3183995	-8.4375134	-1.2391165
C	4.7242375	-11.5515078	-0.5412789
H	2.7483065	-11.7986842	0.3405949
C	5.1246177	-13.6815990	-1.4746327
C	6.8980246	-8.9090383	-1.9113811
O	5.2530267	-12.7807606	-0.3475846
O	6.4743026	-10.2581680	-1.6603640
H	4.0651798	-13.8424251	-1.7261283
H	5.5780784	-14.6273626	-1.1579281
H	5.6601809	-13.2837646	-2.3490327
H	6.9057360	-8.3166094	-0.9832115
H	6.2545344	-8.4223175	-2.6616756
H	7.9158086	-8.9868226	-2.3060828

HEP complex R_1=H R_2=C_6H_5

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Energy = -6915.9218718360

H	-2.6544535	-5.5731161	3.0637775
C	-2.9378107	-5.9058005	2.0658274
C	-4.1859466	-5.5825236	1.5319334
H	-4.8838756	-4.9921736	2.1261348
C	-4.5565590	-6.0006286	0.2424999
H	-5.5389545	-5.7310151	-0.1459179
C	-3.6936969	-6.7534918	-0.5551763
H	-3.9956968	-7.0679217	-1.5520615
C	-2.4403736	-7.0794961	-0.0257532
C	-2.0747057	-6.6624320	1.2698200
N	-1.3480647	-7.7932600	-0.5199911
N	-0.7863766	-7.1504350	1.4983212
C	-1.2340179	-8.4247278	-1.8555947
C	-1.2682112	-7.3737801	-2.9675595
H	-2.2386506	-6.8625342	-3.0300443
H	-0.4847284	-6.6211249	-2.8092747
H	-1.0841589	-7.8627458	-3.9341459
C	-2.2542309	-9.5517759	-2.0284819
H	-3.2892095	-9.1829809	-2.0251344
H	-2.0804071	-10.0533080	-2.9906490
H	-2.1426740	-10.2958380	-1.2286723
C	-0.0408158	-6.8324299	2.7428337
C	0.7281059	-5.5170107	2.5829538

H	1.5097118	-5.6190917	1.8173505
H	0.0605698	-4.6958916	2.2874117
H	1.2014600	-5.2469809	3.5375526
C	0.8470406	-7.9787448	3.2164298
H	-0.8317815	-6.6939676	3.4957993
H	1.6960420	-8.1379810	2.5356681
H	1.2450144	-7.7250069	4.2092003
H	0.2921136	-8.9223489	3.2876734
C	-0.3405288	-7.8313223	0.4027177
H	-0.2271210	-8.8724080	-1.8358618
Pd	1.4376893	-8.7542313	0.0535495
Br	2.3606347	-6.6208134	-0.8311542
Br	0.4849936	-10.9283225	0.8257214
C	3.1977245	-9.6793017	-0.3576223
N	4.3273687	-9.1496985	-0.8650370
N	3.4935534	-11.0008216	-0.1946671
C	5.3299274	-10.1085593	-1.0404156
H	4.3709121	-8.1513412	-1.0939647
C	4.7798486	-11.2973471	-0.5985437
S	6.9533363	-9.7821189	-1.5870114
S	5.4488065	-12.9111663	-0.5199104
H	2.7749358	-11.6288503	0.1864340
H	6.6510224	-12.5014432	-1.0022009
H	6.7366883	-9.8769706	-2.9273543

HEP complex R_1=H R_2=SH

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Energy = -6915.9218718360

H	-2.6544535	-5.5731161	3.0637775
C	-2.9378107	-5.9058005	2.0658274
C	-4.1859466	-5.5825236	1.5319334
H	-4.8838756	-4.9921736	2.1261348
C	-4.5565590	-6.0006286	0.2424999
H	-5.5389545	-5.7310151	-0.1459179
C	-3.6936969	-6.7534918	-0.5551763
H	-3.9956968	-7.0679217	-1.5520615
C	-2.4403736	-7.0794961	-0.0257532
C	-2.0747057	-6.6624320	1.2698200
N	-1.3480647	-7.7932600	-0.5199911
N	-0.7863766	-7.1504350	1.4983212
C	-1.2340179	-8.4247278	-1.8555947
C	-1.2682112	-7.3737801	-2.9675595
H	-2.2386506	-6.8625342	-3.0300443
H	-0.4847284	-6.6211249	-2.8092747
H	-1.0841589	-7.8627458	-3.9341459
C	-2.2542309	-9.5517759	-2.0284819
H	-3.2892095	-9.1829809	-2.0251344
H	-2.0804071	-10.0533080	-2.9906490
H	-2.1426740	-10.2958380	-1.2286723
C	-0.0408158	-6.8324299	2.7428337
C	0.7281059	-5.5170107	2.5829538
H	1.5097118	-5.6190917	1.8173505
H	0.0605698	-4.6958916	2.2874117

H	1.2014600	-5.2469809	3.5375526
C	0.8470406	-7.9787448	3.2164298
H	-0.8317815	-6.6939676	3.4957993
H	1.6960420	-8.1379810	2.5356681
H	1.2450144	-7.7250069	4.2092003
H	0.2921136	-8.9223489	3.2876734
C	-0.3405288	-7.8313223	0.4027177
H	-0.2271210	-8.8724080	-1.8358618
Pd	1.4376893	-8.7542313	0.0535495
Br	2.3606347	-6.6208134	-0.8311542
Br	0.4849936	-10.9283225	0.8257214
C	3.1977245	-9.6793017	-0.3576223
N	4.3273687	-9.1496985	-0.8650370
N	3.4935534	-11.0008216	-0.1946671
C	5.3299274	-10.1085593	-1.0404156
H	4.3709121	-8.1513412	-1.0939647
C	4.7798486	-11.2973471	-0.5985437
S	6.9533363	-9.7821189	-1.5870114
S	5.4488065	-12.9111663	-0.5199104
H	2.7749358	-11.6288503	0.1864340
H	6.6510224	-12.5014432	-1.0022009
H	6.7366883	-9.8769706	-2.9273543

HEP complex R_1=$COCH_3$ R_2=H

55

Energy = -6424.8185843940

H	-2.1005629	-4.9095087	2.3719722
C	-2.5319881	-5.5973510	1.6458517
C	-3.8866289	-5.5275281	1.3210322
H	-4.5122761	-4.7757495	1.8028058
C	-4.4581933	-6.4085377	0.3872626
H	-5.5211134	-6.3304178	0.1572339
C	-3.6935858	-7.3839476	-0.2526726
H	-4.1511660	-8.0597640	-0.9717535
C	-2.3334491	-7.4565324	0.0684578
C	-1.7640016	-6.5764774	1.0087487
N	-1.2959061	-8.2837593	-0.3583203
N	-0.4137860	-6.9189185	1.1092377
C	-1.4077884	-9.3588045	-1.3658694
C	-1.8027031	-8.8005487	-2.7357612
H	-2.8176726	-8.3813744	-2.7434050
H	-1.0964920	-8.0205010	-3.0489881
H	-1.7710773	-9.6099380	-3.4786492
C	-2.3016652	-10.4975547	-0.8682912
H	-3.3464001	-10.1828023	-0.7414163
H	-2.2883942	-11.3184042	-1.5992649
H	-1.9331490	-10.8819054	0.0921068
C	0.5206892	-6.1661968	1.9877006
C	1.4946274	-5.3278425	1.1570632
H	2.1328195	-5.9645799	0.5327522
H	0.9521886	-4.6328078	0.5010618
H	2.1373647	-4.7417339	1.8287811
C	1.1936759	-7.0677476	3.0205004

H	-0.1386693	-5.4769933	2.5335699
H	1.8804443	-7.7801951	2.5501382
H	1.7687471	-6.4409347	3.7169006
H	0.4487963	-7.6354568	3.5936584
C	-0.1258603	-7.9654411	0.2774813
H	-0.3771128	-9.7316726	-1.4395150
Pd	1.6326934	-8.9741800	-0.0225811
Br	2.1514714	-7.5983364	-2.0388559
Br	0.9841668	-10.5969483	1.7682441
C	3.3953988	-9.9377246	-0.3449065
N	4.6378392	-9.4260419	-0.0106295
N	3.7087559	-11.1333731	-0.9532927
C	5.6734678	-10.2856892	-0.4138728
C	4.8627888	-8.1561305	0.6371949
C	5.0933327	-11.3558849	-0.9854881
H	6.7177600	-10.0681742	-0.2385694
H	5.4993664	-12.2598132	-1.4188393
C	2.8419006	-12.1331405	-1.5731458
C	1.4004808	-11.8017689	-1.7259500
C	6.2663644	-7.6140102	0.5178755
H	0.9427446	-11.6668387	-0.7311556
H	0.9186836	-12.6197262	-2.2707945
H	1.2917049	-10.8491869	-2.2650491
H	6.9700226	-8.2086532	1.1194243
H	6.2619413	-6.5889588	0.8994751
H	6.6147028	-7.6236494	-0.5241596
O	3.9719360	-7.5923078	1.2252588
O	3.3677959	-13.1599957	-1.9459332

HEP complex R_1=SH R_2=H

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Energy = -6915.8647078700

H	-2.5258265	-5.9205650	3.0919801
C	-2.7542090	-6.1867452	2.0604414
C	-3.9902836	-5.8667199	1.4974922
H	-4.7343364	-5.3481142	2.1024655
C	-4.2905138	-6.1970140	0.1650736
H	-5.2652394	-5.9326368	-0.2457126
C	-3.3665925	-6.8546534	-0.6480053
H	-3.6144196	-7.1016315	-1.6782207
C	-2.1249128	-7.1763104	-0.0894659
C	-1.8297732	-6.8489476	1.2488241
N	-0.9845249	-7.8059021	-0.5891229
N	-0.5334141	-7.3050414	1.4957687
C	-0.7968756	-8.3319480	-1.9616344
C	-0.8393834	-7.2045976	-2.9960693
H	-1.8347939	-6.7469097	-3.0761659
H	-0.1139267	-6.4202290	-2.7431043
H	-0.5778662	-7.6106058	-3.9828772
C	-1.7614707	-9.4829275	-2.2551445
H	-2.8112345	-9.1584107	-2.2548526
H	-1.5384388	-9.8983041	-3.2477288
H	-1.6388631	-10.2836134	-1.5137187

C	0.1398652	-7.0649026	2.7966948
C	0.8521956	-5.7079020	2.7908966
H	1.6748627	-5.7096566	2.0623477
H	0.1614319	-4.8939207	2.5315771
H	1.2652071	-5.5031711	3.7886866
C	1.0566936	-8.2106487	3.2123220
H	-0.6900090	-7.0273412	3.5195819
H	1.9378058	-8.2843232	2.5579779
H	1.4071542	-8.0238212	4.2374219
H	0.5334188	-9.1749318	3.1871504
C	-0.0141173	-7.8801804	0.3713631
H	0.2268774	-8.7396738	-1.9386509
Pd	1.8042850	-8.7304629	0.0228257
Br	2.7874335	-6.4904953	-0.4833913
Br	0.8251030	-10.9918833	0.4349933
C	3.5861793	-9.6100645	-0.4019897
N	4.2572828	-9.6155071	-1.5937464
N	4.3868311	-10.3596079	0.4155883
C	5.4442575	-10.3393598	-1.5176827
S	3.7060855	-8.8619689	-3.0525797
C	5.5179956	-10.8248070	-0.2499774
S	4.0592382	-10.7053989	2.0794755
H	6.2542892	-11.4500976	0.2382903
H	6.1133669	-10.4344394	-2.3632264
H	2.7918132	-11.1804424	1.8057446
H	3.4828218	-7.6486449	-2.4286855

HEP complex R_1=OCH_3 R_2=H

53

Energy = -6348.4336465210

H	-2.4523684	-6.1327951	3.1212175
C	-2.6358614	-6.2699153	2.0560991
C	-3.8006210	-5.7798630	1.4638704
H	-4.5341181	-5.2586542	2.0794414
C	-4.0427630	-5.9438806	0.0896666
H	-4.9626328	-5.5489426	-0.3424395
C	-3.1294144	-6.6002156	-0.7367143
H	-3.3304260	-6.7171899	-1.7997041
C	-1.9600169	-7.0936223	-0.1483295
C	-1.7236299	-6.9323611	1.2314297
N	-0.8531647	-7.7774332	-0.6491135
N	-0.4932726	-7.5363093	1.4983343
C	-0.6321774	-8.1849550	-2.0553808
C	-0.4832179	-6.9619744	-2.9640029
H	-1.4056000	-6.3676405	-3.0203557
H	0.3279288	-6.3149789	-2.6029074
H	-0.2360385	-7.2915890	-3.9827925
C	-1.6907204	-9.1890221	-2.5163610
H	-2.6960757	-8.7484336	-2.5592292
H	-1.4367562	-9.5456724	-3.5241856
H	-1.7100508	-10.0550478	-1.8417978
C	0.1118473	-7.5100677	2.8534056
C	1.0208789	-6.2863810	3.0103233

H	1.8799023	-6.3558086	2.3286614
H	0.4800816	-5.3565130	2.7845890
H	1.3879647	-6.2278241	4.0448749
C	0.8040329	-8.8191460	3.2189451
H	-0.7535671	-7.3965214	3.5240394
H	1.6997497	-8.9904675	2.6038611
H	1.1073065	-8.7749253	4.2748004
H	0.1407019	-9.6813206	3.0754308
C	0.0436022	-8.0412761	0.3485377
H	0.3372606	-8.7070290	-2.0139291
Pd	1.7945963	-9.0072255	0.0176854
Br	2.9563476	-6.8222642	-0.3246835
Br	0.6081218	-11.1788098	0.2207338
C	3.4992615	-10.0423903	-0.3678439
N	3.9509303	-10.5369718	-1.5517222
N	4.4466255	-10.5070709	0.4906301
C	5.1009336	-11.3010853	-1.4398280
O	3.2961852	-10.3693537	-2.7556542
C	5.4233154	-11.2816349	-0.1143694
O	4.4167407	-10.2941319	1.8546847
H	6.2202538	-11.7530242	0.4458412
H	5.5545885	-11.7933049	-2.2901955
C	3.7196775	-9.1354860	-3.3957883
H	3.1282252	-9.0948048	-4.3172566
H	4.7923738	-9.1774824	-3.6391859
H	3.4991770	-8.2727751	-2.7502546
C	5.0689643	-9.0380036	2.1855335
H	4.9503028	-8.9515643	3.2713016
H	4.5741199	-8.2017437	1.6704619
H	6.1374948	-9.0799868	1.9244848

HEP complex R_1=$COOCH_3$ R_2=H

55

Energy = -6424.8101697700

H	-2.6363692	-5.7771050	3.0066579
C	-2.8445475	-6.0910295	1.9842545
C	-4.0773169	-5.8141020	1.3925396
H	-4.8368687	-5.2819103	1.9658938
C	-4.3547464	-6.2050504	0.0716559
H	-5.3276093	-5.9727967	-0.3625939
C	-3.4104461	-6.8846072	-0.6983913
H	-3.6384773	-7.1773909	-1.7210968
C	-2.1731635	-7.1672590	-0.1092424
C	-1.8989455	-6.7771169	1.2171518
N	-1.0241730	-7.8106022	-0.5653300
N	-0.6005681	-7.2062648	1.4983472
C	-0.8175492	-8.3906905	-1.9134375
C	-0.8344600	-7.3023256	-2.9889410
H	-1.8195416	-6.8255118	-3.0891700
H	-0.0891097	-6.5294091	-2.7602188
H	-0.5759071	-7.7515755	-3.9574744
C	-1.7829329	-9.5477268	-2.1785215
H	-2.8312550	-9.2213214	-2.2243588

H	-1.5320120	-10.0087631	-3.1439789
H	-1.6853681	-10.3144365	-1.3982842
C	0.0591988	-6.9251846	2.7989698
C	1.0593358	-5.7737771	2.6705915
H	1.8893129	-6.0462639	2.0056650
H	0.5787332	-4.8723195	2.2662420
H	1.4671198	-5.5326535	3.6627389
C	0.6634463	-8.1794435	3.4242032
H	-0.7677725	-6.5953728	3.4442670
H	1.5285861	-8.5348145	2.8521545
H	0.9989886	-7.9419363	4.4439047
H	-0.0702619	-8.9947080	3.4745831
C	-0.0634907	-7.8312067	0.4081858
H	0.2004289	-8.8042630	-1.8618716
Pd	1.7687632	-8.6658809	0.0792574
Br	2.6368873	-6.4907147	-0.7808157
Br	0.9250282	-10.9051061	0.7906343
C	3.5393050	-9.5104412	-0.3692482
N	4.1164095	-9.6298066	-1.6112682
N	4.4545664	-10.1111588	0.4640672
C	5.3588421	-10.2715602	-1.5437322
C	3.5024340	-9.1878970	-2.8627959
C	5.5552754	-10.6025754	-0.2484000
C	4.3216901	-10.1968407	1.9126945
H	6.3831753	-11.1132146	0.2252740
H	5.9720437	-10.4610270	-2.4147608
C	4.4756298	-8.6393966	-3.8731281
H	3.9033463	-8.1881127	-4.6889366
H	5.1051783	-9.4404279	-4.2900023
H	5.1336880	-7.8912539	-3.4112850
C	4.9468788	-11.4228873	2.5270029
H	4.5949577	-11.5016019	3.5600426
H	6.0440630	-11.3318526	2.5415902
H	4.6832678	-12.3282678	1.9648278
O	3.7691745	-9.3212083	2.5266621
O	2.3158674	-9.2979793	-3.0314449

Fe-adduct R_1=CH_1CH_2 R_2=H

30

Energy = -3393.1561058670

Fe	1.4977455	10.3306834	23.7013807
S	3.6659884	10.1804598	23.5641411
C	4.2476736	10.5967006	25.1183544
C	3.3578930	10.8791174	26.1291425
S	1.6773402	10.8181162	25.8242007
S	1.5931058	10.6930470	21.5488210
C	0.2751381	11.7254831	21.2076976
C	-0.5825333	12.0978085	22.2170289
C	0.9121334	8.5243797	23.7539557
N	1.4200025	7.4657324	24.5093196
C	0.7165053	6.2879156	24.2576581

H	0.9576862	5.3547783	24.7466890
C	-0.2366699	6.5725731	23.3499388
H	-0.9929558	5.9383287	22.9088897
N	-0.1267788	7.9274924	23.0381642
S	-0.3294086	11.5147960	23.8056706
H	0.1605832	12.0859940	20.1827320
H	-1.4195353	12.7799672	22.0512814
H	5.3295451	10.6495643	25.2606428
H	3.6855605	11.1656800	27.1311816
C	2.4947579	7.5331125	25.4165166
C	-0.9784004	8.5697898	22.1185657
C	-1.8696117	7.9540212	21.3321481
C	2.9181674	6.5260182	26.1900908
H	2.9775789	8.5032413	25.4340260
H	2.4655520	5.5358785	26.2146479
H	3.7683257	6.6946246	26.8470965
H	-0.8637710	9.6476437	22.1115399
H	-2.0144768	6.8754058	21.2958355
H	-2.4906312	8.5571967	20.6739225

Fe-adduct R_1=CCH_1 R_2=H

26
Energy = -3390.5477839910

Fe	1.5990771	10.1966056	23.6360387
S	3.7064396	9.2867773	23.6079159
C	4.3094551	10.5208094	24.7215963
C	3.5260773	11.3183617	25.5434449
S	1.7490482	11.2411219	25.6708455
S	1.5081187	11.1112092	21.4625342
C	0.1207223	12.1921801	21.5468980
C	-0.7979971	12.0947396	22.5553070
C	0.9341411	8.2515656	23.8192007
N	1.2663537	7.2194748	24.7640914
C	0.5491862	6.0459291	24.4429775
H	0.6054315	5.1011958	24.9753623
C	-0.2156521	6.2867681	23.3620065
H	-0.8882676	5.6010765	22.8543833
N	-0.0112473	7.6156124	22.9624945
S	-0.6246129	10.9456950	23.8588616
H	-0.0275539	12.9449708	20.7619549
H	-1.6745650	12.7542368	22.5482374
H	5.4003938	10.6665106	24.7375831
H	4.0407031	12.0691408	26.1635656
C	2.1106852	7.2771607	25.8367531
C	-0.6736497	8.1321151	21.8968558
C	2.9211524	7.2421774	26.7539066
C	-1.3393137	8.4546727	20.9227766
H	-1.9542094	8.6109302	20.0850733
H	3.5192636	7.1545528	27.6203552

Fe-adduct R_1=Br R_2=H

```
22
 Energy =   -8385.9155785530
Fe    1.4602483   10.2831910   23.6629679
 S    3.6090042    9.8846917   23.3474036
 C    4.3733405   10.4749198   24.7507254
 C    3.6189124   11.0072857   25.7699488
 S    1.9139458   11.0408756   25.6329756
 S    1.4408211   10.9556888   21.6121623
 C    0.0021566   11.8625403   21.4264539
 C   -0.8873810   11.9485731   22.4716293
 C    0.9141773    8.4737050   23.7603161
 N    1.3129156    7.4618454   24.6276473
 C    0.6915144    6.2411201   24.3958195
 H    0.9002239    5.3625914   24.9914881
 C   -0.1411763    6.4364220   23.3447746
 H   -0.8125270    5.7642322   22.8273346
 N    0.0031933    7.7690497   22.9804821
 S   -0.5359571   11.1793566   23.9502618
 H   -0.1583519   12.3743420   20.4749084
 H   -1.8216126   12.5107923   22.3970795
 H    5.4641795   10.4279318   24.7972848
 H    4.0667149   11.4400937   26.6672730
Br    2.5304125    7.6321762   26.0174054
Br   -0.9822444    8.4545954   21.5652577
```

Fe-adduct R_1=Cl R_2=H

```
22
 Energy =   -4157.5436783530
Fe    1.4713518   10.3116689   23.6576889
 S    3.6293220   10.1159244   23.3523097
 C    4.3373604   10.5625484   24.8374112
 C    3.5358984   10.8982900   25.9049132
 S    1.8388049   10.8581332   25.7368445
 S    1.4063749   10.7655889   21.5255949
 C    0.0062412   11.7147940   21.3038348
 C   -0.8169519   11.9803050   22.3746154
 C    0.9302191    8.5172952   23.7550528
 N    1.4484602    7.4568030   24.4953641
 C    0.7796379    6.2516998   24.3181713
 H    1.0752333    5.3478841   24.8335125
 C   -0.2152681    6.5029914   23.4343106
 H   -0.9783349    5.8662390   23.0075097
 N   -0.1106237    7.8507007   23.1121044
 S   -0.4297567   11.3639299   23.9163588
 H   -0.1889307   12.1123995   20.3050743
 H   -1.7130116   12.5987310   22.2815567
 H    5.4279786   10.5921547   24.8955590
 H    3.9467418   11.2178873   26.8654286
Cl    2.7741185    7.5491566   25.5446050
Cl   -1.1923655    8.5508751   22.0137797
```

Fe-adduct R_1=$COOH_3$ R_2=H

```
34
 Energy =   -3694.2551965910
Fe    1.3614497   10.0189559   23.7038113
 S    3.4748599    9.3569380   23.7446129
 C    4.0882905    9.9665441   25.2167544
 C    3.2561201   10.6482361   26.0674044
 S    1.6070738   10.8548591   25.6544957
 S    1.7687260   10.8968581   21.7975934
 C    0.4096551   11.8624997   21.4081388
 C   -0.6808056   11.8673582   22.2396477
 C    0.6858214    8.2512359   23.6638835
 N    1.0708331    7.1438090   24.4156689
 C    0.3288365    6.0014628   24.0939851
 H    0.5042646    5.0505326   24.5783900
 C   -0.5621153    6.3660154   23.1507434
 H   -1.3271653    5.8002377   22.6367772
 N   -0.3342109    7.7196043   22.8777652
 S   -0.6574922   10.9325961   23.6684117
 H    0.4620342   12.4670730   20.5002460
 H   -1.5723618   12.4640245   22.0301016
 H    5.1462361    9.8056361   25.4392446
 H    3.6019711   11.0870829   27.0056788
 C    1.9806826    7.1099377   25.5308577
 C   -0.9997842    8.3423786   21.7646825
 O    2.7733684    6.0256700   25.3881856
 O   -2.3176876    8.0612399   21.8550647
 C   -3.1007684    8.5309612   20.7302685
 H   -4.1249551    8.2091954   20.9395883
 H   -2.7319869    8.0885626   19.7962659
 H   -3.0410323    9.6241091   20.6648776
 C    3.6762299    5.7999425   26.4988063
 H    4.2008577    4.8709095   26.2574340
 H    3.1142091    5.7033206   27.4363300
 H    4.3820801    6.6356706   26.5802444
 O    1.9501925    7.8523135   26.4776419
 O   -0.4522268    8.9094694   20.8550177
```

Fe-adduct R_1=OCH_3 R_2=H

```
30
 Energy =   -3467.3465227140
Fe    1.4946386   10.2657962   23.6798247
 S    3.5790030    9.7421988   23.1547978
 C    4.4913497   10.1518146   24.5358560
 C    3.8613099   10.6719845   25.6433850
 S    2.1592331   10.8600568   25.6352974
 S    1.2957399   11.0262378   21.6794445
 C   -0.1624327   11.9229801   21.6479707
 C   -0.9570329   11.9652124   22.7708742
```

C	0.8826020	8.4643585	23.7398585
N	0.8723346	7.5666728	24.7868230
C	0.3418352	6.3271569	24.4677306
H	0.2583845	5.5327960	25.1978257
C	-0.0029833	6.3993158	23.1554322
H	-0.4349935	5.6750267	22.4774126
N	0.3230943	7.6833602	22.7500361
S	-0.4625804	11.1612766	24.1911581
H	-0.4096282	12.4674813	20.7338706
H	-1.8984766	12.5198589	22.7974453
H	5.5740923	10.0070452	24.4963357
H	4.4093240	11.0005451	26.5295715
O	1.2621271	7.8496814	26.0774772
O	0.1593452	8.0643295	21.4362127
C	-1.1924569	8.5357858	21.2023481
H	-1.2039531	8.8090084	20.1418900
H	-1.4063803	9.4143483	21.8246429
H	-1.9196770	7.7318688	21.3934541
C	2.6214236	7.4008042	26.3156005
H	2.8178644	7.6749275	27.3575445
H	3.3209351	7.9185710	25.6466773
H	2.6943884	6.3091396	26.1922425

Fe-adduct R_1=H R_2= CH_2CH_3

34

Energy = -3395.6472188120

Fe	1.5804649	10.4624065	23.6849708
S	3.6964562	10.0424910	23.4102189
C	4.3777546	10.0931411	24.9779437
C	3.5845683	10.3970193	26.0605860
S	1.9204072	10.7285516	25.8276309
S	1.4320512	10.7247364	21.5215502
C	-0.0834067	11.4817355	21.2686456
C	-0.8629801	11.8275734	22.3489735
C	0.9295844	8.7062313	23.7549608
N	1.0917547	7.7733675	24.7323563
C	0.4267110	6.5723432	24.4570635
C	0.5083164	5.4316790	25.4232662
C	-0.1780553	6.7551404	23.2376244
C	-1.0167831	5.9137800	22.3216922
N	0.1515149	8.0566638	22.8456722
S	-0.3163042	11.4949872	23.9343374
H	-0.3799451	11.7093853	20.2419226
H	-1.8189824	12.3440658	22.2337185
H	5.4501517	9.9087653	25.0775448
H	3.9874135	10.4707932	27.0737284
H	1.5974098	7.9870514	25.5864638
H	-0.1244841	8.4996673	21.9744294
C	-1.5001929	4.5691222	22.8682943
H	-0.4500528	5.7399607	21.3893122
H	-1.8951710	6.5118785	22.0217119
H	-0.6631993	3.9005028	23.1105500

H	-2.1164956	4.0623751	22.1134543
H	-2.1157676	4.6962088	23.7694854
C	1.8722053	4.7169778	25.4301689
H	-0.2860233	4.7112681	25.1987461
H	0.2923001	5.8128057	26.4362843
H	2.0914658	4.2771205	24.4475542
H	1.8822428	3.9113662	26.1780065
H	2.6904306	5.4089081	25.6727621

Fe-adduct R_1=H R_2= CCH_1

26

Energy = -3390.6835763970

Fe	1.4939583	10.3327312	23.6722669
S	3.6272645	9.9824538	23.4085636
C	4.2927475	10.0647213	24.9810430
C	3.4821341	10.3671096	26.0532195
S	1.8160309	10.6581976	25.8028339
S	1.3443167	10.5777850	21.5118837
C	-0.1955731	11.2705324	21.2452307
C	-1.0011461	11.5822642	22.3183035
C	0.9554077	8.5581474	23.7714720
N	1.4835535	7.5565690	24.5353965
C	0.8256692	6.3394822	24.3571737
C	1.1773524	5.1597944	25.0289260
C	-0.1753693	6.5868370	23.4279833
C	-1.1378599	5.7297427	22.8757104
N	-0.0609926	7.9385050	23.1011133
S	-0.4563076	11.2720765	23.9079440
H	-0.4923728	11.4815023	20.2151895
H	-1.9781011	12.0552294	22.1933637
H	5.3676992	9.9040851	25.0932983
H	3.8732727	10.4630001	27.0689718
H	2.2675835	7.7041696	25.1632654
H	-0.6529549	8.4245877	22.4349789
C	1.4986639	4.1503402	25.6228089
C	-1.9772382	5.0003213	22.3876371
H	-2.7133438	4.3502861	21.9618763
H	1.7750952	3.2557189	26.1416066

Fe-adduct R_1=H R_2= C_6H_6

42

Energy = -3700.6229775940

Fe	1.2841788	9.6721399	23.2142915
S	3.2494792	8.8847021	22.6988028
C	4.2782471	9.3761686	23.9740006
C	3.7800601	10.1584717	24.9924525
S	2.1367751	10.6318722	24.9751406
S	0.6438023	9.1856146	21.1899766
C	-0.8606471	9.9748578	20.9939830
C	-1.3580768	10.7624863	22.0088489

C	0.6119085	8.1515777	24.0615647
N	1.2227574	7.3593935	24.9863353
C	0.4217100	6.2950781	25.4056019
C	-0.7705652	6.4356500	24.7206881
N	-0.6075758	7.5618198	23.9105700
S	-0.4677853	10.9440067	23.4577770
H	-1.3807318	9.8607906	20.0398885
H	-2.2974810	11.3117673	21.9109486
H	5.3289534	9.0796641	23.9300481
H	4.4110246	10.5220589	25.8071917
H	2.1903155	7.5001641	25.2595949
H	-1.3348033	7.9687098	23.3305860
H	0.8676337	1.9350750	26.9678212
C	1.1101298	2.9899982	27.1037996
H	2.3254320	2.6488299	28.8612814
C	1.9318142	3.3886039	28.1632647
H	-0.0077243	3.6091008	25.3665933
C	0.6108766	3.9308046	26.2045909
C	2.2494119	4.7401927	28.3181130
C	0.9160419	5.2970431	26.3558724
C	1.7452857	5.6870972	27.4259186
H	2.8860088	5.0625836	29.1431569
H	1.9757776	6.7437500	27.5759936
H	-4.1656646	4.1498822	26.9306097
C	-3.7703162	4.5166363	25.9822356
H	-5.4417604	3.7846183	24.8192466
C	-4.4895625	4.3161075	24.7993648
H	-2.0150540	5.3796849	26.8915966
C	-2.5570862	5.2025109	25.9626062
C	-3.9830194	4.8061659	23.5931522
C	-2.0317485	5.6917206	24.7516560
C	-2.7648919	5.4862155	23.5667934
H	-4.5337972	4.6513922	22.6644070
H	-2.3644125	5.8379330	22.6139550

Fe-adduct R_1=H R_2= Br

22

Energy = -8386.0073946180

Fe	1.5491072	10.6024348	23.6380405
S	3.6855887	10.2560337	23.3859319
C	4.3405588	10.3348404	24.9636482
C	3.5225360	10.6397435	26.0299828
S	1.8596051	10.9348218	25.7679836
S	1.4095918	10.8486227	21.4780490
C	-0.1443595	11.5028552	21.2001142
C	-0.9650959	11.7962970	22.2672566
C	1.0267899	8.8216312	23.7367219
N	1.6356654	7.7949868	24.4064873
C	0.9495372	6.5959010	24.2559392
Br	1.5047010	5.0020359	25.0416800

C	-0.1298556	6.8673676	23.4647585
Br	-1.4885734	5.7554302	22.8453946
N	-0.0609881	8.2219883	23.1614748
S	-0.4220881	11.5044120	23.8617724
H	-0.4399206	11.7037569	20.1676230
H	-1.9518665	12.2461306	22.1339402
H	5.4145623	10.1724082	25.0829761
H	3.9065944	10.7326467	27.0486419
H	2.4924127	7.9194705	24.9376660
H	-0.7319829	8.7321950	22.5955372

Fe-adduct R_1=H R_2= $COOCH_3$

34

Energy = -3694.2933516820

Fe	1.3503554	10.1977512	23.7839104
S	3.5184058	10.0368300	23.6604978
C	4.0618324	10.0523714	25.2797027
C	3.1561221	10.2072310	26.3059747
S	1.4935457	10.3815262	25.9503395
S	1.3353923	10.6028599	21.6411166
C	-0.2345839	11.1936035	21.3073031
C	-1.1372989	11.3572963	22.3346026
C	0.9547805	8.3908918	23.7127112
N	1.4267676	7.3722249	24.4858419
C	0.8867391	6.1412797	24.1382734
C	0.0183922	6.3872361	23.0929142
N	0.0936119	7.7466857	22.8561401
S	-0.6832038	10.9690609	23.9359211
H	-0.4743059	11.4589286	20.2747912
H	-2.1395464	11.7597358	22.1685276
H	5.1356903	9.9655438	25.4607962
H	3.4655677	10.2526795	27.3525894
H	2.1172119	7.4884683	25.2236063
H	-0.3854366	8.2281157	22.0990412
C	1.3952420	4.9393414	24.8074173
C	-0.7780254	5.5302305	22.1606553
O	-1.7170530	4.6963695	22.6552367
O	0.8923654	3.7974213	24.2791313
C	1.4035931	2.5751214	24.8669862
H	2.4921660	2.5221908	24.7415780
H	0.9098586	1.7660748	24.3212889
H	1.1602172	2.5335407	25.9361507
C	-2.1561365	4.7790417	24.0317642
H	-3.1682837	4.3607492	24.0347903
H	-2.1855268	5.8191232	24.3806802
H	-1.5012581	4.1798198	24.6745929
O	-0.6063977	5.6167520	20.9621968
O	2.2015197	4.9878934	25.7225399

Fe-adduct R_1=H R_2= OCH_3

```
30
 Energy =   -3467.4681371960
Fe    1.5754430   10.5626326   23.6281503
 S    3.7284920   10.2625098   23.7347580
 C    4.1277228   10.4545817   25.3859581
 C    3.1474043   10.7938041   26.2925955
 S    1.5388059   11.0229001   25.7579937
 S    1.7650466   10.6380477   21.4572777
 C    0.2580463   11.2239916   20.8970325
 C   -0.7162583   11.5823638   21.8026026
 C    1.0603264    8.7693104   23.7607795
 N    1.4406703    7.8481097   24.6960786
 C    0.8547217    6.6030074   24.4798354
 O    1.0947378    5.5891213   25.3391512
 C    0.0687834    6.7379622   23.3658326
 O   -0.6893774    5.8426119   22.6896637
 N    0.2232296    8.0678487   22.9466574
 S   -0.4130960   11.4355579   23.4790899
 H    0.1175606   11.3345159   19.8190041
 H   -1.6782137   11.9943232   21.4881519
 H    5.1729429   10.3329514   25.6798619
 H    3.3666716   10.9587408   27.3502627
 H    2.0677512    8.0665091   25.4643338
 H   -0.1810581    8.4674992   22.1053622
 C   -2.0861153    5.8192232   23.0845520
 H   -2.5650472    5.0632449   22.4528359
 H   -2.5562266    6.7992451   22.9145586
 H   -2.1809672    5.5423879   24.1448965
 C    1.4448377    4.3281266   24.7217060
 H    1.6427332    3.6386287   25.5489957
 H    2.3468189    4.4454634   24.1030415
 H    0.6187537    3.9489597   24.1044108
```

Fe-adduct R_1=H R_2= I

```
22
 Energy =   -3832.8332448540
Fe    1.5569125   10.6079150   23.6378069
 S    3.6936846   10.2642025   23.3840044
 C    4.3521374   10.3555872   24.9593987
 C    3.5347534   10.6578177   26.0268083
 S    1.8692616   10.9414109   25.7677017
 S    1.4189031   10.8551414   21.4780803
 C   -0.1308240   11.5197335   21.2007059
 C   -0.9495728   11.8173936   22.2682662
 C    1.0235499    8.8292272   23.7371426
 N    1.6154681    7.8052273   24.4244642
 C    0.9314096    6.6034798   24.2687130
 I    1.5326517    4.8394840   25.1562240
 C   -0.1341637    6.8733705   23.4528868
 I   -1.6261538    5.6385405   22.7382495
 N   -0.0540735    8.2284819   23.1452795
 S   -0.4090198   11.5194877   23.8623621
```

H	-0.4255842	11.7223422	20.1683577
H	-1.9341867	12.2720846	22.1360825
H	5.4275712	10.2021926	25.0771944
H	3.9206127	10.7562794	27.0443306
H	2.4583220	7.9365908	24.9753478
H	-0.7091493	8.7400095	22.5621829

Fe-adduct R_1=H R_2= $COCH_3$

32
Energy = -3543.7637585610

Fe	1.5026675	10.2986599	23.6886504
S	3.6338856	9.9971247	23.3496378
C	4.3586328	10.1339366	24.8907529
C	3.5823261	10.4301316	25.9887860
S	1.8992679	10.6593631	25.8008883
S	1.2764454	10.5448650	21.5347987
C	-0.2778803	11.2216564	21.3202654
C	-1.0513496	11.5215845	22.4194973
C	1.0001380	8.5258722	23.8101772
N	1.5573274	7.5240131	24.5553800
C	0.9221633	6.3053057	24.4064523
C	-0.1187558	6.5401965	23.4995342
N	-0.0252508	7.8806454	23.1766284
S	-0.4515484	11.2134557	23.9887638
H	-0.6118935	11.4276063	20.3007199
H	-2.0381657	11.9813916	22.3282735
H	5.4413214	10.0062059	24.9620362
H	4.0092966	10.5538426	26.9868667
H	2.3592160	7.6291192	25.1756736
H	-0.6761166	8.3125305	22.5218871
C	1.5034433	5.1988750	25.2138211
C	-1.2279225	5.8139758	22.8245488
C	-1.4935731	4.3487416	23.0491806
H	-0.6176730	3.7375467	22.7923707
H	-2.3393977	4.0556483	22.4184740
H	-1.7417639	4.1492989	24.1011841
C	0.9533641	3.7975150	25.1799347
H	1.0218430	3.3700320	24.1697405
H	-0.1036582	3.7748472	25.4777228
H	1.5394801	3.1836738	25.8719009
O	2.4705037	5.4789505	25.9219567
O	-1.9353630	6.4710385	22.0610555

Fe-adduct R_1=H R_2= SH

24
Energy = -4034.8376437500

Fe	1.5748777	10.6004762	23.6426976
S	3.7127524	10.2848816	23.3645368
C	4.3918249	10.4132277	24.9283559
C	3.5844783	10.7177714	26.0023215

S	1.9102978	10.9643181	25.7633828
S	1.4027236	10.8182159	21.4823457
C	-0.1688962	11.4371186	21.2178066
C	-0.9790221	11.7316318	22.2926961
C	1.0727454	8.8117224	23.7594893
N	1.6813868	7.7901313	24.4147585
C	0.9920695	6.5745261	24.2712850
S	1.5361828	5.0401421	24.8873667
C	-0.0952980	6.8598947	23.4768468
S	-1.3853758	5.8418824	22.8827841
N	-0.0243649	8.2119729	23.1859052
S	-0.4051979	11.4770834	23.8836228
H	-0.4831122	11.6173778	20.1870300
H	-1.9760862	12.1609804	22.1684428
H	5.4711370	10.2787440	25.0326306
H	3.9830833	10.8400263	27.0121675
H	2.5455185	7.9075991	24.9343533
H	-0.6858791	8.7384527	22.6229554
H	0.9848743	5.1104876	26.1311342
H	-0.8509101	4.7301154	23.4511749

Fe-adduct R_1= $COCH_3$ R_2= H

32
Energy = -3543.7198395200

Fe	1.4482160	10.0653405	23.6818413
S	3.5812024	9.6369659	24.0196011
C	3.9201494	10.2799882	25.5654278
C	2.9097823	10.8490424	26.2988454
S	1.3226100	10.9031859	25.6605432
S	2.0018144	10.4666286	21.6409017
C	0.6983081	11.3413619	20.9595194
C	-0.4241288	11.5857134	21.7099618
C	0.8373840	8.2817797	23.7680682
N	1.2927993	7.2461398	24.5706509
C	0.6038841	6.0600052	24.3235091
H	0.8091499	5.1432990	24.8616423
C	-0.3220248	6.3326725	23.3753433
H	-1.0496221	5.6882266	22.8981675
N	-0.1683902	7.6745564	23.0322911
S	-0.5038013	11.0139355	23.3179064
H	0.8064970	11.6962322	19.9325071
H	-1.2783596	12.1434169	21.3189473
H	4.9484353	10.2258916	25.9310260
H	3.0762484	11.2881760	27.2847468
C	2.2389020	7.3116830	25.7009383
C	-0.9195874	8.2186770	21.8819031
C	-2.4135762	8.2221044	22.0772565
H	-2.7923708	7.1871461	22.0757773
H	-2.8799139	8.7634310	21.2479848
H	-2.6862036	8.6750780	23.0378449
C	3.4095484	6.3706860	25.5731796
H	3.0738194	5.3340620	25.7399879

```
 H     4.1479044     6.6189838    26.3420919
 H     3.8576699     6.4223624    24.5740205
 O    -0.3428937     8.4966120    20.8617325
 O     1.9801776     7.9808160    26.6688140
```

Fe-adduct R_1= SH R_2= H

```
24
 Energy =   -4034.7718684520
Fe     1.3777085    10.2478062    23.6940770
 S     3.5109076     9.7334990    23.3539094
 C     4.3305529    10.3720402    24.7137823
 C     3.6174829    10.9887959    25.7119020
 S     1.9095037    11.0839424    25.5998159
 S     1.3297171    10.8727358    21.6370753
 C    -0.1029844    11.7907781    21.4485063
 C    -0.9805747    11.8963785    22.4997392
 C     0.7929318     8.4568186    23.8595835
 N     1.2197789     7.4809545    24.7531269
 C     0.6006704     6.2490962    24.5263875
 H     0.8279928     5.3831375    25.1345747
 C    -0.2386871     6.4165746    23.4815610
 H    -0.9103676     5.7324819    22.9799278
 N    -0.1180112     7.7489880    23.0744498
 S    -0.6166780    11.1458845    23.9854879
 H    -0.2677176    12.2882412    20.4902836
 H    -1.9159560    12.4565215    22.4250167
 H     5.4198037    10.2858124    24.7419947
 H     4.0964877    11.4488892    26.5788392
 S     2.2324566     7.6875047    26.1314658
 S    -1.0571189     8.3703441    21.7805027
 H     3.3248172     8.0962296    25.4313705
 H    -0.1779264     8.0646253    20.7896102
```

carbene-phosphinidene adduct R_2=CH_3 R_1=H

```
27
 Energy =    -878.0991688064
 C    -2.7679272     1.5491942     0.5244140
 C    -3.7488493     1.8933509    -0.4074648
 C    -3.4106379     2.4839259    -1.6455758
 C    -2.0428475     2.7410609    -1.8863790
 H    -1.7484467     3.2003421    -2.8330276
 C    -1.0647149     2.4165478    -0.9454783
 H    -0.0163101     2.6312355    -1.1628863
 C    -1.4181923     1.8092120     0.2641605
 H    -0.6536278     1.5497050     0.9976882
 P    -4.6190598     3.1219940    -2.8654256
 C    -7.9949910     1.0493364    -3.1609831
 C    -7.1667548     0.0040959    -2.8950058
 N    -5.8901732     0.5177105    -2.7080778
 N    -7.2309425     2.2039143    -3.1083336
 C    -5.9059437     1.8984464    -2.8341597
```

H	-7.3739537	-1.0564530	-2.8237748
H	-9.0574932	1.0706635	-3.3684280
C	-4.6840575	-0.2864623	-2.6324038
C	-7.7213040	3.5532489	-3.3102778
H	-3.0625963	1.0920847	1.4716482
H	-4.8006216	1.7285523	-0.1625247
H	-8.7923203	3.5871684	-3.0755311
H	-7.5632195	3.8884757	-4.3462198
H	-7.1587429	4.2257081	-2.6447265
H	-4.9088324	-1.2935678	-3.0033431
H	-4.2959048	-0.3441518	-1.6059187
H	-3.9123650	0.1810015	-3.2607754

carbene-phosphinidene adduct R_2=CH_3 R_1=Br

27
Energy = -6025.7783283480

C	-1.9960757	2.3884440	0.7561459
C	-3.3544186	2.5179445	0.4619630
C	-3.8400267	2.3448284	-0.8523670
C	-2.8977803	2.0455635	-1.8599542
H	-3.2297144	1.9547609	-2.8964590
C	-1.5423010	1.8978394	-1.5616423
H	-0.8369165	1.6654105	-2.3623590
C	-1.0808972	2.0695599	-0.2521340
H	-0.0197942	1.9636760	-0.0226374
P	-5.6062850	2.7234655	-1.1616226
C	-7.2742619	0.6629266	-4.1130010
C	-6.4207265	-0.3071544	-3.6744557
N	-5.6748194	0.2252419	-2.6256456
N	-7.0382039	1.8032461	-3.3547932
C	-6.0472161	1.5487156	-2.4130418
C	-4.8649168	-0.5448810	-1.6966189
C	-7.7085917	3.0838758	-3.4843516
H	-1.6513534	2.5296773	1.7823404
H	-4.0596350	2.7532618	1.2626056
H	-8.0571209	3.2096788	-4.5154956
H	-6.9805535	3.8647022	-3.2182980
H	-8.5641199	3.1587775	-2.7972711
H	-5.1333705	-1.6030787	-1.7867068
H	-5.0761066	-0.1814819	-0.6812418
H	-3.7922273	-0.4157398	-1.8940484
Br	-8.5106511	0.5860032	-5.5079771
Br	-6.1829358	-2.0328038	-4.3493126

carbene-phosphinidene adduct R_2=CH_3 R_1=CH_3

33
Energy = -956.7653405130

C	-2.8495883	1.5493971	0.5631817
C	-3.7547257	1.8801341	-0.4470404
C	-3.3350441	2.5407281	-1.6240057

C	-1.9658908	2.8781273	-1.7193870
H	-1.6080339	3.3915561	-2.6151631
C	-1.0658574	2.5664839	-0.6999053
H	-0.0153050	2.8452843	-0.8057938
C	-1.4978181	1.8910235	0.4469957
H	-0.7933330	1.6404486	1.2412282
P	-4.4456825	3.1616148	-2.9398975
C	-7.7778963	1.0333045	-3.4751785
C	-6.9361932	-0.0098300	-3.1984578
N	-5.6760750	0.5393575	-2.9314720
N	-7.0298135	2.2051973	-3.3445589
C	-5.7183969	1.9184602	-3.0132606
C	-7.1980163	-1.4753994	-3.1575503
C	-9.2253728	1.0418252	-3.8260466
C	-4.4445897	-0.2193597	-2.8166036
C	-7.5291187	3.5551501	-3.5188491
H	-3.2076428	1.0371425	1.4591077
H	-4.8138972	1.6483473	-0.3123286
H	-8.5868094	3.6021393	-3.2325724
H	-7.4203042	3.8979474	-4.5591191
H	-6.9278585	4.2177258	-2.8771230
H	-4.5692645	-1.1918652	-3.3062894
H	-4.1502266	-0.3693772	-1.7677827
H	-3.6457090	0.3500292	-3.3127701
H	-9.8353641	1.5613447	-3.0695967
H	-9.6020336	0.0146364	-3.9022196
H	-9.4093050	1.5363747	-4.7927349
H	-8.2578623	-1.6748640	-3.3559028
H	-6.9545286	-1.9073572	-2.1740342
H	-6.6137334	-2.0269572	-3.9115196

carbene-phosphinidene adduct R_2=CH_3 R_1=Cl

27
Energy = -1797.4207084120

C	-2.0087643	2.3838889	0.7636535
C	-3.3653623	2.5120166	0.4614406
C	-3.8437439	2.3375486	-0.8554029
C	-2.8950214	2.0414609	-1.8580096
H	-3.2207536	1.9516001	-2.8967317
C	-1.5406925	1.8960190	-1.5517576
H	-0.8301594	1.6657180	-2.3485381
C	-1.0872500	2.0666642	-0.2392896
H	-0.0274622	1.9615480	-0.0036002
P	-5.6088301	2.7157493	-1.1719416
C	-7.2782263	0.6601326	-4.1246915
C	-6.4167934	-0.3075297	-3.6965840
N	-5.6677399	0.2236557	-2.6480567
N	-7.0437578	1.7972630	-3.3605524
C	-6.0472075	1.5428434	-2.4251179
C	-4.8553017	-0.5552913	-1.7287133
C	-7.7221088	3.0735840	-3.4870822

H	-1.6703393	2.5255107	1.7918832
H	-4.0755677	2.7467720	1.2578215
H	-8.0927073	3.1890784	-4.5115103
H	-6.9933558	3.8608268	-3.2427145
H	-8.5635078	3.1503420	-2.7829322
H	-5.1128249	-1.6141967	-1.8402128
H	-5.0745339	-0.2132949	-0.7074775
H	-3.7827705	-0.4122714	-1.9181823
Cl	-8.4137866	0.5987620	-5.3919952
Cl	-6.2024610	-1.8859501	-4.3025047

carbene-phosphinidene adduct R_2=CH_3 R_1=$COOCH_3$

39

Energy = -1334.0437003940

C	-1.8002367	2.2859402	0.2812962
C	-3.1210449	2.6665358	0.0349825
C	-3.7665564	2.3272312	-1.1716350
C	-3.0231849	1.6065612	-2.1297804
H	-3.4767773	1.3754999	-3.0962396
C	-1.7078629	1.2127339	-1.8775360
H	-1.1554115	0.6563512	-2.6375626
C	-1.0879733	1.5494269	-0.6694084
H	-0.0573417	1.2491504	-0.4759304
P	-5.4364430	3.0244927	-1.4811698
C	-7.9137962	0.6649116	-3.4802073
C	-7.1466040	-0.3276046	-2.9003420
N	-6.1690792	0.3040956	-2.1248887
N	-7.3684918	1.8760087	-3.1008146
C	-6.2791931	1.6853049	-2.2552171
C	-7.3855701	-1.7821344	-2.9953207
C	-9.2243992	0.6234937	-4.1986786
C	-5.4834656	-0.3151284	-0.9961680
C	-7.8137478	3.1949800	-3.5243638
H	-1.3266332	2.5618704	1.2253482
H	-3.6690270	3.2331618	0.7913024
H	-8.3417921	3.1202836	-4.4798042
H	-6.9211985	3.8314652	-3.6171880
H	-8.4902600	3.6348572	-2.7792868
H	-5.9147298	-1.3054064	-0.8130867
H	-5.6304767	0.3258704	-0.1147320
H	-4.4038188	-0.4008392	-1.1752833
O	-10.1496151	1.2981384	-3.7910053
O	-9.3850907	-0.1182280	-5.3161148
O	-8.5095432	-2.2470069	-3.0025381
O	-6.3163598	-2.6328849	-3.0737139
C	-5.0307268	-2.1997122	-3.5674924
C	-8.3086302	-0.8386716	-5.9477999
H	-4.7206976	-2.9402479	-4.3147606
H	-4.3033676	-2.1878426	-2.7457624
H	-5.0848038	-1.2071878	-4.0325026
H	-8.5455588	-0.8456381	-7.0174607

```
 H    -8.2817414    -1.8675478    -5.5678845
 H    -7.3418693    -0.3423140    -5.7877602
```

carbene-phosphinidene adduct R_2=CH_3 R_1=F

```
27
 Energy =   -1076.6517716190
 C    -2.0333289     2.3777712     0.7786022
 C    -3.3843438     2.5155751     0.4570390
 C    -3.8476873     2.3307907    -0.8641608
 C    -2.8881537     2.0175814    -1.8512049
 H    -3.2005573     1.9193467    -2.8932232
 C    -1.5394642     1.8622555    -1.5252809
 H    -0.8209389     1.6172208    -2.3105498
 C    -1.1016341     2.0406488    -0.2085340
 H    -0.0463206     1.9262719     0.0425143
 P    -5.6101402     2.7057772    -1.1955349
 C    -7.2845199     0.6539594    -4.1346008
 C    -6.4116363    -0.2988952    -3.7299208
 N    -5.6377154     0.2310098    -2.7052977
 N    -7.0449417     1.7942411    -3.3838933
 C    -6.0320626     1.5452222    -2.4642154
 C    -4.8518304    -0.5783338    -1.7861901
 C    -7.7531042     3.0543239    -3.5159590
 H    -1.7071146     2.5265256     1.8098311
 H    -4.1027939     2.7653935     1.2413602
 H    -8.1414170     3.1462627    -4.5367844
 H    -7.0385246     3.8612017    -3.2968133
 H    -8.5854651     3.1235457    -2.8001935
 H    -5.0971587    -1.6337195    -1.9495890
 H    -5.1067214    -0.2809272    -0.7589632
 H    -3.7755029    -0.4211545    -1.9352357
 F    -8.1860869     0.6448839    -5.1147741
 F    -6.2118452    -1.5343486    -4.1872579
```

carbene-phosphinidene adduct R_2=CH_3 R_1=I

```
27
 Energy =   -1472.6031786000
 C    -1.9838497     2.4090081     0.7546036
 C    -3.3399730     2.5404378     0.4530246
 C    -3.8215596     2.3518302    -0.8606984
 C    -2.8766683     2.0347382    -1.8606908
 H    -3.2048063     1.9302692    -2.8972405
 C    -1.5227587     1.8847135    -1.5545135
 H    -0.8152300     1.6380576    -2.3493174
 C    -1.0657924     2.0727983    -0.2453695
 H    -0.0060078     1.9661183    -0.0097848
 P    -5.5846211     2.7386289    -1.1754963
 C    -7.2873927     0.6677749    -4.1028813
 C    -6.4346508    -0.3081071    -3.6620620
 N    -5.6791712     0.2303142    -2.6207574
```

N	-7.0367073	1.8112789	-3.3507942
C	-6.0394375	1.5580314	-2.4164785
C	-4.8727014	-0.5308271	-1.6810206
C	-7.7112746	3.0923527	-3.4551419
H	-1.6424538	2.5632987	1.7798774
H	-4.0479017	2.7903481	1.2466436
H	-8.1032581	3.2164220	-4.4709241
H	-6.9745223	3.8755927	-3.2223557
H	-8.5365680	3.1687561	-2.7320785
H	-5.1434966	-1.5897007	-1.7582168
H	-5.0855093	-0.1554980	-0.6701098
H	-3.7986746	-0.4069348	-1.8761673
I	-8.6690051	0.5727879	-5.6392612
I	-6.1570379	-2.2100400	-4.4415989

carbene-phosphinidene adduct R_2=CH_3 R_1=NH_2

31

Energy = -988.8642113279

C	-1.9724958	2.4379298	0.6447602
C	-3.3465372	2.5431044	0.4280674
C	-3.9167387	2.2847128	-0.8396892
C	-3.0313272	1.9273441	-1.8818192
H	-3.4240276	1.7701441	-2.8889939
C	-1.6589166	1.8034376	-1.6594717
H	-1.0031991	1.5246734	-2.4875031
C	-1.1165540	2.0575532	-0.3949418
H	-0.0428894	1.9676130	-0.2241638
P	-5.7077807	2.6081054	-1.0415161
C	-7.4358518	0.5113268	-3.9739937
C	-6.5612469	-0.4459641	-3.5282334
N	-5.8044485	0.1091957	-2.5052925
N	-7.1612564	1.6747094	-3.2234803
C	-6.1753998	1.4379232	-2.2999914
C	-4.9500870	-0.6417306	-1.6050813
C	-7.8336656	2.9480406	-3.3858031
H	-1.5668855	2.6450237	1.6374035
H	-4.0018563	2.8255282	1.2557069
H	-8.2882109	2.9777753	-4.3821667
H	-7.0917014	3.7493627	-3.2557826
H	-8.6201318	3.0855811	-2.6283930
H	-5.2918567	-1.6840632	-1.5494998
H	-5.0253528	-0.1832735	-0.6091947
H	-3.8975980	-0.6178992	-1.9198546
N	-8.3941230	0.5029449	-4.9961126
N	-6.3038594	-1.7209023	-4.0343796
H	-6.9884684	-1.9836146	-4.7425521
H	-6.2461254	-2.4528558	-3.3255475
H	-8.0306078	0.4137497	-5.9436042
H	-9.1905403	-0.1152560	-4.8500963

carbene-phosphinidene adduct R_2=CH_3 R_1=NO_2

```
31
 Energy =   -1287.3269660050
 C    -2.0750960    2.4347824    0.6341269
 C    -3.4226818    2.5832729    0.3003057
 C    -3.8858625    2.2894028   -0.9984239
 C    -2.9451298    1.8586880   -1.9560887
 H    -3.2644331    1.6675473   -2.9826695
 C    -1.6004815    1.6991104   -1.6167157
 H    -0.8898274    1.3629825   -2.3739766
 C    -1.1584887    1.9861755   -0.3207647
 H    -0.1054544    1.8699186   -0.0614013
 P    -5.6274127    2.7160430   -1.3795226
 C    -7.5108045    0.3835198   -3.9266145
 C    -6.5999183   -0.5511028   -3.4852005
 N    -5.8026929    0.0600217   -2.5334641
 N    -7.2460198    1.5662857   -3.2934439
 C    -6.1668717    1.4032048   -2.4101768
 C    -4.9925991   -0.6439654   -1.5398946
 C    -7.9024675    2.8471486   -3.5255293
 H    -1.7416004    2.6683709    1.6465538
 H    -4.1312888    2.9304286    1.0554312
 H    -8.3290475    2.8717699   -4.5323631
 H    -7.1407056    3.6301465   -3.4069604
 H    -8.7016352    3.0077256   -2.7901917
 H    -5.3551899   -1.6709007   -1.4389125
 H    -5.0972839   -0.1056519   -0.5902838
 H    -3.9358428   -0.6611432   -1.8309586
 N    -8.5645524    0.2564105   -4.9132413
 N    -6.4498709   -1.9137729   -3.9016176
 O    -5.3119684   -2.4059400   -3.8018575
 O    -7.4599584   -2.4928872   -4.3198800
 O    -8.2715319   -0.2563033   -5.9924345
 O    -9.6722421    0.7022715   -4.5817699
```

carbene-phosphinidene adduct R_2=CH_3 R_1=OH

```
29
 Energy =   -1028.6148108290
 C    -2.0336484    2.4325948    0.6869446
 C    -3.3966293    2.5451969    0.4118322
 C    -3.9125908    2.2837778   -0.8776441
 C    -2.9888926    1.9116487   -1.8795743
 H    -3.3399214    1.7515116   -2.9015363
 C    -1.6282079    1.7784049   -1.5978859
 H    -0.9406363    1.4855621   -2.3946031
 C    -1.1382389    2.0388645   -0.3134877
 H    -0.0731893    1.9435123   -0.0977467
 P    -5.6873115    2.6346231   -1.1545007
 C    -7.4173466    0.5343708   -4.0533253
 C    -6.5526882   -0.4215280   -3.6142521
 N    -5.7762786    0.1279533   -2.6071982
```

N	-7.1282430	1.7048556	-3.3367674
C	-6.1361318	1.4597441	-2.4088404
C	-4.9681834	-0.6543977	-1.6862329
C	-7.7732260	2.9864480	-3.5359524
H	-1.6685200	2.6454933	1.6937153
H	-4.0848831	2.8377981	1.2085502
H	-8.1180316	3.0568312	-4.5751176
H	-7.0347581	3.7712963	-3.3148804
H	-8.6284245	3.1234126	-2.8562894
H	-5.2544435	-1.7081041	-1.7748601
H	-5.1591374	-0.2870871	-0.6678318
H	-3.8959204	-0.5435826	-1.8965640
O	-6.3507454	-1.7083796	-3.9975344
H	-6.8934088	-1.8727771	-4.7907299
O	-8.2609991	0.4930294	-5.1299189
H	-9.1857441	0.4075468	-4.8289184

carbene-phosphinidene adduct R_2=CH_3 R_1=COH

31

Energy = -1104.8607868710

C	-2.7194767	1.4676229	0.5867681
C	-3.7467658	1.8358794	-0.2843700
C	-3.4704586	2.5287242	-1.4814694
C	-2.1300878	2.8722638	-1.7485695
H	-1.8925075	3.4212877	-2.6623623
C	-1.1048935	2.5173869	-0.8690516
H	-0.0749508	2.7957089	-1.0995736
C	-1.3929321	1.8057968	0.2989493
H	-0.5926044	1.5268287	0.9856453
P	-4.7725942	3.2148280	-2.5820086
C	-7.7879147	0.8354956	-3.5015228
C	-6.8665161	-0.1648001	-3.1910968
N	-5.6808248	0.4667144	-2.8388945
N	-7.1573273	2.0426107	-3.3035260
C	-5.8412376	1.8525803	-2.8700045
C	-7.0463884	-1.6145920	-3.1359556
C	-9.1872122	0.6276307	-3.8950504
C	-4.3829353	-0.1903374	-2.7575650
C	-7.7259535	3.3747166	-3.4694259
H	-2.9585285	0.9293843	1.5060661
H	-4.7817482	1.6046478	-0.0237891
H	-8.8033048	3.2819274	-3.6219796
H	-7.2693884	3.8690236	-4.3394394
H	-7.4835386	3.9672780	-2.5747593
H	-4.4104241	-1.1193687	-3.3372582
H	-4.0958771	-0.4044747	-1.7191050
H	-3.6318128	0.4842679	-3.1868726
O	-9.9592046	1.5213427	-4.2291223
H	-9.4921361	-0.4384114	-3.8680394
O	-7.9963189	-2.2277547	-3.6117494
H	-6.2348564	-2.1582782	-2.5957481

carbene-phosphinidene adduct R_2=CH_3 R_1=$COCH_3$

37
 Energy =   -1183.5265867110
 C   -1.7934975   2.4538939   0.5281395
 C   -3.1479955   2.7240951   0.3246199
 C   -3.7668764   2.4684500   -0.9166884
 C   -2.9625721   1.9465888   -1.9517494
 H   -3.3975583   1.7857977   -2.9407095
 C   -1.6119494   1.6623652   -1.7435057
 H   -1.0131808   1.2594015   -2.5629944
 C   -1.0181775   1.9138223   -0.5020378
 H   0.0397106   1.7002690   -0.3434320
 P   -5.4999329   3.0324707   -1.1323213
 C   -7.6972627   0.8058022   -3.5802422
 C   -6.8299528   -0.1883064   -3.1373648
 N   -5.9503888   0.4056785   -2.2366688
 N   -7.2947789   1.9867721   -2.9761702
 C   -6.2051948   1.7707766   -2.1402301
 C   -6.7699528   -1.6156109   -3.5183189
 C   -8.8795053   0.7540003   -4.4841774
 C   -5.1994189   -0.3175363   -1.2172623
 C   -7.8197429   3.3248778   -3.2240258
 H   -1.3427674   2.6622707   1.5003113
 H   -3.7440831   3.1380682   1.1413752
 H   -8.2153600   3.3917001   -4.2404104
 H   -6.9885828   4.0290953   -3.0731808
 H   -8.6263676   3.5624027   -2.5186234
 H   -5.6254608   -1.3201852   -1.1001322
 H   -5.2964429   0.2377272   -0.2736569
 H   -4.1313241   -0.3872739   -1.4628066
 O   -9.7775949   1.5785139   -4.3265637
 C   -8.9570118   -0.2727288   -5.5891618
 O   -7.7959431   -2.2544664   -3.7444905
 C   -5.4030802   -2.2624507   -3.6845084
 H   -4.5687209   -1.5528467   -3.6347027
 H   -5.3960116   -2.7678827   -4.6602816
 H   -5.2603647   -3.0420738   -2.9218285
 H   -7.9719887   -0.5808809   -5.9598052
 H   -9.5542798   0.1585857   -6.4016869
 H   -9.4654080   -1.1718428   -5.2170975

carbene-phosphinidene adduct R_2=SH R_1= CH_3

carbene-phosphinidene adduct R_2=SH R_1= CH_3

29
 Energy =   -1674.6052939090
 C   -2.3692259   1.8837556   0.7637035
 C   -3.5840538   2.2230570   0.1609083

C	-3.6671400	2.4676445	-1.2228413
C	-2.4776130	2.4093959	-1.9736879
H	-2.5131588	2.6358750	-3.0414598
C	-1.2607099	2.0696472	-1.3744127
H	-0.3528486	2.0231715	-1.9790760
C	-1.2039202	1.7992444	-0.0038163
H	-0.2542150	1.5380432	0.4656050
P	-5.2425968	3.0808255	-1.9800900
C	-7.7213240	0.5044647	-3.6953465
C	-6.8029730	-0.4186095	-3.2604922
N	-5.7839133	0.2593392	-2.6067499
N	-7.2405639	1.7642170	-3.2863951
C	-6.0413752	1.6342478	-2.6107932
C	-4.6388002	-0.3846940	-1.9829344
C	-7.8755417	3.0432466	-3.5120786
H	-2.3321184	1.6900877	1.8373601
H	-4.4890844	2.2994449	0.7667750
H	-8.8212297	2.8761150	-4.0397089
H	-7.2159048	3.6941804	-4.1078783
H	-8.0670695	3.5450355	-2.5500657
H	-4.7117111	-1.4658632	-2.1493390
H	-4.6235364	-0.1882882	-0.9035886
H	-3.7014219	-0.0178020	-2.4179162
S	-6.7957642	-2.1611236	-3.4483258
S	-9.2439886	0.2098859	-4.4784077
H	-7.9721588	-2.1348874	-4.1294360
H	-8.8797188	0.4384432	-5.7742120

carbene-phosphinidene adduct R_2=OCH_3 R_1= CH_3

35

Energy = -1107.2389025370

C	-2.0298317	2.5326069	0.7402020
C	-3.3644276	2.7012030	0.3697536
C	-3.8253968	2.3343789	-0.9148011
C	-2.8750160	1.8010855	-1.8138593
H	-3.1811418	1.5534314	-2.8328711
C	-1.5436813	1.6154276	-1.4361648
H	-0.8334578	1.1997633	-2.1546741
C	-1.1093198	1.9796084	-0.1566597
H	-0.0670029	1.8411036	0.1336895
P	-5.5556611	2.7593414	-1.3361591
C	-7.3098500	0.3997049	-4.0095744
C	-6.5068114	-0.5502044	-3.4392653
N	-5.7319748	0.0994664	-2.4580423

N	-7.0049245	1.6168235	-3.4102480
C	-6.0320147	1.4475162	-2.4346231
C	-5.0385207	-0.6053303	-1.3948874
C	-7.6137632	2.8896467	-3.7493228
H	-1.7075888	2.8270586	1.7411209
H	-4.0740317	3.1201231	1.0872249
H	-7.9439400	2.8670780	-4.7935397
H	-6.8569311	3.6726257	-3.5935326
H	-8.4752446	3.1078856	-3.1005358
H	-5.3664276	-1.6514422	-1.4046752
H	-5.2970513	-0.1322037	-0.4361985
H	-3.9470693	-0.5540793	-1.5144139
O	-8.2264300	0.3844146	-5.0029694
O	-6.4186269	-1.8870708	-3.6598726
C	-5.3223685	-2.2827171	-4.5226577
C	-8.9528521	-0.8481706	-5.1717662
H	-5.3866621	-3.3728260	-4.6145128
H	-4.3545030	-2.0040979	-4.0799513
H	-5.4230372	-1.8125187	-5.5126596
H	-9.7452518	-0.6273461	-5.8947233
H	-9.3890157	-1.1703103	-4.2147904
H	-8.3024521	-1.6433462	-5.5617695

carbene-phosphinidene adduct R_2=C_6H_5 R_1= CH_3

47

Energy = -1340.3888411250

C	-1.8582372	2.3016291	0.3837197
C	-3.2304036	2.5112223	0.2372949
C	-3.8827991	2.2775705	-0.9928905
C	-3.0888638	1.8334629	-2.0726024
H	-3.5505749	1.6872207	-3.0518202
C	-1.7200574	1.6072604	-1.9214085
H	-1.1333727	1.2633074	-2.7760519
C	-1.0932034	1.8406448	-0.6925071
H	-0.0216774	1.6711211	-0.5775188
P	-5.6487971	2.7493451	-1.1271185
C	-7.7579124	0.5774962	-3.7183676
C	-6.8982611	-0.4150983	-3.2955333
N	-6.0234313	0.1665845	-2.3689352
N	-7.3730412	1.7511684	-3.0655800
C	-6.3000347	1.5154432	-2.2223407
C	-6.8436426	-1.8319749	-3.6727967
C	-8.8653466	0.5166139	-4.6813513
C	-5.2049136	-0.5749673	-1.4214800

C	-7.8849201	3.0843976	-3.3317389
H	-1.3841540	2.4916585	1.3489343
H	-3.8168500	2.8571779	1.0919683
H	-8.2842700	3.1267956	-4.3512425
H	-7.0498581	3.7904986	-3.2075456
H	-8.6753655	3.3664769	-2.6213354
H	-5.5461882	-1.6152753	-1.3935711
H	-5.3224656	-0.1065320	-0.4338307
H	-4.1395865	-0.5421582	-1.6877527
C	-10.1409924	1.0150991	-4.3503548
C	-8.6791447	-0.0565026	-5.9538266
C	-8.0155393	-2.6124440	-3.7035989
C	-5.6219266	-2.4429051	-4.0207733
C	-11.1938738	0.9414247	-5.2616480
H	-10.3109988	1.4447267	-3.3620663
C	-10.9974520	0.3649697	-6.5199907
C	-9.7372698	-0.1352126	-6.8597069
H	-11.8216753	0.3074007	-7.2320512
H	-12.1751943	1.3282332	-4.9836679
H	-9.5733552	-0.5825889	-7.8412743
H	-7.6951070	-0.4368996	-6.2293934
C	-7.9674481	-3.9537645	-4.0834040
H	-8.9656829	-2.1587299	-3.4205264
C	-5.5774063	-3.7866383	-4.3930029
C	-6.7497753	-4.5480052	-4.4286085
H	-6.7137700	-5.5982928	-4.7205082
H	-8.8864668	-4.5414733	-4.0996653
H	-4.6223524	-4.2391744	-4.6645404
H	-4.7043109	-1.8524424	-4.0167394

Fe-adduct R_1=CH_3 R_2=H

28
Energy = -3316.9595031560

Fe	0.3093524	1.1256895	-0.0336802
S	2.4331241	0.6092662	-0.3820596
C	3.2540136	1.1890185	0.9989433
C	2.5524301	1.8049215	2.0054099
S	0.8446416	1.9446341	1.8828936
S	0.2396699	1.8358402	-2.0556787
C	-1.2463697	2.6790446	-2.2194404
C	-2.1231658	2.7166781	-1.1620998
C	-0.2290763	-0.7182854	0.0529463

N	0.1733044	-1.6899692	0.9442511
C	-0.4226397	-2.9097295	0.6624399
H	-0.2367413	-3.7921348	1.2619146
C	-1.2164118	-2.7211637	-0.4217480
H	-1.8599405	-3.4066228	-0.9589469
N	-1.1007044	-1.3868837	-0.7798408
S	-1.7155756	1.9475331	0.3075510
H	-1.4382528	3.1968486	-3.1617079
H	-3.0805738	3.2408209	-1.2182535
H	4.3401267	1.0715881	1.0355051
H	3.0384403	2.2472963	2.8777060
C	1.1126555	-1.5331871	2.0479839
C	-1.7807663	-0.8412215	-1.9483652
H	-2.6249506	-1.4981882	-2.1900470
H	-1.0978276	-0.7927974	-2.8063208
H	-2.1549712	0.1628290	-1.7299200
H	1.0520527	-0.5108668	2.4321519
H	2.1395078	-1.7326647	1.7161169
H	0.8386483	-2.2382939	2.8422952

Fe-adduct R_1=CH_3 R_2=OH

30
Energy = -3467.4751138480

Fe	1.4638300	10.3702680	23.6674347
S	3.5957786	9.8647514	23.3599198
C	4.3839314	10.4450492	24.7596979
C	3.6557080	11.0466300	25.7564735
S	1.9486322	11.1694188	25.6008154
S	1.4347361	11.1065151	21.6540290
C	-0.0508408	11.9475435	21.4688250
C	-0.9507830	11.9686225	22.5064522
C	0.9159501	8.5259347	23.7360873
N	1.3215055	7.5413694	24.6215015
C	0.7032008	6.3376095	24.3379784
O	0.9687937	5.2466178	25.1000820
C	-0.1099774	6.5351358	23.2670569
O	-0.8467039	5.6195164	22.5684885
N	0.0329620	7.8827019	22.9029728
S	-0.5752644	11.1810100	23.9755205
H	-0.2230749	12.4773217	20.5293047
H	-1.9075155	12.4920953	22.4347621
H	5.4695722	10.3342500	24.8207940
H	4.1179497	11.4819411	26.6448877
C	2.2366633	7.6639493	25.7493164
C	-0.6022665	8.4309353	21.7121580
H	-1.4075059	7.7522413	21.4084458
H	0.1223714	8.5138778	20.8918754
H	-1.0147123	9.4199278	21.9322230
H	2.5522089	8.7048044	25.8328555
H	3.1112951	7.0192952	25.5949236
H	1.7264152	7.3607636	26.6733932
H	-1.7837097	5.6649153	22.8393771
H	0.5590799	4.4731378	24.6706178

Fe-adduct R_1=CH_3 R_2=SH

```
30
 Energy =   -4113.4680844100
Fe    1.4745476   10.4016245   23.6676883
 S    3.6112758    9.9162330   23.3658843
 C    4.3868347   10.4811418   24.7786809
 C    3.6490860   11.0643241   25.7799142
 S    1.9423954   11.1802234   25.6174046
 S    1.4622394   11.1614850   21.6611879
 C   -0.0180064   12.0094069   21.4776422
 C   -0.9231691   12.0256506   22.5116050
 C    0.9254492    8.5601401   23.7032077
 N    1.3204348    7.5681726   24.5920056
 C    0.7232055    6.3585063   24.2889752
 S    1.0081769    4.9186149   25.2401493
 C   -0.0719504    6.5565743   23.1875086
 S   -0.9859404    5.3615251   22.3092456
 N    0.0660273    7.9183549   22.8503823
 S   -0.5578902   11.2237286   23.9740527
 H   -0.1847615   12.5472810   20.5418167
 H   -1.8778785   12.5529032   22.4407243
 H    5.4731445   10.3779401   24.8420032
 H    4.1056129   11.4920060   26.6751090
 C    2.2229153    7.7030007   25.7280653
 C   -0.5619137    8.4990487   21.6699569
 H   -1.4111837    7.8672101   21.3884799
 H    0.1509275    8.5365103   20.8356110
 H   -0.9094001    9.5098057   21.8973452
 H    2.5473204    8.7414526   25.8067083
 H    3.0979067    7.0537331   25.5882852
 H    1.6992583    7.4180612   26.6520762
 H   -2.1944313    5.5263496   22.9174373
 H    0.2054071    4.1715618   24.4361171
```

Fe-adduct R_1=CH_3 R_2=I

```
28
 Energy =   -3911.4621396460
Fe    1.4637127   10.3865425   23.6780143
 S    3.6013433    9.9265607   23.3554258
 C    4.3861485   10.5132706   24.7532732
 C    3.6529400   11.0959556   25.7590548
 S    1.9444376   11.1913641   25.6175686
 S    1.4334824   11.0804375   21.6430253
 C   -0.0354852   11.9466827   21.4578615
 C   -0.9241925   12.0094849   22.5048683
 C    0.9198038    8.5427607   23.7702760
 N    1.3481498    7.5646894   24.6481494
 C    0.7373711    6.3440291   24.3716905
 I    1.0559817    4.6050612   25.4476991
```

C	-0.0863445	6.5420980	23.3004617
I	-1.2932683	5.1554388	22.3474902
N	0.0212137	7.8858976	22.9486720
S	-0.5490421	11.2475001	23.9862522
H	-0.2099938	12.4584064	20.5088467
H	-1.8716286	12.5494143	22.4319160
H	5.4744506	10.4258943	24.8037807
H	4.1155706	11.5359859	26.6451014
C	2.2959502	7.7265539	25.7434584
C	-0.6674760	8.4610389	21.7996224
H	-1.6346468	7.9588122	21.6821473
H	-0.0730663	8.3240361	20.8861078
H	-0.8319333	9.5253617	21.9755530
H	2.6250749	8.7652675	25.7740050
H	3.1598124	7.0673690	25.5892109
H	1.8102543	7.4700663	26.6945876

Fe-adduct R_1=CH_3 R_2=F

28
Energy = -3515.5120827710

Fe	1.4584077	10.3667216	23.6801781
S	3.6044413	9.9560791	23.4070209
C	4.3439414	10.4980627	24.8472701
C	3.5758154	11.0304239	25.8553421
S	1.8721300	11.1095886	25.6718155
S	1.4462519	10.9200063	21.5929997
C	0.0122847	11.8266238	21.3566277
C	-0.8645202	11.9998295	22.4020303
C	0.9087117	8.5343056	23.7751512
N	1.3762220	7.5413030	24.6184017
C	0.7536305	6.3338102	24.3481679
F	1.0320759	5.2337016	25.0431838
C	-0.1181820	6.5458356	23.3373884
F	-0.9612466	5.7142041	22.7297703
N	-0.0331814	7.8861551	22.9937986
S	-0.5102977	11.3222886	23.9298226
H	-0.1510459	12.2761438	20.3746041
H	-1.7854714	12.5791993	22.2994433
H	5.4320888	10.4279173	24.9211063
H	4.0097667	11.4387607	26.7707581
C	2.3796523	7.6422871	25.6719548
C	-0.7979163	8.4291972	21.8761853
H	-1.7224461	7.8498579	21.7736041
H	-0.2203800	8.3628764	20.9451633
H	-1.0438212	9.4727257	22.0835436
H	2.5036722	8.6948139	25.9330159
H	3.3367983	7.2259465	25.3339879
H	2.0312077	7.0872850	26.5517738

Fe-adduct R_1=CH_3 R_2=Cl

```
28
 Energy =   -4236.2801349110
Fe    1.4572315   10.3738493   23.6816558
 S    3.5965327    9.9226429   23.3820673
 C    4.3657522   10.4956067   24.7940083
 C    3.6214254   11.0685717   25.7972617
 S    1.9152131   11.1646331   25.6387202
 S    1.4378114   10.9969943   21.6202848
 C   -0.0100653   11.8901709   21.4104388
 C   -0.8927487   12.0113410   22.4578961
 C    0.9092738    8.5360924   23.7756373
 N    1.3587825    7.5519922   24.6367580
 C    0.7540033    6.3317249   24.3549913
Cl    1.0653426    4.9000109   25.2220985
 C   -0.0910259    6.5345941   23.3072040
Cl   -1.1016497    5.4118046   22.5213092
 N   -0.0027977    7.8813972   22.9667741
 S   -0.5311235   11.2887794   23.9625026
 H   -0.1766118   12.3720299   20.4444586
 H   -1.8248827   12.5752509   22.3709900
 H    5.4536763   10.4103802   24.8540510
 H    4.0751154   11.5006479   26.6918537
 C    2.3216572    7.6927939   25.7218594
 C   -0.7344815    8.4472515   21.8396378
 H   -1.6858370    7.9138401   21.7366857
 H   -0.1558702    8.3412833   20.9124451
 H   -0.9297477    9.5033004   22.0336192
 H    2.5227541    8.7541225   25.8730499
 H    3.2530861    7.1671681   25.4753635
 H    1.8978041    7.2677066   26.6405001
```

Fe-adduct R_1=CH_3 R_2=Br

```
28
 Energy =   -8464.6375751780
Fe    1.4591755   10.3798076   23.6796587
 S    3.5955387    9.9179587   23.3631679
 C    4.3780167   10.4970149   24.7653696
 C    3.6435936   11.0785338   25.7710193
 S    1.9360742   11.1787727   25.6253355
 S    1.4280657   11.0377193   21.6313576
 C   -0.0300670   11.9191237   21.4385697
 C   -0.9125944   12.0120657   22.4888114
 C    0.9154210    8.5393091   23.7724779
 N    1.3555126    7.5582000   24.6420892
 C    0.7522960    6.3380839   24.3582074
Br    1.0738045    4.7686202   25.3142103
 C   -0.0779934    6.5368594   23.2977429
Br   -1.1635362    5.2920263   22.4288537
 N    0.0141739    7.8818688   22.9533127
 S   -0.5403646   11.2689891   23.9805448
 H   -0.2027233   12.4161449   20.4814398
 H   -1.8519486   12.5654601   22.4122353
```

H	5.4659381	10.4073363	24.8184029
H	4.1055186	11.5146373	26.6594064
C	2.2956094	7.7119415	25.7453459
C	-0.6999503	8.4529094	21.8174498
H	-1.6509640	7.9218094	21.6997734
H	-0.1082791	8.3478947	20.8984199
H	-0.8953678	9.5088761	22.0119761
H	2.5983639	8.7574723	25.8038842
H	3.1752963	7.0774803	25.5792677
H	1.8100099	7.4190644	26.6857901

Fe-adduct R_1=CH_3 R_2=NH_2

32
Energy = -3427.7267000460

Fe	1.4877008	10.3695307	23.6643566
S	3.5996541	9.8497285	23.2351953
C	4.4673309	10.4230385	24.5921752
C	3.7965253	11.0233060	25.6286833
S	2.0833643	11.1553408	25.5616684
S	1.3535234	11.2251723	21.7112165
C	-0.1769254	12.0010637	21.6192925
C	-1.0429288	11.9113697	22.6809530
C	0.9513483	8.5188475	23.7260376
N	1.3000827	7.5747985	24.6719256
C	0.6750358	6.3591737	24.4179353
N	0.9245419	5.2236470	25.1948061
C	-0.0629230	6.5120472	23.2758652
N	-0.8984311	5.6323439	22.5751966
N	0.1248287	7.8512166	22.8697949
S	-0.5773717	11.0618841	24.0888136
H	-0.4035951	12.5767760	20.7193684
H	-2.0300538	12.3804624	22.6674478
H	5.5540584	10.3056936	24.5931636
H	4.3080017	11.4543381	26.4920548
C	2.1684613	7.7773869	25.8229876
C	-0.4748122	8.3884091	21.6562229
H	-1.2277520	7.6686745	21.3166525
H	0.2867517	8.5226351	20.8772090
H	-0.9430696	9.3549005	21.8679120
H	2.9776473	8.4614767	25.5561711
H	2.5922079	6.8051597	26.1036344
H	1.6091870	8.1986229	26.6705942
H	-1.6593099	5.2343973	23.1229958
H	-0.4251195	4.9102161	22.0343100
H	0.5077272	4.3925378	24.7770523
H	0.6136330	5.3047443	26.1646276

Fe-adduct R_1=CH_3 R_2= CH_3

34
Energy = -3395.6258026200

Fe	1.4609436	10.3818724	23.6832404

S	3.5558770	9.7576382	23.2776000
C	4.4615491	10.4584222	24.5476317
C	3.8245094	11.1849989	25.5200395
S	2.1094004	11.3394432	25.4659071
S	1.3703185	11.4034239	21.8234182
C	-0.1765051	12.1580656	21.7430648
C	-1.0789724	11.9420479	22.7523413
C	0.9307414	8.5114634	23.7551532
N	1.2867467	7.5662397	24.6842196
C	0.6983646	6.3280176	24.4094125
C	0.9079705	5.1280264	25.2657785
C	-0.0398832	6.4933446	23.2714480
C	-0.8789252	5.5286868	22.5081440
N	0.1092658	7.8303339	22.8920874
S	-0.6435866	10.9687324	24.0897563
H	-0.3799973	12.8115194	20.8921650
H	-2.0799514	12.3808301	22.7410307
H	5.5449385	10.3131540	24.5460891
H	4.3563826	11.6994129	26.3230966
C	2.1569825	7.7736320	25.8331972
C	-0.5406154	8.3774783	21.7094323
H	-1.6324775	8.3378748	21.8202458
H	-0.2449722	7.8051804	20.8189757
H	-0.2282099	9.4168122	21.5856980
H	2.3739918	8.8408517	25.9246299
H	3.0978535	7.2209892	25.7087472
H	1.6538482	7.4313845	26.7478812
H	-0.5323539	5.4109340	21.4695467
H	-1.9342897	5.8404778	22.4684911
H	-0.8427298	4.5402608	22.9822081
H	0.3446707	4.2765488	24.8654792
H	0.5674581	5.2938753	26.2999236
H	1.9680967	4.8344765	25.3128301

Fe-adduct R_1=CH_3 R_2= COH

32
Energy = -3543.7040582890

Fe	1.4273133	10.2306594	23.7031243
S	3.5971644	10.1576409	23.5498350
C	4.1782603	10.6660432	25.0761962
C	3.2894374	10.9574424	26.0856097
S	1.6092823	10.8148618	25.8066987
S	1.4883441	10.4758302	21.5276710
C	0.1676382	11.4916651	21.1529557
C	-0.6689941	11.9269476	22.1545734
C	0.9031481	8.4015376	23.8165981
N	1.4660121	7.3806760	24.5690297
C	0.8387234	6.1598566	24.3489485
C	1.3144191	4.9085523	24.9660660
C	-0.1748031	6.4015465	23.4356830
C	-1.1890112	5.5098716	22.8398170
N	-0.1175939	7.7537072	23.1323872

S	-0.3938539	11.4282546	23.7685136
H	0.0380676	11.7977438	20.1121634
H	-1.4997319	12.6109647	21.9671630
H	5.2583316	10.7733338	25.2000891
H	3.6169580	11.3048978	27.0682412
C	2.6085388	7.5071832	25.4708459
C	-1.0909968	8.3851553	22.2435706
H	-2.1035229	8.0757158	22.5305530
H	-0.9008894	8.1038890	21.1999856
H	-1.0110411	9.4664011	22.3495027
H	2.8999167	8.5543096	25.5226438
H	3.4534570	6.9119257	25.1007976
H	2.3301901	7.1660285	26.4760970
O	-1.5505389	4.4492594	23.3135829
O	1.0040638	3.7888542	24.6021469
H	-1.6302808	5.8924927	21.8882545
H	2.0223418	5.0556524	25.8157557

Fe-adduct R_1=CH_3 R_2= OCH_3

36

Energy = -3546.0998427860

Fe	1.5040243	10.4328597	23.6636014
S	3.6641711	9.9427187	23.5152286
C	4.3529031	10.6137548	24.9282137
C	3.5516381	11.2508120	25.8426787
S	1.8568333	11.3331679	25.5664169
S	1.5871751	11.2185732	21.6795517
C	0.0569414	11.9401039	21.3729857
C	-0.9314740	11.8545310	22.3213978
C	1.0153310	8.5756316	23.7579347
N	1.2885379	7.6818315	24.7661199
C	0.7456364	6.4254978	24.4818465
O	0.8341347	5.3915140	25.3503879
C	0.1277165	6.5276360	23.2683726
O	-0.5111391	5.5920379	22.5264562
N	0.3027908	7.8474610	22.8362656
S	-0.6204410	11.0661574	23.8056536
H	-0.0727605	12.4803428	20.4327170
H	-1.9227022	12.2894786	22.1690314
H	5.4341297	10.5271482	25.0630929
H	3.9477546	11.7431774	26.7334284
C	1.9698230	7.9738790	26.0213165
C	-0.1457581	8.3096158	21.5286254
H	-0.7301234	9.2297060	21.6359396
H	-0.7613256	7.5193646	21.0854241
H	0.7153510	8.5055553	20.8780533
H	1.3428983	8.6098396	26.6585340
H	2.9144213	8.4891718	25.8191565
H	2.1587539	7.0232013	26.5310851
C	-1.8916623	5.3637080	22.9126297
C	1.6958641	4.3097019	24.9145212
H	2.7249873	4.6710462	24.7703682

H	1.3207970	3.8707161	23.9794733
H	1.6700025	3.5638363	25.7166598
H	-2.2684009	4.5863874	22.2389588
H	-2.4845649	6.2828068	22.7941032
H	-1.9463743	5.0191684	23.9548998

Fe-adduct R_1=CH_3 R_2= $COOCH_3$

40

Energy = -3772.9273806390

Fe	1.3816457	10.5313833	23.8045518
S	3.5147727	10.1621571	23.3912159
C	4.3281526	10.6263717	24.8184072
C	3.6129916	11.0934715	25.8945185
S	1.9012812	11.1665165	25.8089265
S	1.2733838	11.3111053	21.7963778
C	-0.1787451	12.2153674	21.7196135
C	-1.0139741	12.2571685	22.8115278
C	0.8846722	8.6818590	23.7400062
N	1.4280616	7.6214461	24.4443885
C	0.8520071	6.4142338	24.0628872
C	1.1328466	5.0785776	24.6352138
C	-0.0879677	6.7116239	23.1046179
C	-1.0190891	5.8008046	22.3922702
N	-0.0666044	8.0851835	22.9295148
S	-0.5891568	11.4202894	24.2372668
H	-0.3866637	12.7677574	20.8005201
H	-1.9458625	12.8277843	22.8103044
H	5.4190722	10.5619221	24.8299195
H	4.0932686	11.4560269	26.8059982
C	2.3888674	7.7343524	25.5395881
C	-0.8632235	8.7618025	21.9063127
H	-1.7771559	8.1833813	21.7448737
H	-0.2914652	8.8384927	20.9726405
H	-1.1178388	9.7629982	22.2581687
H	2.4198525	8.7763459	25.8604979
H	3.3828941	7.4091818	25.2159187
H	2.0579264	7.1084752	26.3764849
O	-2.2011511	6.0313183	22.2058120
O	0.2903575	4.2134245	24.7848368
O	-0.3789193	4.6903310	21.9693323
O	2.4450420	4.9241278	24.9540156
C	-1.2354010	3.6713518	21.3994693
C	2.7826041	3.6341562	25.5176889
H	-0.5580385	2.8799227	21.0664071
H	-1.8083837	4.0781388	20.5570630
H	-1.9260108	3.2941508	22.1644438
H	2.6156697	2.8421221	24.7767863
H	2.1704564	3.4306880	26.4053136
H	3.8426356	3.7013484	25.7793300

Fe-adduct R_1=CH_3 R_2=C_6H_5

```
48
 Energy =   -3779.2457023760
Fe    1.3626256    9.9368690   23.7291104
 S    3.4957173    9.4694785   23.3258786
 C    4.3519361   10.2607261   24.5761611
 C    3.6660147   10.9620812   25.5350788
 S    1.9482957   11.0039282   25.4856184
 S    1.1838661   10.6283927   21.7167795
 C   -0.3820366   11.3207370   21.5731732
 C   -1.2376014   11.2829140   22.6452582
 C    0.9462013    8.0698792   23.9790130
 N    1.4630563    7.2029293   24.9127656
 C    0.9430573    5.9124406   24.7563919
 C    1.3709904    4.7512347   25.5501630
 C    0.0589567    5.9750246   23.7052681
 C   -0.7831871    4.9125677   23.1298487
 N    0.0791770    7.2956013   23.2445474
 S   -0.7318126   10.5654755   24.1123524
 H   -0.6350258   11.8128180   20.6314830
 H   -2.2426953   11.7099061   22.6022924
 H    5.4433618   10.2012517   24.5684547
 H    4.1654942   11.5331461   26.3207344
 C    2.3139806    7.5964442   26.0322107
 C   -0.5974464    7.7316931   22.0256802
 H   -1.0534506    6.8596662   21.5483977
 H    0.1327153    8.1848471   21.3466383
 H   -1.3692652    8.4746823   22.2568455
 H    1.9518340    8.5467821   26.4363686
 H    3.3538824    7.7273369   25.7094569
 H    2.2615496    6.8202201   26.8020236
 C   -2.1812186    5.0647485   23.0596122
 C    2.7371449    4.4298210   25.6701305
 C   -0.2118700    3.7126021   22.6709115
 C   -1.0166741    2.6938913   22.1579187
 C   -2.4025893    2.8582466   22.0881689
 C   -2.9819298    4.0479471   22.5390396
 H   -4.0637259    4.1821597   22.4948375
 H   -2.6409733    5.9823091   23.4306430
 H   -0.5572038    1.7692441   21.8055799
 H   -3.0296355    2.0627176   21.6835497
 H    0.8703060    3.5850988   22.7163127
 C    0.4257496    3.9151632   26.1717069
 C    0.8345342    2.7871211   26.8845573
 C    2.1930255    2.4795886   26.9988061
 C    3.1423880    3.3062054   26.3906359
 H    2.5109534    1.6002906   27.5606886
 H    0.0874316    2.1504834   27.3605081
 H   -0.6343787    4.1588332   26.0941888
 H    3.4827514    5.0552594   25.1769247
 H    4.2046030    3.0698358   26.4693654
```

Fe-adduct R_1=CH_3 R_2=$COCH_3$

```
38
 Energy =   -3622.3804342340
Fe    1.5096082   10.3611137   23.6287057
 S    3.6257489   10.1589522   23.0078063
 C    4.5210657   10.7762428   24.3232018
 C    3.8663485   11.2158831   25.4487271
 S    2.1561621   11.1138447   25.5254939
 S    1.1664824   11.3229497   21.7353826
 C   -0.4307033   11.9534851   21.7965893
 C   -1.2092584   11.7174781   22.9019301
 C    1.1442946    8.4783263   23.6971498
 N    1.7234451    7.5382884   24.5400447
 C    1.1502069    6.2960853   24.3789605
 C    1.5900542    5.0723560   25.1428011
 C    0.1955372    6.4130339   23.3873712
 C   -0.6172220    5.2823355   22.9048326
 N    0.2133242    7.7552659   22.9851632
 S   -0.5682740   10.8472566   24.2243085
 H   -0.7702894   12.5596568   20.9541249
 H   -2.2335168   12.0902795   22.9831677
 H    5.6089625   10.8179355   24.2286024
 H    4.3877327   11.6648751   26.2968395
 C    2.7350839    7.8267652   25.5572561
 C   -0.5485713    8.2780241   21.8560973
 H   -1.6167782    8.3345548   22.0954224
 H   -0.3958640    7.6376636   20.9786200
 H   -0.1779441    9.2807887   21.6310751
 H    3.4460745    8.5536405   25.1585566
 H    3.2612766    6.8977630   25.7930163
 H    2.2605348    8.2410282   26.4557640
 O   -0.2539735    4.1420008   23.2042942
 O    2.7652362    4.7397981   25.1002557
 C   -1.8961754    5.4908591   22.1204812
 C    0.5855424    4.3934615   26.0399431
 H   -1.6755364    5.7527040   21.0752380
 H   -2.5151947    6.2957536   22.5393405
 H   -2.4524074    4.5472380   22.1286059
 H    0.6411350    4.8871775   27.0256164
 H    0.8600600    3.3402258   26.1683895
 H   -0.4417674    4.4786897   25.6720157
```

Fe-adduct R_1=CH_3 R_2=NO_2

```
32
 Energy =   -3726.1805777660
Fe    1.4213768   10.2259040   23.7041502
 S    3.5828674    9.9565788   23.5116788
 C    4.2435040   10.5354372   24.9740558
 C    3.4115204   11.0077634   25.9630438
 S    1.7180803   10.9882018   25.7297011
 S    1.4731411   10.5699110   21.5528208
```

C	0.1221465	11.5596406	21.2169371
C	-0.7364980	11.9168432	22.2315394
C	0.8929730	8.4106735	23.8387685
N	1.4591204	7.3965993	24.6060401
C	0.8409838	6.1859507	24.3560299
N	1.2024681	4.9303207	24.9601936
C	-0.1551706	6.4229383	23.4464550
N	-1.0824714	5.4753565	22.8467488
N	-0.1270710	7.7591971	23.1358183
S	-0.4495302	11.3609603	23.8208581
H	-0.0072584	11.9130199	20.1913858
H	-1.5954608	12.5712864	22.0666588
H	5.3313279	10.5413537	25.0754053
H	3.7926620	11.4262367	26.8972612
C	2.4729936	7.5693504	25.6495966
C	-0.9892261	8.3455721	22.1083544
H	-1.9977005	7.9363095	22.2208896
H	-0.5971966	8.1119549	21.1104064
H	-1.0108042	9.4249742	22.2531729
H	2.5193350	8.6305113	25.8956525
H	3.4445024	7.2059711	25.3019775
H	2.1753111	7.0017041	26.5382420
O	-2.2816728	5.7703753	22.8949728
O	-0.5947628	4.4699073	22.3348047
O	0.2972672	4.1027103	25.1063868
O	2.3918826	4.7752565	25.2728734

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=H

46
Energy = -3552.8984009240

Fe	1.5367758	10.1388343	23.6194721
S	3.2966316	9.2019317	22.6219049
C	4.6233483	10.1229599	23.1874825
C	4.4273290	11.0827753	24.1473021
S	2.8469666	11.3178256	24.7862241
S	1.2084123	11.4667399	22.0064840
C	-0.0473738	12.5367779	22.4935619
C	-0.7140019	12.2939640	23.6672781
C	0.8262463	8.2578043	23.9421087
N	1.0507272	7.4374886	25.0402634
C	0.4343822	6.2088627	24.8553719
C	-0.1837537	6.2375045	23.6557139
N	0.0447608	7.4846362	23.0939493
S	-0.2723283	10.9556276	24.6375830
H	-0.2781437	13.3804470	21.8396518
H	-1.5422018	12.9229830	24.0033334
H	5.6128912	9.9073135	22.7767959
H	5.2318391	11.7086881	24.5389086
C	1.8324599	7.7106813	26.3165330
C	-0.5368939	7.8223889	21.7293219
C	-1.3687618	6.6322058	21.2162792
C	0.5981821	8.0587004	20.7235388

C	-1.4831570	9.0242080	21.8466093
C	1.2255575	8.9111780	27.0535199
C	3.3198251	7.9056283	25.9898531
C	1.7233119	6.4944478	27.2555840
H	-0.7630165	5.7287191	21.0592825
H	-1.7820861	6.9211046	20.2415314
H	-2.2156041	6.3952978	21.8749969
H	1.2571664	7.1806716	20.6710532
H	1.2011499	8.9328056	20.9833297
H	0.1679124	8.2276136	19.7263689
H	3.5030016	8.7979870	25.3874138
H	3.7110838	7.0330226	25.4480614
H	3.8792196	8.0067990	26.9306269
H	1.2667562	9.8245344	26.4543837
H	1.7899191	9.0874665	27.9802520
H	0.1777160	8.7128152	27.3193766
H	0.6850466	6.2781897	27.5437470
H	2.2734619	6.7413170	28.1727327
H	2.1825312	5.5905662	26.8316995
H	-2.2966098	8.8069198	22.5526252
H	-1.9249898	9.2263213	20.8605766
H	-0.9682707	9.9279432	22.1802778
H	0.4713748	5.4086202	25.5769806
H	-0.7621835	5.4638428	23.1765647

Fe-adduct R_1=CH_3 R_2=OCH_3

54

Energy = -3782.0107741160

Fe	1.5391516	10.2646653	23.6718919
S	3.1842987	9.1313816	22.6653667
C	4.6037478	9.9634002	23.1380815
C	4.5264548	10.9683435	24.0661948
S	2.9969791	11.3590448	24.7520235
S	1.3432814	11.5299108	21.9917370
C	0.2074491	12.7445081	22.4280639
C	-0.4654982	12.6387867	23.6210118
C	0.7550041	8.3610685	23.9859123
N	1.2278816	7.4826712	24.9457773
C	1.1552317	6.1697248	24.4692612
C	0.5037655	6.2049718	23.2687292
N	0.2027794	7.5548979	23.0030851
S	-0.1521884	11.3257869	24.6680851
H	0.0538637	13.5698340	21.7296342
H	-1.2202274	13.3694169	23.9225396
H	5.5530064	9.6553245	22.6930448
H	5.3939751	11.5389834	24.4039411
C	1.6966186	7.7995681	26.3574874
C	-0.6340492	7.9880429	21.8064148
C	-1.6874924	6.9098906	21.4704362
C	0.2835824	8.1918931	20.5920063
C	-1.4295564	9.2520900	22.1464277
C	1.0445967	9.0947940	26.8494792

C	3.2288206	7.8922607	26.3749509
C	1.2195072	6.6953410	27.3300693
H	-1.2608219	6.0590203	20.9333564
H	-2.4384141	7.3732993	20.8171276
H	-2.2099408	6.5564370	22.3709544
H	0.8292140	7.2663130	20.3616316
H	1.0095880	8.9933941	20.7672094
H	-0.3238442	8.4609044	19.7157917
H	3.5823973	8.7089877	25.7342448
H	3.6790323	6.9517687	26.0304762
H	3.5715768	8.0840880	27.4021266
H	1.3498776	9.9647311	26.2664937
H	1.3592488	9.2616598	27.8888829
H	-0.0512803	9.0202479	26.8269446
H	0.1568765	6.4581864	27.1731885
H	1.3215663	7.0848123	28.3516733
H	1.8110785	5.7791428	27.2622893
H	-2.1065960	9.0707079	22.9927284
H	-2.0360477	9.5148145	21.2686886
H	-0.8016296	10.1091253	22.3886452
O	1.8511777	5.1688364	25.0582417
O	0.3525621	5.2092344	22.3638882
C	1.1608662	3.9619039	25.4253027
H	1.0681084	3.2878370	24.5633994
H	0.1658642	4.1842238	25.8384351
H	1.7776029	3.4770965	26.1920066
C	-0.6085319	4.1621408	22.6233919
H	-0.0743672	3.2048189	22.6917407
H	-1.3144248	4.1181972	21.7820769
H	-1.1608922	4.3523195	23.5531007

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=COOCH$_3$

58

Energy = -4008.8379164960

Fe	1.5921682	10.1301206	23.6779488
S	3.1150494	8.7436525	22.8053380
C	4.6114468	9.4109197	23.2986641
C	4.6311957	10.4702212	24.1669779
S	3.1433670	11.0943645	24.7620555
S	1.6131623	11.3326926	21.9431442
C	0.6826975	12.7302722	22.3010867
C	-0.0178010	12.7869804	23.4813747
C	0.5415881	8.3916563	24.0247176
N	0.8663290	7.4870524	25.0179748
C	0.4023103	6.2149025	24.6733586
C	-0.3426428	6.3496563	23.5333428
N	-0.2712268	7.6801568	23.1361264
S	0.0621517	11.4874005	24.5849420
H	0.6752718	13.5373158	21.5653762
H	-0.6476738	13.6422699	23.7379035
H	5.5276878	8.9564599	22.9138448
H	5.5528453	10.9440499	24.5111004

C	1.3399414	7.8113165	26.4412538
C	-0.8916176	8.2040514	21.8371278
C	-2.0352587	7.2959275	21.3587991
C	0.1912725	8.2152030	20.7481319
C	-1.5191829	9.5810932	22.0774947
C	0.7811884	9.1719877	26.8748643
C	2.8719860	7.7932229	26.5103001
C	0.7381886	6.7847894	27.4237305
H	-1.6871381	6.3278555	20.9795457
H	-2.5087844	7.8099412	20.5120537
H	-2.7995674	7.1372085	22.1277366
H	0.5719623	7.1985643	20.5768932
H	1.0329771	8.8635153	21.0055888
H	-0.2473304	8.5794209	19.8085954
H	3.3044727	8.5438193	25.8385747
H	3.2657185	6.8072642	26.2394903
H	3.1864862	8.0293813	27.5370977
H	1.2055305	9.9973693	26.3005640
H	1.0443021	9.3284780	27.9300255
H	-0.3132539	9.2006128	26.7836921
H	-0.3515371	6.7074249	27.3094441
H	0.9421771	7.1461296	28.4402638
H	1.1821687	5.7885928	27.3470258
H	-2.3489096	9.5024596	22.7942876
H	-1.9206110	9.9491103	21.1239599
H	-0.8085390	10.3160667	22.4569896
C	0.8087241	4.8741651	25.1544748
C	-1.1247813	5.1957166	22.9633664
O	-2.2756663	4.9481333	23.2478669
O	0.0732000	3.9030996	25.1564722
O	2.1311495	4.8141154	25.4666303
O	-0.3450837	4.4430180	22.1533706
C	2.6031526	3.5026074	25.8552827
H	2.4746214	2.7921225	25.0292310
H	2.0521874	3.1373258	26.7317520
H	3.6635405	3.6358868	26.0895682
C	-0.9620067	3.2144331	21.6912697
H	-1.2125840	2.5806354	22.5508097
H	-0.2110612	2.7362001	21.0556601
H	-1.8740308	3.4344612	21.1216586

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=OH

48
Energy = -3703.3967398720

Fe	1.4952049	10.1868332	23.6783910
S	3.1432089	9.0797945	22.6456026
C	4.5588485	9.9205634	23.1139238
C	4.4788301	10.9173165	24.0510055
S	2.9508262	11.2864276	24.7517195
S	1.2618728	11.4553662	22.0041368
C	0.1097876	12.6476819	22.4589472
C	-0.5522146	12.5212919	23.6560224
C	0.7441388	8.2764637	23.9878862

N	1.2429641	7.3909402	24.9417814
C	1.1762574	6.0987737	24.4469932
C	0.5333630	6.1340675	23.2545317
N	0.2265013	7.4776480	22.9844207
S	-0.2074441	11.2063327	24.6903097
H	-0.0641973	13.4751056	21.7679016
H	-1.3191009	13.2349444	23.9674146
H	5.5076106	9.6258431	22.6587225
H	5.3434388	11.4932092	24.3871721
C	1.7046905	7.6892327	26.3599902
C	-0.6635503	7.8722033	21.8181645
C	-1.7007037	6.7504418	21.5611011
C	0.1989924	8.0719929	20.5638911
C	-1.4773419	9.1248149	22.1569261
C	1.0642441	8.9837278	26.8667389
C	3.2376767	7.7689259	26.3761978
C	1.2097134	6.5712388	27.3055585
H	-1.2831754	5.9075181	20.9983002
H	-2.5103016	7.1692091	20.9498489
H	-2.1536147	6.3970858	22.5001679
H	0.7718043	7.1619967	20.3372335
H	0.8999209	8.9047718	20.6943991
H	-0.4486763	8.2955332	19.7040017
H	3.5956895	8.5839057	25.7349045
H	3.6825546	6.8257520	26.0310666
H	3.5842746	7.9568406	27.4025365
H	1.3914403	9.8618867	26.3078554
H	1.3625229	9.1211282	27.9153029
H	-0.0318264	8.9256840	26.8251628
H	0.1283964	6.4080509	27.1901257
H	1.3879111	6.9059176	28.3360438
H	1.7286016	5.6200138	27.1631368
H	-2.1008271	8.9607610	23.0464206
H	-2.1365340	9.3387565	21.3041705
H	-0.8560786	10.0042787	22.3291819
O	1.7538303	5.0197550	25.0380950
O	0.4572491	5.0657983	22.3973204
H	1.6989577	4.2951842	24.3835595
H	-0.4503564	4.7078808	22.3831256

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=COH

50
Energy = -3779.6213777150

Fe	1.5122137	10.1157002	23.6424201
S	3.1424035	8.9774929	22.6095482
C	4.5775617	9.7834100	23.0769705
C	4.5198970	10.7893372	24.0046554
S	3.0009537	11.1984387	24.6989706
S	1.2602272	11.3820888	21.9670774
C	0.1516017	12.6074135	22.4320701
C	-0.4823643	12.5100091	23.6464108
C	0.7384468	8.2549229	23.9861167

N	1.2118012	7.3953951	24.9490996
C	1.0380595	6.0682553	24.5315267
C	0.2779805	6.0998441	23.3845812
N	0.0701648	7.4252444	23.0601827
S	-0.1389463	11.1999646	24.6852006
H	-0.0156059	13.4317546	21.7359899
H	-1.2220927	13.2449881	23.9728810
H	5.5176660	9.4617520	22.6225056
H	5.3954162	11.3531666	24.3326610
C	1.6574754	7.7141031	26.3733014
C	-0.7241426	7.8797038	21.8338101
C	-1.7043035	6.7829131	21.3925083
C	0.2476300	8.1451868	20.6742057
C	-1.5687394	9.1066152	22.1936394
C	1.0425112	9.0303464	26.8578564
C	3.1907215	7.7671787	26.4322995
C	1.0958557	6.6276673	27.3185254
H	-1.2050195	5.9282502	20.9194054
H	-2.3562439	7.2246938	20.6273581
H	-2.3347650	6.4180020	22.2119580
H	0.8157835	7.2359897	20.4305878
H	0.9539093	8.9484424	20.8987387
H	-0.3293405	8.4325191	19.7839262
H	3.5790592	8.5610734	25.7821333
H	3.6451801	6.8152661	26.1250733
H	3.5084525	7.9770810	27.4632885
H	1.4367225	9.8976337	26.3268919
H	1.2911452	9.1466524	27.9217471
H	-0.0513091	9.0189605	26.7606283
H	0.0096728	6.5202858	27.1954441
H	1.2880867	6.9504073	28.3501242
H	1.5600657	5.6425189	27.2040197
H	-2.2798134	8.8645242	22.9954253
H	-2.1412690	9.4011626	21.3037944
H	-0.9696995	9.9619875	22.5103122
C	1.7396392	4.8565403	24.9334059
C	-0.1656501	4.8018115	22.7335507
O	-1.2284517	4.2734644	22.9821759
O	1.5091362	3.7719257	24.4025738
H	2.5523144	4.9513910	25.6829465
H	0.5707919	4.3589742	22.0247156

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=CH$_3$

52
 Energy = -3631.5370203970

Fe	1.5269852	10.0693755	23.6511845
S	3.0952338	8.8135746	22.6532154
C	4.5609971	9.5925721	23.0721515
C	4.5506665	10.6308688	23.9660026
S	3.0552083	11.1245361	24.6625032
S	1.3684011	11.2552698	21.9107243
C	0.3089543	12.5511921	22.3042109

C	-0.3431598	12.5455927	23.5131577
C	0.6773135	8.2090163	24.0577858
N	1.1591088	7.3405068	25.0172010
C	1.1051623	6.0205163	24.5437390
C	1.7238126	4.8078792	25.1646463
C	0.4711712	6.0529400	23.3332420
C	0.2956332	4.8862347	22.4123357
N	0.1378352	7.3942760	23.0788802
S	-0.0823207	11.2735814	24.6226874
H	0.1853497	13.3466431	21.5662826
H	-1.0483149	13.3336041	23.7891532
H	5.4861162	9.2274007	22.6192201
H	5.4518203	11.1692614	24.2668460
C	1.5837127	7.7064118	26.4276483
C	-0.8241664	7.8163764	21.9767798
C	-1.9540874	6.7677840	21.8529942
C	-0.0713865	7.9608539	20.6454557
C	-1.5255400	9.1301965	22.3392893
C	0.9274044	9.0241644	26.8540922
C	3.1143923	7.8142500	26.5048693
C	1.0632609	6.6428922	27.4222081
H	-1.6517680	5.8483300	21.3448783
H	-2.7627297	7.2119931	21.2584130
H	-2.3664778	6.5129327	22.8394868
H	0.4213843	7.0249478	20.3489190
H	0.6924275	8.7452437	20.7133302
H	-0.7794146	8.2367069	19.8512209
H	3.4847824	8.6057606	25.8419095
H	3.6037421	6.8717311	26.2243936
H	3.4123930	8.0575394	27.5349363
H	1.2757603	9.8720481	26.2617574
H	1.1921447	9.2165693	27.9028777
H	-0.1668155	8.9664746	26.7773136
H	0.0081460	6.4017650	27.2304912
H	1.1304117	7.0668831	28.4327286
H	1.6451199	5.7175436	27.4247356
H	-2.0357082	9.0546133	23.3084445
H	-2.2779614	9.3324608	21.5646457
H	-0.8446115	9.9816518	22.3741598
H	1.9495703	4.0812309	24.3733822
H	1.0668898	4.3012753	25.8868672
H	2.6704558	5.0350556	25.6693401
H	-0.6639449	4.3645593	22.5404225
H	1.0882630	4.1538396	22.6134980
H	0.3883466	5.1723838	21.3584323

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=F

46

Energy = -3751.4371853510

Fe	1.4918995	10.2088901	23.6911040
S	3.1775177	9.1564851	22.6613235
C	4.5652798	10.0256303	23.1591998
C	4.4493688	11.0055531	24.1105984

S	2.9053167	11.3261088	24.8000890
S	1.2646715	11.4969369	22.0289765
C	0.0830158	12.6597604	22.4815201
C	-0.5995112	12.5019430	23.6634416
C	0.7946079	8.2814962	23.9710954
N	1.3029054	7.3995688	24.9167997
C	1.2771063	6.1144509	24.3982942
C	0.6729915	6.1617266	23.1925360
N	0.3090713	7.4769812	22.9444134
S	-0.2503241	11.1771574	24.6831263
H	-0.0934979	13.4945810	21.8000547
H	-1.3858573	13.1955839	23.9712874
H	5.5263877	9.7626991	22.7105876
H	5.2962940	11.5967819	24.4648358
C	1.7629925	7.6832950	26.3406656
C	-0.6009878	7.8423579	21.7735336
C	-1.6265589	6.7048535	21.5576396
C	0.2591967	8.0290359	20.5167623
C	-1.4144515	9.0967905	22.0993418
C	1.0553867	8.9292907	26.8783368
C	3.2895033	7.8406639	26.3464028
C	1.3414594	6.5122141	27.2567487
H	-1.1946462	5.8074324	21.1069387
H	-2.3989290	7.0812146	20.8748459
H	-2.1212582	6.4306771	22.5001992
H	0.8265870	7.1162053	20.2877480
H	0.9646868	8.8598858	20.6403112
H	-0.3905599	8.2502375	19.6584883
H	3.6044172	8.6913266	25.7301952
H	3.7786220	6.9318533	25.9695219
H	3.6336047	8.0111088	27.3765384
H	1.3134249	9.8321627	26.3218826
H	1.3703431	9.0743702	27.9208413
H	-0.0356197	8.8019732	26.8619820
H	0.2796554	6.2615951	27.1221540
H	1.4763925	6.8407160	28.2955186
H	1.9423458	5.6095604	27.1140524
H	-2.0126495	8.9561139	23.0091903
H	-2.0980581	9.2746715	21.2579156
H	-0.7956060	9.9867334	22.2223118
F	1.8332797	5.0464157	24.9708312
F	0.5135937	5.1495702	22.3392189

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=Cl

46
Energy = -4472.1945973410

Fe	1.5318116	10.2306755	23.6627237
S	3.1865654	9.1710770	22.5779207
C	4.5922270	10.0159634	23.0612181
C	4.5086385	10.9792653	24.0333010
S	2.9833275	11.3077662	24.7572692
S	1.3024949	11.5159491	21.9958913
C	0.1558453	12.7064081	22.4665618

C	-0.5080722	12.5696580	23.6616328
C	0.8463690	8.2892309	23.9489350
N	1.4277058	7.4184404	24.8566081
C	1.5579232	6.1612550	24.2657613
C	0.9442643	6.2105074	23.0502437
N	0.4292790	7.4977120	22.8872151
S	-0.1695487	11.2435323	24.6822847
H	-0.0135936	13.5429330	21.7853543
H	-1.2716537	13.2833611	23.9809209
H	5.5394508	9.7541676	22.5833173
H	5.3692607	11.5552650	24.3792589
C	1.7071310	7.6785307	26.3317485
C	-0.6251250	7.8403135	21.8353595
C	-1.6723750	6.7046773	21.8128303
C	0.0537112	8.0152273	20.4696855
C	-1.3895085	9.1093409	22.2192854
C	1.0097971	8.9600249	26.7926753
C	3.2235714	7.7799675	26.5542619
C	1.0826630	6.5313703	27.1556967
H	-1.2907323	5.7586255	21.4209129
H	-2.5002964	7.0227657	21.1656369
H	-2.0800745	6.5338103	22.8191526
H	0.5917556	7.1099863	20.1616434
H	0.7615523	8.8540034	20.4968304
H	-0.7099669	8.2334281	19.7104420
H	3.6405084	8.6156597	25.9769009
H	3.7407700	6.8570473	26.2636901
H	3.4216671	7.9629922	27.6198011
H	1.4405308	9.8561578	26.3415613
H	1.1374512	9.0343705	27.8816301
H	-0.0658704	8.9355870	26.5744979
H	0.0107897	6.4340375	26.9329141
H	1.1824709	6.7872911	28.2189208
H	1.5651728	5.5625462	27.0018854
H	-1.8393074	9.0233855	23.2163221
H	-2.1962634	9.2386099	21.4845202
H	-0.7661027	10.0053254	22.1959529
Cl	2.4913037	4.8386644	24.8226221
Cl	1.0059414	4.9578064	21.8855716

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=Br

46

Energy = -8700.5498026160

Fe	1.5477862	10.2294222	23.6540518
S	3.1943562	9.1576668	22.5661895
C	4.6070285	9.9884918	23.0518220
C	4.5316838	10.9527380	24.0237136
S	3.0088263	11.2959605	24.7457334
S	1.3179972	11.5040613	21.9793643
C	0.1809262	12.7050652	22.4461208
C	-0.4763594	12.5829908	23.6464061
C	0.8559585	8.2903210	23.9444443

N	1.4388891	7.4195434	24.8510042
C	1.5751303	6.1642213	24.2559390
C	0.9610529	6.2152355	23.0391206
N	0.4397596	7.5009424	22.8806967
S	-0.1404124	11.2639554	24.6766387
H	0.0122306	13.5366566	21.7587458
H	-1.2331010	13.3047514	23.9639346
H	5.5525031	9.7177434	22.5752961
H	5.3973247	11.5214324	24.3695325
C	1.6933481	7.6852965	26.3306258
C	-0.6363127	7.8499130	21.8502160
C	-1.6837243	6.7153584	21.8457719
C	0.0120487	8.0372553	20.4716717
C	-1.3932475	9.1164936	22.2565043
C	0.9883792	8.9683425	26.7759307
C	3.2048770	7.7937271	26.5820299
C	1.0530483	6.5416922	27.1458110
H	-1.3055883	5.7647236	21.4612285
H	-2.5162461	7.0269126	21.2009011
H	-2.0831640	6.5554508	22.8571526
H	0.5436185	7.1361099	20.1422094
H	0.7194580	8.8765947	20.4906247
H	-0.7694508	8.2619404	19.7324933
H	3.6280076	8.6316435	26.0123556
H	3.7336998	6.8738955	26.3033905
H	3.3811684	7.9789709	27.6510455
H	1.4320768	9.8635112	26.3353980
H	1.0924372	9.0417640	27.8674385
H	-0.0820974	8.9476086	26.5340149
H	-0.0168744	6.4523329	26.9109488
H	1.1442462	6.7942379	28.2106649
H	1.5299688	5.5693033	26.9947722
H	-1.8219968	9.0258016	23.2623700
H	-2.2154897	9.2475276	21.5393748
H	-0.7718046	10.0134948	22.2240453
Br	2.6322738	4.7204176	24.8324444
Br	1.0791896	4.8531908	21.7491615

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=I

46

Energy = -4147.3712327010

Fe	1.5681575	10.2230154	23.6409884
S	3.2060724	9.1345877	22.5555214
C	4.6248832	9.9546539	23.0406273
C	4.5577119	10.9212214	24.0106722
S	3.0373986	11.2810325	24.7295186
S	1.3451809	11.4837464	21.9553822
C	0.2237783	12.7023112	22.4151042
C	-0.4287549	12.6001123	23.6198308
C	0.8655013	8.2881565	23.9396381
N	1.4461006	7.4176820	24.8463107
C	1.5848136	6.1579203	24.2527763

C	0.9651604	6.2092686	23.0320619
N	0.4428770	7.4989759	22.8797332
S	-0.1038871	11.2878443	24.6620463
H	0.0623886	13.5292571	21.7203775
H	-1.1746927	13.3343715	23.9341405
H	5.5680405	9.6757018	22.5644986
H	5.4279878	11.4829882	24.3559939
C	1.6773498	7.6963800	26.3284337
C	-0.6514203	7.8604212	21.8718396
C	-1.7031569	6.7311123	21.8795686
C	-0.0337255	8.0633796	20.4816228
C	-1.3978083	9.1261010	22.3014361
C	0.9595033	8.9795457	26.7552017
C	3.1824845	7.8205107	26.6072936
C	1.0280125	6.5580109	27.1424021
H	-1.3328250	5.7761203	21.4963232
H	-2.5383407	7.0422153	21.2377810
H	-2.0953731	6.5760997	22.8944934
H	0.4951431	7.1690834	20.1298546
H	0.6688675	8.9066228	20.4933974
H	-0.8320223	8.2907471	19.7613210
H	3.6069839	8.6614971	26.0433174
H	3.7280158	6.9062518	26.3424238
H	3.3364057	8.0097763	27.6791392
H	1.4131022	9.8745486	26.3244126
H	1.0383370	9.0549399	27.8486634
H	-0.1050264	8.9582994	26.4889498
H	-0.0384271	6.4654975	26.8935530
H	1.1058144	6.8156526	28.2072216
H	1.5073331	5.5841569	27.0043945
H	-1.7999972	9.0338448	23.3179822
H	-2.2388601	9.2589462	21.6067105
H	-0.7783215	10.0236980	22.2550164
I	2.7882198	4.5611955	24.8638726
I	1.1344441	4.7072084	21.5875020

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=SH

48

Energy = -4349.3817163140

Fe	1.5381094	10.1956377	23.6628423
S	3.1516690	9.0343468	22.6225481
C	4.5908831	9.8242116	23.1030682
C	4.5424460	10.8150880	24.0486508
S	3.0264134	11.2357696	24.7456460
S	1.3774587	11.4517409	21.9696975
C	0.2784001	12.6999930	22.4036091
C	-0.3965270	12.6209458	23.5978333
C	0.7451283	8.3006882	23.9665820
N	1.2527517	7.4045865	24.9046950
C	1.2935747	6.1262154	24.3602784
C	0.6705715	6.1794398	23.1336986
N	0.2682112	7.5202357	22.9390689

S	-0.1199678	11.3082483	24.6539139
H	0.1471215	13.5256401	21.7011056
H	-1.1304400	13.3745051	23.8941390
H	5.5303648	9.5045026	22.6457189
H	5.4257245	11.3585851	24.3903051
C	1.6107808	7.7059858	26.3521404
C	-0.7349261	7.9276506	21.8630709
C	-1.8383337	6.8482826	21.7855824
C	-0.0158132	8.0801664	20.5153693
C	-1.4489398	9.2276420	22.2425886
C	0.9417729	9.0046445	26.8105123
C	3.1377099	7.7921025	26.4910847
C	1.0319825	6.5938854	27.2515238
H	-1.4973391	5.9165316	21.3264335
H	-2.6554863	7.2428762	21.1674481
H	-2.2459405	6.6326350	22.7834678
H	0.4738642	7.1455241	20.2127556
H	0.7380494	8.8762578	20.5660511
H	-0.7477990	8.3476292	19.7404771
H	3.5360932	8.6137817	25.8824348
H	3.6230548	6.8572358	26.1797122
H	3.3980637	7.9805482	27.5422965
H	1.3385450	9.8823407	26.2968975
H	1.1398733	9.1251805	27.8846462
H	-0.1459961	8.9692048	26.6628020
H	-0.0409730	6.4505633	27.0615967
H	1.1525402	6.9097879	28.2962511
H	1.5363612	5.6266201	27.1507726
H	-1.9297324	9.1497851	23.2260223
H	-2.2278777	9.4068007	21.4886714
H	-0.7847680	10.0934625	22.2496730
S	2.1233851	4.7221809	25.0162544
S	0.7583775	4.9029039	21.9358389
H	2.0566946	4.1012328	23.7987987
H	-0.2870763	4.1345671	22.3475751

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=NH$_2$

50

Energy = -3663.6454851980

Fe	1.5087403	10.1151988	23.6554837
S	3.0760336	8.9127777	22.5884193
C	4.5464437	9.6667838	23.0367833
C	4.5395281	10.6701403	23.9691602
S	3.0437273	11.1392767	24.6831377
S	1.2661705	11.3417072	21.9515579
C	0.1658040	12.5856138	22.3998726
C	-0.4560584	12.5229985	23.6226578
C	0.6971433	8.2404466	24.0413523
N	1.2406511	7.3707306	24.9833683
C	1.2793251	6.0820488	24.4578786
C	0.6195822	6.0941153	23.2633603
N	0.1924064	7.4297367	23.0505457

S	-0.1139232	11.2357108	24.6920571
H	-0.0050066	13.3940005	21.6858398
H	-1.1876605	13.2718956	23.9361672
H	5.4695525	9.3166946	22.5680208
H	5.4410951	11.1970446	24.2881827
C	1.6092627	7.6807776	26.4213896
C	-0.7814948	7.8111882	21.9530887
C	-1.8564064	6.7055305	21.8172611
C	-0.0311773	7.9880347	20.6242432
C	-1.5426389	9.0900186	22.3195311
C	1.0090269	9.0170059	26.8675467
C	3.1393190	7.7143690	26.5665997
C	0.9787796	6.6093295	27.3394344
H	-1.5055528	5.8214834	21.2752505
H	-2.6993916	7.1189545	21.2484293
H	-2.2370718	6.3998689	22.8020866
H	0.5039986	7.0718572	20.3354945
H	0.6976546	8.8047799	20.6918533
H	-0.7462006	8.2254928	19.8239920
H	3.5743892	8.4741713	25.9041359
H	3.6051593	6.7457548	26.3333898
H	3.4050360	7.9637051	27.6035074
H	1.4749912	9.8725178	26.3745889
H	1.1759660	9.1153661	27.9495981
H	-0.0725816	9.0489079	26.6828785
H	-0.1143903	6.6050097	27.2226006
H	1.2051383	6.8802871	28.3795789
H	1.3460979	5.5964581	27.1541481
H	-2.0807661	8.9711497	23.2693009
H	-2.2762630	9.2844355	21.5247320
H	-0.8939794	9.9637281	22.3982172
N	1.8603398	4.9580430	25.0451642
N	0.5403474	4.9719570	22.4232825
H	1.8289315	4.1965777	24.3614996
H	2.8238127	5.1114324	25.3455062
H	0.8522611	5.1418029	21.4670834
H	-0.3633121	4.5000337	22.4073211

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=NO$_2$

50

Energy = -3962.0941018150

Fe	1.5478716	10.0869015	23.6397157
S	3.2124446	8.9426669	22.6729528
C	4.6216852	9.7763571	23.1590654
C	4.5294434	10.8003877	24.0660696
S	2.9938642	11.2070137	24.7169420
S	1.3813856	11.3047475	21.9140098
C	0.2863612	12.5643078	22.3129523
C	-0.3865698	12.5201184	23.5098883
C	0.7909865	8.2317324	23.9876429
N	1.2755739	7.3706730	24.9589757
C	1.0486336	6.0536202	24.5651547

C	0.3054241	6.0963776	23.4192471
N	0.1141016	7.4110746	23.0625266
S	-0.1124061	11.2356617	24.5990788
H	0.1614214	13.3738730	21.5910515
H	-1.1118142	13.2870782	23.7921471
H	5.5768764	9.4579260	22.7349024
H	5.3920163	11.3769933	24.4057744
C	1.6450624	7.7355860	26.4166129
C	-0.7240437	7.8532166	21.8443022
C	-1.7991631	6.7992225	21.5137620
C	0.2150762	8.0229412	20.6430011
C	-1.4831709	9.1380572	22.1850648
C	0.8629890	8.9836858	26.8386258
C	3.1555134	7.9626136	26.5398753
C	1.1767182	6.5983368	27.3481714
H	-1.4098574	5.9159494	20.9984367
H	-2.5015584	7.2757525	20.8187515
H	-2.3703219	6.4923784	22.3992615
H	0.7244841	7.0785731	20.4087425
H	0.9693450	8.7956837	20.8224042
H	-0.3789370	8.3191218	19.7669711
H	3.4799017	8.7994567	25.9103358
H	3.7139865	7.0636943	26.2608191
H	3.3889109	8.2123749	27.5847304
H	1.1791000	9.8769759	26.2977168
H	1.0582942	9.1546511	27.9058412
H	-0.2190335	8.8487824	26.7054069
H	0.1223203	6.3415076	27.1733697
H	1.2571936	6.9690088	28.3782471
H	1.7925111	5.6976584	27.2856759
H	-2.1546448	8.9834257	23.0408540
H	-2.0946558	9.4028131	21.3122674
H	-0.8299319	9.9817047	22.4037251
N	1.7748456	4.8724163	24.9764541
N	-0.0509578	4.9062877	22.6209845
O	1.2220130	3.7848743	24.7693491
O	2.9078673	5.0200727	25.4491944
O	-1.0437060	4.2790305	22.9660014
O	0.6949701	4.6522256	21.6755566

Fe-adduct R_1=$C(CH_3)_3$ R_2=$COCH_3$

56
Energy = -3858.2928049030

Fe	1.5553333	10.0771393	23.5676589
S	3.0149868	8.8001204	22.4453240
C	4.5280864	9.5372085	22.7519485
C	4.6095010	10.5789652	23.6383299
S	3.1847661	11.1051126	24.4457586
S	1.2259563	11.2868699	21.8659476
C	0.2250289	12.5901849	22.3658269
C	-0.3050985	12.5782733	23.6324376
C	0.7308599	8.2571735	24.0332742

N	1.1008717	7.4077474	25.0652527
C	0.7168877	6.0952056	24.7761081
C	0.0590663	6.1211340	23.5739307
N	0.0318325	7.4540341	23.1419308
S	0.0575260	11.2945814	24.6980362
H	0.0405493	13.3932423	21.6493896
H	-0.9732062	13.3670569	23.9867479
H	5.4066442	9.1390772	22.2386878
H	5.5429985	11.0963690	23.8686674
C	1.7582732	7.7844620	26.3921605
C	-0.9374766	7.9224401	22.0465816
C	-1.9935450	6.8293100	21.8034633
C	-0.2007862	8.2046760	20.7298686
C	-1.7034956	9.1606732	22.5332732
C	1.2601536	9.1542395	26.8648593
C	3.2842278	7.7585170	26.2229485
C	1.3270499	6.7897171	27.4871731
H	-1.5938732	5.9394512	21.3028733
H	-2.7515762	7.2482564	21.1285497
H	-2.4967549	6.5235051	22.7302123
H	0.2039576	7.2859900	20.2867478
H	0.6163783	8.9187040	20.8651571
H	-0.9115850	8.6344512	20.0098486
H	3.6106966	8.4861117	25.4711756
H	3.6247978	6.7600979	25.9209347
H	3.7577554	8.0188333	27.1806640
H	1.5989804	9.9651220	26.2196069
H	1.6659869	9.3375633	27.8692620
H	0.1636454	9.1815017	26.9263190
H	0.2335365	6.6913306	27.5343659
H	1.6623750	7.1962606	28.4500347
H	1.7859805	5.8004378	27.3949812
H	-2.1973368	8.9635773	23.4948006
H	-2.4758424	9.3999123	21.7896407
H	-1.0595785	10.0352138	22.6475256
C	1.2709385	4.8254096	25.4059943
C	-0.1546629	4.8720400	22.7619697
C	0.3015006	3.8705928	26.0474444
H	-0.3858331	3.4893156	25.2770449
H	-0.3227445	4.3925312	26.7866413
H	0.8473148	3.0442027	26.5165231
C	0.6980239	4.7020650	21.5203928
H	1.5942052	4.1413292	21.8345168
H	1.0441942	5.6482034	21.0921478
H	0.1685809	4.0954436	20.7752346
O	-0.8537531	3.9572196	23.1769708
O	2.4685004	4.5986169	25.3135943

Fe-adduct R_1=C(CH$_3$)$_3$ R_2=C$_6$H$_5$

66
 Energy = -4015.1559027820

Fe	1.5858673	9.9078107	23.5116726
S	2.9800309	8.3853189	22.6388162
C	4.5322010	9.0643474	22.8915279
C	4.6620282	10.2097703	23.6310391
S	3.2560907	10.9372002	24.3101290
S	1.4317851	10.8691455	21.6399702
C	0.5347872	12.3107732	21.9035120
C	-0.0382532	12.5311087	23.1323503
C	0.5859230	8.2048749	24.1570608
N	0.9733157	7.4209857	25.2284339
C	0.6620665	6.0729426	24.9775107
C	1.1513127	4.8697648	25.6961366
C	-0.0065182	6.0297979	23.7834780
C	-0.2754402	4.7835527	23.0237977
N	-0.1115193	7.3532622	23.3172295
S	0.1612593	11.3898315	24.3862494
H	0.4453009	13.0116720	21.0706363
H	-0.6430211	13.4187214	23.3347244
H	5.3953737	8.5499857	22.4617235
H	5.6230134	10.6927754	23.8199808
C	1.5428034	7.9226064	26.5516548
C	-1.0571940	7.7599936	22.1842333
C	-2.2570303	6.7909716	22.1351916
C	-0.3261218	7.7322938	20.8342481
C	-1.6552651	9.1435504	22.4637367
C	1.0211424	9.3348492	26.8412430
C	3.0774870	7.9047103	26.5059446
C	1.0450041	7.0386740	27.7124875
C	-1.2618447	3.8674127	23.4244200
C	2.4901496	4.4669951	25.5536978
C	0.5499290	4.4480349	21.9366867
C	0.3705867	3.2455628	21.2499800
C	-0.6272249	2.3513075	21.6466582
C	-1.4377529	2.6631247	22.7413778
H	-2.2130565	1.9666307	23.0643935
H	-1.9077416	4.1131264	24.2676180
H	1.0220987	3.0019752	20.4094587
H	-0.7668226	1.4117685	21.1102308
H	1.3517850	5.1282019	21.6457500
C	0.2807392	4.0558269	26.4387553
C	0.7404038	2.8866992	27.0462921
C	2.0787057	2.5063044	26.9147171
C	2.9505332	3.2971650	26.1619916
H	2.4387065	1.5933342	27.3909541
H	0.0508579	2.2713233	27.6261062
H	-0.7607630	4.3566944	26.5562892

H	3.1662596	5.0693591	24.9450640
H	3.9925515	2.9984986	26.0385653
H	-2.0073899	5.8089852	21.7245466
H	-3.0173723	7.2385454	21.4813409
H	-2.7067599	6.6576365	23.1292888
H	0.0263236	6.7213058	20.5948669
H	0.5283333	8.4184289	20.8259466
H	-1.0223100	8.0443865	20.0424054
H	3.4599266	8.5209376	25.6844854
H	3.4574548	6.8813862	26.3897281
H	3.4712977	8.3066428	27.4505082
H	1.4199560	10.0778852	26.1488050
H	1.3407875	9.6185141	27.8531900
H	-0.0760163	9.3687088	26.8024003
H	-0.0457373	6.9091673	27.6808571
H	1.2928513	7.5561794	28.6489574
H	1.5187537	6.0547202	27.7463332
H	-2.1825424	9.1567551	23.4271187
H	-2.3802604	9.3639118	21.6683714
H	-0.9105754	9.9409465	22.4715836

Fe-adduct R_1=C_6H_5 R_2=CH_3

48

Energy = -3779.2414128790

Fe	1.8583502	10.1235101	23.4490180
S	3.5505316	9.2065483	22.3195063
C	4.9492896	9.7617767	23.1292662
C	4.8220037	10.5639929	24.2334742
S	3.2470837	10.9505197	24.8073639
S	1.2518633	11.2338907	21.7495405
C	-0.0955299	12.1934256	22.2259767
C	-0.6178424	12.0364487	23.4821714
C	1.2276107	8.3209632	23.7538888
N	1.5242648	7.4917364	24.8050976
C	0.9971265	6.2002316	24.6118849
C	1.1628213	5.1045198	25.6060968
C	0.3482366	6.2242918	23.4126577
C	-0.4168207	5.1640053	22.7004401
N	0.4949204	7.5298929	22.9066217
S	0.1081818	10.9300686	24.5679315
H	-0.4847342	12.9163636	21.5057665
H	-1.4903800	12.5980385	23.8264365
H	5.9238785	9.4633515	22.7342704
H	5.6773470	10.9882055	24.7633966
C	2.1773389	7.8823484	26.0251013
C	-0.1521794	7.9644837	21.6983904
C	0.3643870	7.5968086	20.4537033
C	-1.3321307	8.7075013	21.7903350
C	1.4479886	8.5838740	26.9891011

C	3.5040745	7.5151007	26.2598621
H	0.5839174	4.2260042	25.2966581
H	0.8148416	5.4083499	26.6046145
H	2.2144543	4.7971266	25.7095326
H	-1.4442411	5.4872904	22.4766504
H	-0.4718811	4.2614031	23.3208907
H	0.0513089	4.8877336	21.7437707
C	4.1038377	7.8545643	27.4748168
C	2.0567681	8.9240177	28.1978598
C	3.3824153	8.5563269	28.4437808
H	3.8564056	8.8232860	29.3891875
H	5.1428892	7.5784340	27.6585590
H	0.4181523	8.8736516	26.7782438
H	1.4935795	9.4821290	28.9465810
H	4.0635467	6.9905616	25.4849797
C	-1.9996713	9.0839200	20.6240174
C	-0.3096688	7.9778449	19.2912558
C	-1.4918472	8.7178991	19.3746106
H	1.2983899	7.0368862	20.4011777
H	-1.7042745	9.0010199	22.7719136
H	-2.9157476	9.6715689	20.6937781
H	-2.0135141	9.0161174	18.4642795
H	0.0966979	7.7016566	18.3176325

NHC R_1=CH_3 R_2=H

15
Energy = -304.9268189014

C	0.5606789	8.4809343	24.1015301
N	0.7121952	7.5653887	25.1106127
C	0.1431932	6.3291704	24.8180513
C	-0.3953561	6.4517134	23.5724036
N	-0.1304745	7.7550441	23.1647461
C	1.3937595	7.8767183	26.3571540
C	-0.5348890	8.3142326	21.8810159
H	1.7428360	8.9118642	26.2878612
H	2.2541824	7.2094300	26.5097549
H	0.7090485	7.7786214	27.2120169
H	-1.0918958	7.5579158	21.3146962
H	0.3469688	8.6194776	21.3034135
H	-1.1748594	9.1919020	22.0359107
H	0.1634463	5.4842592	25.4973245
H	-0.9316140	5.7323981	22.9630083

NHC R_1=CH_3 R_2=I

15
Energy = -899.4365904326

C	0.5833804	8.5490908	24.0913964
N	0.7414232	7.6512248	25.1133438
C	0.1679976	6.4191801	24.8214587
C	-0.3764034	6.5366501	23.5641160
N	-0.1100541	7.8369777	23.1457237

C	1.4335490	7.9893976	26.3480535
C	-0.4948350	8.4318782	21.8702824
H	1.7591996	9.0299377	26.2531126
H	2.3053012	7.3376954	26.4961335
H	0.7610720	7.8864629	27.2105668
H	-1.0432630	7.6945483	21.2735893
H	0.4019667	8.7488473	21.3245086
H	-1.1337080	9.3050559	22.0484192
I	0.1693144	4.7655717	26.0852629
I	-1.3977106	5.0765615	22.4835426

NHC R_1=CH_3 R_2=F

15

Energy = -503.4833337572

C	0.5704014	8.5004419	24.1006053
N	0.7257957	7.5891944	25.1188510
C	0.1532091	6.3686225	24.8147848
C	-0.3851114	6.4909558	23.5721501
N	-0.1246195	7.7833484	23.1539105
C	1.4064315	7.8954228	26.3679430
C	-0.5323315	8.3363629	21.8670743
H	1.7473602	8.9326235	26.2897430
H	2.2687474	7.2316420	26.5176992
H	0.7219555	7.7941615	27.2213162
H	-1.0840008	7.5739275	21.3057908
H	0.3523977	8.6424126	21.2957400
H	-1.1753950	9.2100242	22.0267822
F	0.1714919	5.3175881	25.6438728
F	-1.0490922	5.5923419	22.8332269

NHC R_1=CH_3 R_2=Cl

15

Energy = -1224.2529420670

C	0.5765544	8.5265362	24.0943056
N	0.7326438	7.6234751	25.1141339
C	0.1597930	6.3928076	24.8205176
C	-0.3825422	6.5106874	23.5682511
N	-0.1171747	7.8104580	23.1502591
C	1.4202056	7.9435040	26.3560418
C	-0.5125145	8.3854442	21.8689651
H	1.7534998	8.9823464	26.2712033
H	2.2868342	7.2847698	26.5030854
H	0.7427066	7.8387107	27.2143346
H	-1.0598791	7.6362349	21.2869391
H	0.3789581	8.7002645	21.3133707
H	-1.1548608	9.2577345	22.0384605
Cl	0.1686070	5.0392746	25.8685119
Cl	-1.2255911	5.3268120	22.6611201

NHC R_1=CH_3 R_2=Br

15

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 Energy =   -5452.6113320360
 C    0.5796771    8.5369917   24.0929659
 N    0.7368343    7.6360884   25.1143864
 C    0.1635370    6.4068525   24.8200073
 C   -0.3791841    6.5244837   23.5671389
 N   -0.1144154    7.8226756   23.1477923
 C    1.4266310    7.9632006   26.3534423
 C   -0.5051864    8.4054065   21.8686343
 H    1.7563812    9.0028002   26.2645333
 H    2.2955046    7.3072950   26.5001706
 H    0.7512064    7.8584360   27.2134259
 H   -1.0514493    7.6601176   21.2806325
 H    0.3884950    8.7223507   21.3181148
 H   -1.1468417    9.2774568   22.0411251
Br    0.1679561    4.9184474   25.9634589
Br   -1.3019156    5.2164773   22.5836814
```

NHC R_1=CH_3 R_2=CH_3

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21
 Energy =    -383.5889228047
 C    0.5509951    8.4635579   24.0911667
 N    0.7125920    7.5669689   25.1110829
 C    0.1456665    6.3159439   24.8461955
 C   -0.4076129    6.4119647   23.5955443
 N   -0.1437552    7.7243051   23.1688595
 C    1.4013027    7.9115112   26.3427014
 C   -0.5315710    8.3126968   21.8929044
 C   -1.1482453    5.3662052   22.8214733
 C    0.1797967    5.1661721   25.7948673
 H    1.7376712    8.9485150   26.2444649
 H    2.2722511    7.2601081   26.5078276
 H    0.7297104    7.8282211   27.2102329
 H   -1.1000618    7.5930752   21.2941070
 H    0.3610678    8.6150938   21.3303233
 H   -1.1536080    9.1999638   22.0651089
 H   -0.3304834    4.2974335   25.3590010
 H   -0.3207559    5.3992269   26.7488370
 H    1.2096758    4.8572973   26.0367316
 H   -1.4694132    5.7320552   21.8387525
 H   -2.0547178    5.0348861   23.3513788
 H   -0.5257349    4.4759181   22.6431392
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NHC R_1=CH_3 R_2=OH

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17
 Energy =    -455.4389092724
 C    0.5438452    8.4497490   24.0850650
 N    0.7001124    7.5472703   25.1057727
 C    0.1316512    6.3128737   24.8247234
 C   -0.4125325    6.4145404   23.5790040
 N   -0.1504674    7.7179685   23.1494031
```

C	1.3867545	7.8597659	26.3479227
C	-0.5469541	8.2837809	21.8698148
H	1.7207828	8.8993277	26.2693118
H	2.2532784	7.1993078	26.4931842
H	0.7103022	7.7495236	27.2073230
H	-1.0977229	7.5451316	21.2690798
H	0.3373863	8.5955408	21.2999254
H	-1.1989914	9.1526401	22.0234839
O	0.1899812	5.2861406	25.7270176
O	-1.0740659	5.4196774	22.9017458
H	-0.2673987	4.5171614	25.3413069
H	-1.3746313	5.7549104	22.0401358

NHC R_1=CH_3 R_2=NO_2

19
Energy = -714.1583596197

C	-0.2259133	-0.6410834	0.0948462
N	0.2042911	-1.6231853	0.9540264
C	-0.3788111	-2.8441642	0.6774559
N	-0.1410510	-4.0503360	1.4398456
C	-1.2225484	-2.6369461	-0.3946723
N	-2.0504321	-3.5860269	-1.1057196
N	-1.1060371	-1.3015608	-0.7279936
C	1.1233483	-1.3276108	2.0546804
C	-1.7535037	-0.6256220	-1.8540606
H	-2.8368281	-0.5813842	-1.7013751
H	-1.5468532	-1.1547882	-2.7926270
H	-1.3254175	0.3806061	-1.8883107
H	1.2689548	-0.2437051	2.0436329
H	2.0751908	-1.8482598	1.9063556
H	0.6898775	-1.6386560	3.0130585
O	-3.1217702	-3.1551106	-1.5534493
O	-1.6201952	-4.7326633	-1.2281975
O	1.0079024	-4.2072319	1.8748477
O	-1.0945241	-4.8082414	1.6152164

NHC R_1=CH_3 R_2=CO_2CH_3

27
Energy = -760.8987712268

C	0.5656834	8.3721191	24.0584579
N	0.4725120	7.6244314	25.2015131
C	-0.1678311	6.4002069	24.9975616
C	-0.4929051	6.3677773	23.6563302
N	-0.0384666	7.5698099	23.1235381
C	1.0689977	8.0904664	26.4505998
C	-0.2187729	8.0191619	21.7462759
H	1.5730512	9.0335950	26.2184124
H	1.7988290	7.3616522	26.8268506
H	0.2997728	8.2502109	27.2147772
H	-1.2807343	7.9971313	21.4675203
H	0.3460841	7.3855198	21.0525354
H	0.1515376	9.0477864	21.7044202

C	-0.3825895	5.3233941	25.9857821
C	-1.2568111	5.3273271	22.9270420
O	-0.5687906	5.8207140	27.2419048
O	-0.7060648	5.0816957	21.7053947
C	-1.3987118	4.0816230	20.9217198
O	-2.2526453	4.7747324	23.3478825
O	-0.3922258	4.1369402	25.7204204
C	-0.7827329	4.8160281	28.2604910
H	-1.7007436	4.2523681	28.0505642
H	-0.8743822	5.3696106	29.2000315
H	0.0645308	4.1192756	28.2981643
H	-0.8788273	4.0560546	19.9592670
H	-2.4531525	4.3561723	20.7910858
H	-1.3413513	3.1055655	21.4202771

NHC R_1=CH_3 R_2=OCH_3

23
Energy = -534.0673166999

C	0.5225890	8.7446345	24.2349356
N	0.8200158	7.7344582	25.1095360
C	0.2780439	6.5010120	24.7235787
C	-0.3793086	6.7400576	23.5420355
N	-0.2197667	8.0942704	23.2757447
C	1.6487540	7.9283257	26.2868845
C	-0.7773161	8.7658904	22.1134885
H	1.9905997	8.9683791	26.2642039
H	2.5134070	7.2501777	26.2722883
H	1.0793581	7.7540221	27.2122915
H	-1.8761270	8.7639882	22.1434774
H	-0.4508573	8.2756300	21.1860146
H	-0.4098180	9.7969169	22.1395841
O	0.4765449	5.3421914	25.4167337
O	-1.0961323	5.9589364	22.6930160
C	-0.5384698	5.0536601	26.4045188
H	-0.2484510	4.1059460	26.8737276
H	-1.5265950	4.9509744	25.9301393
H	-0.5838319	5.8456258	27.1685069
C	-0.6048428	4.6163983	22.5160607
H	-0.7347469	4.0176105	23.4288264
H	0.4609690	4.6299569	22.2416066
H	-1.1984881	4.1854975	21.7020906

NHC R_1=CH_3 R_2=$COCH_3$

25
Energy = -610.3541192644

C	0.3909058	8.5867863	24.2590214
N	0.4446300	7.6377930	25.2417065
C	-0.1264763	6.4129976	24.8511994

```
 C   -0.5598329    6.6150730   23.5462069
 N   -0.2380581    7.9239871   23.2323124
 C    0.9695644    7.9927757   26.5562933
 C   -0.4709077    8.5673097   21.9407933
 H    1.2671924    9.0438938   26.4931582
 H    1.8431304    7.3820860   26.8176952
 H    0.2012261    7.8802148   27.3328912
 H   -1.5407935    8.5785077   21.7077334
 H    0.0616520    8.0339893   21.1417483
 H   -0.0817526    9.5860901   22.0242458
 C   -0.3322437    5.1827391   25.6355990
 C   -1.2810427    5.7178264   22.5882429
 C    0.4513572    4.9311352   26.9092236
 H    0.2868750    3.8900545   27.2075955
 H    0.1024324    5.5863813   27.7206165
 H    1.5264285    5.1164954   26.7756392
 C   -0.6972680    4.3619686   22.2680019
 H   -0.0812806    3.9560260   23.0760092
 H   -0.0675385    4.4822342   21.3698060
 H   -1.5063736    3.6642539   22.0217305
 O   -2.2658954    6.1523859   22.0029935
 O   -1.1373402    4.3412753   25.2321465
```

NHC R_1=CH_3 R_2=NH_2

```
19
 Energy =    -415.6932205784
 C   -0.2641408   -0.6330108    0.0976632
 N    0.1632054   -1.6351876    0.9457074
 C   -0.3940568   -2.8718793    0.6450877
 N   -0.1887842   -4.0092584    1.4396519
 C   -1.2170510   -2.6740855   -0.4362995
 N   -2.0019760   -3.5573651   -1.2011438
 N   -1.1138721   -1.3009251   -0.7320005
 C    1.0981298   -1.4025584    2.0312812
 C   -1.8472866   -0.6474953   -1.8023756
 H   -2.9308012   -0.6793503   -1.6171706
 H   -1.6468960   -1.1342290   -2.7664979
 H   -1.5103036    0.3937501   -1.8299572
 H    1.2595156   -0.3209698    2.0887425
 H    2.0648494   -1.8976746    1.8464975
 H    0.6873313   -1.7712243    2.9821028
 H   -1.4985304   -4.3695498   -1.5567437
 H   -2.8763951   -3.8517158   -0.7657759
 H   -0.7562307   -4.7937801    1.1176788
 H    0.7873430   -4.3046209    1.4971217
```

NHC R_1=CH_3 R_2=SH

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17
 Energy =   -1101.4402144220
 C    0.4960890    8.5749600   24.1125454
 N    0.6675110    7.6177567   25.0942805
```

C	0.1018114	6.3991800	24.7594935
C	-0.4596628	6.5601293	23.5098037
N	-0.2019099	7.9000465	23.1591719
C	1.3755143	7.8851157	26.3360149
C	-0.6235605	8.5172168	21.9112271
H	1.6407300	8.9470744	26.3326064
H	2.2904117	7.2786149	26.4044128
H	0.7351205	7.6674248	27.2028619
H	-1.7146554	8.4592755	21.7977935
H	-0.1539597	8.0219957	21.0497747
H	-0.3081185	9.5645488	21.9514583
S	0.1598460	4.9932960	25.8036345
S	-1.4127028	5.4098562	22.6061088
H	-0.5755870	4.2418455	24.9405671
H	-0.4352773	4.8948133	21.8085149

NHC R_1=CH_3 R_2=COH

19
Energy = -531.6782960115

C	-0.2211604	-0.6455890	0.0900806
N	0.2048105	-1.6374098	0.9369296
C	-0.3831075	-2.8747927	0.6863576
C	-0.0994347	-4.0524935	1.5178906
C	-1.2379365	-2.6653436	-0.3976283
C	-2.0992195	-3.5675828	-1.1737459
N	-1.1081479	-1.3153126	-0.7146102
C	1.1663963	-1.3504129	1.9992042
C	-1.7991578	-0.6231907	-1.8005381
H	-2.8870475	-0.6459503	-1.6524431
H	-1.5549861	-1.0712892	-2.7727138
H	-1.4506031	0.4138252	-1.7777146
H	1.3924490	-0.2817825	1.9326333
H	2.0896303	-1.9287592	1.8602887
H	0.7418942	-1.5761051	2.9863049
O	-2.1095893	-4.7833480	-1.1038867
O	-0.7186874	-5.1010439	1.5094630
H	-2.7724854	-3.0327516	-1.8893085
H	0.7632128	-3.9064479	2.2144768

NHC R_1=CH_3 R_2=C_6H_5

35
Energy = -767.2155173325

C	-0.2019699	-1.0382626	0.1966746
N	0.0218516	-1.9571627	1.1855886
C	-0.6752855	-3.1592243	0.9919329
C	-0.6459779	-4.3031232	1.9154667
C	-1.3864241	-2.9908799	-0.1793685
C	-2.2669403	-3.9323566	-0.8865845
N	-1.0691225	-1.6998935	-0.6296379
C	0.8431435	-1.6347321	2.3450157

C	-1.5225596	-1.1051495	-1.8802442
H	-2.5671864	-0.7699828	-1.8139270
H	-1.4341936	-1.8246991	-2.7046280
H	-0.8820620	-0.2383353	-2.0710105
H	1.0085365	-0.5530810	2.3260856
H	1.8149268	-2.1464467	2.3086980
H	0.3296571	-1.9180748	3.2731345
C	-1.8365076	-5.2459940	-1.1566640
C	-1.8473377	-4.8751131	2.3768465
C	-3.5573429	-3.5546799	-1.3058067
C	0.5694903	-4.8608433	2.3571132
C	-4.3842626	-4.4558934	-1.9782539
C	-3.9435385	-5.7565156	-2.2385956
C	-2.6680649	-6.1479666	-1.8208362
H	-0.8374177	-5.5522887	-0.8447476
H	-2.3141507	-7.1604712	-2.0210333
H	-4.5903214	-6.4608814	-2.7634046
H	-5.3812133	-4.1425203	-2.2921873
H	-3.9227527	-2.5513938	-1.0831298
C	-1.8321007	-5.9649268	3.2471295
H	-2.7972651	-4.4513796	2.0495584
C	0.5822108	-5.9463756	3.2339887
C	-0.6180715	-6.5027700	3.6838562
H	1.5355089	-6.3649483	3.5607712
H	1.5129757	-4.4536062	1.9913312
H	-0.6073377	-7.3506842	4.3700810
H	-2.7748347	-6.3908839	3.5940871

NHC R_1=C(CH$_3$)$_3$ R_2=H

33

Energy = -540.8964395829

C	-0.1192150	-0.8368280	0.1760643
N	0.0594396	-1.7335266	1.1970270
C	-0.6248016	-2.9284590	0.9802857
C	-1.2670025	-2.7889784	-0.2107360
N	-0.9424371	-1.5181394	-0.6825210
C	0.9453498	-1.4947483	2.3722206
C	-1.5025039	-0.9361282	-1.9366224
C	-2.9947179	-0.6327272	-1.7086550
C	-1.3314126	-1.9479157	-3.0829294
C	-0.7540290	0.3561127	-2.2784566
C	1.3577259	-0.0196093	2.4100067
C	2.1949998	-2.3838407	2.2308545
C	0.1808538	-1.8474935	3.6602193
H	-1.6967892	-1.5080119	-4.0212817
H	-1.9000612	-2.8719172	-2.9083832
H	-0.2726067	-2.2112065	-3.2147603
H	-1.1704801	0.7685654	-3.2093184
H	0.3179500	0.1662519	-2.4198855
H	-0.8521131	1.0958627	-1.4757755
H	1.9073619	0.2619156	1.5046693
H	1.9954088	0.1460872	3.2908400

H	0.4795118	0.6349688	2.4757425
H	2.7317990	-2.1417254	1.3032470
H	1.9271156	-3.4499231	2.2052989
H	2.8753660	-2.2238393	3.0789169
H	-0.0906207	-2.9115322	3.7020852
H	-0.7386748	-1.2520411	3.7429815
H	0.8108282	-1.6326758	4.5345172
H	-3.4347086	-0.1861492	-2.6116714
H	-3.1171148	0.0737544	-0.8761424
H	-3.5576370	-1.5471946	-1.4714096
H	-0.6095575	-3.7715888	1.6610943
H	-1.9111267	-3.4865893	-0.7325525

NHC R_1=C(CH_3)$_3$ R_2=CH_3

39

Energy = -619.5486177373

C	-0.1654328	-0.9830178	0.1838388
N	0.0164373	-1.8657496	1.2108276
C	-0.6963686	-3.0634843	1.0113481
C	-0.7477672	-4.2492106	1.9236117
C	-1.3594492	-2.9165083	-0.1821243
C	-2.2476399	-3.9246259	-0.8413631
N	-1.0099655	-1.6405204	-0.6661728
C	0.9449241	-1.5489223	2.3434235
C	-1.5150269	-0.9805959	-1.9124832
C	-3.0127594	-0.6570397	-1.7505403
C	-1.2701439	-1.8845403	-3.1351541
C	-0.7559626	0.3366258	-2.1305017
C	1.3525509	-0.0701370	2.2641881
C	2.2133612	-2.4143712	2.2182216
C	0.2442450	-1.7790360	3.6955948
H	-1.5339770	-1.3361529	-4.0503108
H	-1.8698880	-2.8011901	-3.1161023
H	-0.2087148	-2.1621155	-3.1992155
H	-1.1351411	0.8021939	-3.0527903
H	0.3222920	0.1630388	-2.2327402
H	-0.8959724	1.0239296	-1.2896021
H	1.8546808	0.1574844	1.3179734
H	2.0319319	0.1440401	3.1027640
H	0.4777569	0.5884119	2.3347986
H	2.7160442	-2.2083082	1.2630306
H	1.9929866	-3.4888759	2.2647451
H	2.9115932	-2.1800652	3.0341902
H	0.0625951	-2.8389109	3.9086861
H	-0.7166651	-1.2466974	3.7258797
H	0.8764061	-1.3849906	4.5036185
H	-3.3815080	-0.1380948	-2.6468395
H	-3.1646100	0.0010155	-0.8842286
H	-3.6255609	-1.5566640	-1.6104413
H	-1.1885719	-5.1048606	1.3961746
H	-1.3593106	-4.0672683	2.8212539
H	0.2475077	-4.5655929	2.2647080

H	-3.1862229	-3.4888062	-1.2082698
H	-2.5219915	-4.7049583	-0.1204554
H	-1.7624427	-4.4234289	-1.6947516

NHC R_1=C(CH$_3$)$_3$ R_2=NO$_2$

37

Energy = -950.1159616906

C	-0.1472030	-1.0362454	0.2062839
N	0.1170890	-1.9200882	1.2075651
C	-0.5516372	-3.1293381	0.9795019
C	-1.2534913	-2.9648569	-0.1933620
N	-0.9801947	-1.6997621	-0.6646268
C	0.9509650	-1.4986333	2.4086863
C	-1.4911121	-1.0368267	-1.9292318
C	-2.9058867	-0.5041350	-1.6507190
C	-1.4838446	-2.0390748	-3.0941995
C	-0.5511862	0.1268648	-2.2684914
C	1.0990369	0.0291248	2.3721203
C	2.3434832	-2.1396542	2.3003763
C	0.2235942	-1.8902261	3.7043984
H	-1.6777920	-1.4870727	-4.0232582
H	-2.2640211	-2.8042778	-3.0114584
H	-0.5058783	-2.5292336	-3.1933741
H	-0.9219138	0.6004053	-3.1884385
H	0.4753634	-0.2222642	-2.4427301
H	-0.5228892	0.8717432	-1.4663728
H	1.6116691	0.3679148	1.4656389
H	1.6907381	0.3238151	3.2505796
H	0.1254646	0.5333244	2.4173583
H	2.8367819	-1.8158672	1.3730252
H	2.2916730	-3.2323966	2.3169602
H	2.9592625	-1.8054217	3.1473002
H	0.1656220	-2.9733716	3.8517554
H	-0.7898761	-1.4651274	3.7253400
H	0.7783706	-1.4724856	4.5554544
H	-3.2900223	-0.0029844	-2.5500683
H	-2.8813762	0.2285150	-0.8322681
H	-3.5951074	-1.3141641	-1.3825944
N	-0.5241222	-4.3646161	1.7286613
N	-2.1179097	-3.9574051	-0.8346226
O	0.5062580	-4.6577807	2.3487413
O	-1.5468792	-5.0579120	1.6815024
O	-1.5698094	-4.9553128	-1.2987421
O	-3.3215288	-3.6943328	-0.8820214

NHC R_1=C(CH$_3$)$_3$ R_2=C$_6$H$_5$

53

Energy = -1003.1676819870

C	-0.1949690	-1.0083829	0.1946737
N	-0.0175545	-1.8815277	1.2271878

C	-0.6940727	-3.1005778	1.0016276
C	-0.7279472	-4.3155321	1.8528737
C	-1.3374524	-2.9613519	-0.2050558
C	-2.2102171	-3.9866370	-0.8283007
N	-0.9971876	-1.6766774	-0.6833147
C	0.8280235	-1.5115074	2.4141611
C	-1.4358165	-1.0307156	-1.9678234
C	-2.8909028	-0.5506073	-1.8217090
C	-1.3004813	-2.0143300	-3.1420658
C	-0.5368860	0.1828908	-2.2473677
C	1.0799253	0.0036403	2.3932193
C	2.1788926	-2.2437821	2.3263155
C	0.1019333	-1.8652937	3.7223504
C	-1.6470745	-5.1241841	-1.4332135
C	-1.8627496	-4.6107808	2.6285569
C	-3.6115523	-3.8981077	-0.7537435
C	0.3306967	-5.2403731	1.8451886
C	-4.4228913	-4.9003680	-1.2897834
C	-3.8485549	-6.0187939	-1.8993660
C	-2.4570622	-6.1301412	-1.9633202
H	-0.5609686	-5.2136119	-1.4846370
H	-1.9992652	-7.0062422	-2.4254980
H	-4.4823915	-6.8043129	-2.3133883
H	-5.5082731	-4.8128366	-1.2185595
H	-4.0669612	-3.0437571	-0.2508813
C	-1.9288765	-5.7807781	3.3869788
H	-2.6974369	-3.9083317	2.6338920
C	0.2690376	-6.4079756	2.6089289
C	-0.8596578	-6.6805931	3.3858405
H	1.1017774	-7.1128200	2.5871938
H	1.2021042	-5.0483782	1.2176353
H	-0.9095009	-7.5941414	3.9801853
H	-2.8199959	-5.9908878	3.9806609
H	-1.5144341	-1.4804795	-4.0786661
H	-1.9967996	-2.8571345	-3.0703480
H	-0.2768069	-2.4099909	-3.2029892
H	-0.8562390	0.6331792	-3.1992752
H	0.5169274	-0.1135039	-2.3306749
H	-0.6057107	0.9289315	-1.4486297
H	1.6124590	0.3121358	1.4874940
H	1.6802482	0.2620215	3.2784316
H	0.1370754	0.5639605	2.4267065
H	2.6758516	-2.0108069	1.3740863
H	2.0592761	-3.3310010	2.4074370
H	2.8339198	-1.9150179	3.1459016
H	-0.0290146	-2.9451251	3.8541242
H	-0.8864763	-1.3858606	3.7594547
H	0.6928542	-1.4917666	4.5706157
H	-3.1969936	-0.0037688	-2.7252499
H	-2.9820961	0.1264144	-0.9610038
H	-3.5835418	-1.3909199	-1.6868670

NHC R_1=$C(CH_3)_3$ R_2=COH

```
37
 Energy =    -767.6365194523
 C   -0.1897135   -1.0275188    0.2002636
 N    0.0668066   -1.9300929    1.1951970
 C   -0.5907089   -3.1480125    0.9836298
 C   -1.2951957   -2.9999151   -0.2005149
 N   -1.0247784   -1.6987658   -0.6477966
 C    1.0026268   -1.6074430    2.3287394
 C   -1.5957145   -1.0393858   -1.8742787
 C   -3.1306114   -1.1378493   -1.8465575
 C   -1.0037201   -1.7119067   -3.1264486
 C   -1.1981919    0.4428847   -1.8756153
 C    1.6832272   -0.2610612    2.0492547
 C    2.0876561   -2.6936617    2.4294785
 C    0.1894161   -1.4933890    3.6304378
 H   -1.3722849   -1.2016823   -4.0271400
 H   -1.2779590   -2.7717073   -3.2083703
 H    0.0923584   -1.6394623   -3.1136583
 H   -1.6228527    0.9079506   -2.7772418
 H   -0.1096047    0.5679036   -1.8827449
 H   -1.5836286    0.9623272   -0.9897715
 H    2.2677533   -0.2925909    1.1214648
 H    2.3580930   -0.0415569    2.8894461
 H    0.9518586    0.5489396    1.9520751
 H    2.6156531   -2.8020559    1.4720187
 H    1.6885535   -3.6751480    2.7162020
 H    2.8207471   -2.4023470    3.1936485
 H   -0.3207180   -2.4295106    3.8936550
 H   -0.5683234   -0.7029510    3.5374161
 H    0.8583149   -1.2325921    4.4620218
 H   -3.5430647   -0.6087089   -2.7165533
 H   -3.5317690   -0.6687985   -0.9375533
 H   -3.4953646   -2.1721608   -1.8897587
 C   -0.4897589   -4.3660556    1.8174937
 C   -2.2092051   -3.9808568   -0.8207919
 O   -0.4327074   -5.4952497    1.3644233
 H   -0.4623753   -4.1950755    2.9197000
 O   -2.9085256   -4.7513322   -0.1860201
 H   -2.2344486   -3.9821316   -1.9356302
```

NHC R_1=C(CH$_3$)$_3$ R_2=Br

```
33
 Energy =   -5688.5729465310
 C   -0.1478688   -0.9572705    0.1873545
 N    0.1076897   -1.8474471    1.1960123
 C   -0.5780026   -3.0391936    0.9790988
 C   -1.2749605   -2.8885207   -0.1934347
 N   -1.0005156   -1.6076431   -0.6637852
 C    1.0130029   -1.5028487    2.3466477
 C   -1.5312826   -0.9511331   -1.9092955
 C   -3.0629637   -0.8464675   -1.8113884
 C   -1.0939169   -1.7656252   -3.1388561
```

C	-0.9406383	0.4603237	-2.0112833
C	1.5343376	-0.0736570	2.1513961
C	2.2084027	-2.4715813	2.3618479
C	0.2122233	-1.5696890	3.6583959
H	-1.4288166	-1.2534476	-4.0516092
H	-1.5193281	-2.7758153	-3.1420323
H	0.0013353	-1.8467016	-3.1736266
H	-1.3337422	0.9231842	-2.9282059
H	0.1542924	0.4383250	-2.0623272
H	-1.2194647	1.0790268	-1.1502989
H	2.0944776	0.0280903	1.2145864
H	2.1994771	0.1603806	2.9951047
H	0.7156709	0.6555629	2.1285781
H	2.7604314	-2.4119964	1.4137385
H	1.8985618	-3.5113462	2.5213753
H	2.8926024	-2.1935854	3.1750320
H	-0.1638067	-2.5791755	3.8641301
H	-0.6409222	-0.8780639	3.6201875
H	0.8583690	-1.2712502	4.4955821
H	-3.4514344	-0.3355690	-2.7033765
H	-3.3491180	-0.2589913	-0.9278175
H	-3.5440280	-1.8298346	-1.7480466
Br	-0.5957222	-4.6092530	2.0363054
Br	-2.3834819	-4.2202766	-0.9556592

NHC R_1=C(CH$_3$)$_3$ R_2=Cl

33

Energy = -1460.2158081000

C	-0.1418398	-0.9421098	0.1862157
N	0.1075946	-1.8350703	1.1949431
C	-0.5770443	-3.0282610	0.9785283
C	-1.2698591	-2.8786410	-0.1941728
N	-0.9923218	-1.5976846	-0.6647683
C	1.0084684	-1.5075803	2.3520633
C	-1.5307508	-0.9580931	-1.9131099
C	-3.0624127	-0.8541037	-1.8046676
C	-1.1058081	-1.7907517	-3.1356093
C	-0.9392388	0.4508136	-2.0397317
C	1.5305308	-0.0761978	2.1797912
C	2.2012965	-2.4803233	2.3567363
C	0.2039362	-1.5951657	3.6610158
H	-1.4453941	-1.2884047	-4.0519231
H	-1.5349317	-2.7992690	-3.1236870
H	-0.0111879	-1.8765482	-3.1781254
H	-1.3408836	0.9039515	-2.9578399
H	0.1550755	0.4245757	-2.1022306
H	-1.2055693	1.0801096	-1.1825349
H	2.0909602	0.0396679	1.2448074
H	2.1940465	0.1465322	3.0277615
H	0.7108910	0.6524011	2.1657113
H	2.7599749	-2.4041706	1.4136201
H	1.8864126	-3.5219323	2.4932149
H	2.8809468	-2.2211639	3.1799043

H	-0.1675506	-2.6087350	3.8538859
H	-0.6527593	-0.9075793	3.6285593
H	0.8461346	-1.3030281	4.5035282
H	-3.4596704	-0.3610290	-2.7026748
H	-3.3430104	-0.2509770	-0.9299642
H	-3.5401747	-1.8374340	-1.7186233
Cl	-0.5809493	-4.4472797	1.9555481
Cl	-2.2841018	-4.0779883	-0.9018421

NHC R_1=C(CH$_3$)$_3$ R_2=COOCH$_3$

45

Energy = -996.8530323498

C	-0.1276512	-0.9102740	0.1480437
N	0.2681401	-1.8348049	1.0871702
C	-0.3517460	-3.0552709	0.8892482
C	-1.1744945	-2.9206119	-0.2139480
N	-0.9976485	-1.5813552	-0.6510137
C	1.1540703	-1.4434431	2.2421672
C	-1.6295901	-0.8725975	-1.8259085
C	-3.1522477	-0.8029720	-1.6192376
C	-1.2334354	-1.5860298	-3.1303337
C	-1.0903965	0.5648213	-1.8920044
C	1.8012086	-0.0870662	1.9324833
C	2.2674049	-2.4833052	2.4444785
C	0.2740405	-1.3197437	3.4981524
H	-1.6506132	-1.0343555	-3.9847677
H	-1.6041520	-2.6137615	-3.1741606
H	-0.1395197	-1.5972185	-3.2357269
H	-1.5624107	1.0534898	-2.7575487
H	-0.0017760	0.5841832	-2.0188926
H	-1.3262631	1.1324190	-0.9847921
H	2.4278494	-0.1407450	1.0326689
H	2.4334166	0.1905165	2.7885579
H	1.0490745	0.6909575	1.7667059
H	2.8241326	-2.6468246	1.5117242
H	1.8963816	-3.4526270	2.7949304
H	2.9682861	-2.1059691	3.2015929
H	-0.2331077	-2.2648778	3.7320135
H	-0.4881576	-0.5414888	3.3530775
H	0.8957597	-1.0372805	4.3593802
H	-3.6110693	-0.2611099	-2.4582177
H	-3.3792654	-0.2531107	-0.6946532
H	-3.6103762	-1.7950844	-1.5634484
C	-0.0859502	-4.3436072	1.6130949
C	-2.0000639	-4.0640967	-0.6426668
O	0.7598617	-5.1439739	1.2702876
O	-0.8762069	-4.4770706	2.7039365
O	-2.0137934	-5.1229835	-0.0290773
O	-2.7508246	-3.8733686	-1.7606125
C	-0.7502575	-5.7479513	3.3871759
H	-1.4380340	-5.6902350	4.2361173
H	0.2811313	-5.9028412	3.7286342

```
 H    -1.0342794   -6.5621652    2.7088048
 C    -3.5481464   -5.0150268   -2.1517966
 H    -4.0957852   -4.6912029   -3.0425686
 H    -4.2402595   -5.2935320   -1.3475326
 H    -2.9031657   -5.8726347   -2.3816877
```

NHC R_1=C(CH$_3$)$_3$ R_2=F

```
33
 Energy =    -739.4522219328
 C    -0.1221343   -0.8886545    0.1812258
 N     0.1184938   -1.7889564    1.1917574
 C    -0.5743593   -2.9680723    0.9756738
 C    -1.2656571   -2.8179013   -0.1833938
 N    -0.9841006   -1.5493166   -0.6618633
 C     1.0099725   -1.5161422    2.3638001
 C    -1.5361131   -0.9632939   -1.9242411
 C    -3.0694808   -0.8956633   -1.8092444
 C    -1.1095764   -1.8493404   -3.1085531
 C    -0.9675932    0.4466642   -2.1049863
 C     1.5548004   -0.0898069    2.2483889
 C     2.1759893   -2.5212845    2.3445134
 C     0.1850173   -1.6524674    3.6564038
 H    -1.4755743   -1.4109107   -4.0470154
 H    -1.5161979   -2.8652660   -3.0280055
 H    -0.0141439   -1.9135048   -3.1640148
 H    -1.3750858    0.8629079   -3.0374665
 H     0.1271685    0.4322271   -2.1659690
 H    -1.2416547    1.1011523   -1.2689692
 H     2.1221892    0.0495091    1.3204577
 H     2.2149908    0.0964444    3.1075937
 H     0.7441513    0.6494125    2.2524162
 H     2.7583354   -2.4148193    1.4188680
 H     1.8227454   -3.5582106    2.4184861
 H     2.8441947   -2.3301980    3.1951002
 H    -0.1975396   -2.6717550    3.7945001
 H    -0.6656481   -0.9567177    3.6427240
 H     0.8146388   -1.4062804    4.5224429
 H    -3.4892551   -0.4534036   -2.7231758
 H    -3.3620758   -0.2670549   -0.9568906
 H    -3.5144116   -1.8907202   -1.6793735
 F    -0.5421362   -4.0431887    1.7818690
 F    -2.0790896   -3.7068679   -0.7787386
```

NHC R_1=C(CH$_3$)$_3$ R_2=I

```
33
 Energy =   -1135.3959453570
 C    -0.1554998   -0.9762017    0.1895786
 N     0.1019118   -1.8617765    1.1988424
 C    -0.5835031   -3.0572404    0.9845945
 C    -1.2842607   -2.9046319   -0.1933923
```

N	-1.0066308	-1.6215015	-0.6627277
C	1.0120715	-1.4960231	2.3405970
C	-1.5251003	-0.9449646	-1.9049386
C	-3.0549998	-0.8208004	-1.8128409
C	-1.0890891	-1.7452418	-3.1435811
C	-0.9193338	0.4620046	-1.9884576
C	1.5153871	-0.0617206	2.1288910
C	2.2213790	-2.4466266	2.3543839
C	0.2237874	-1.5547406	3.6598760
H	-1.4120227	-1.2146723	-4.0502747
H	-1.5268485	-2.7503455	-3.1676534
H	0.0055203	-1.8396592	-3.1724664
H	-1.3042500	0.9378883	-2.9024838
H	0.1756956	0.4302859	-2.0360951
H	-1.1961322	1.0754152	-1.1226550
H	2.0681386	0.0399935	1.1875018
H	2.1839238	0.1860763	2.9660295
H	0.6884352	0.6582982	2.1072804
H	2.7605257	-2.3917912	1.3986782
H	1.9295934	-3.4888095	2.5318742
H	2.9115402	-2.1483316	3.1553115
H	-0.1323147	-2.5665882	3.8884396
H	-0.6419099	-0.8792863	3.6176163
H	0.8719336	-1.2303286	4.4857505
H	-3.4325418	-0.2864384	-2.6959332
H	-3.3371138	-0.2479066	-0.9183001
H	-3.5508538	-1.7983107	-1.7727229
I	-0.6095742	-4.8113915	2.1449953
I	-2.5170538	-4.3961125	-1.0213781

NHC R_1=C(CH$_3$)$_3$ R_2=COCH$_3$

43

Energy = -846.3022312303

C	-0.1411370	-0.9035687	0.1882736
N	0.2427591	-1.8488745	1.1021640
C	-0.4601388	-3.0440036	0.9341632
C	-1.2758839	-2.8675911	-0.1625651
N	-1.0573331	-1.5375643	-0.5918640
C	1.2734383	-1.5118600	2.1479845
C	-1.8091373	-0.7871833	-1.6590322
C	-3.3040139	-1.1340293	-1.5751238
C	-1.2148182	-1.1216036	-3.0374746
C	-1.6514673	0.7214925	-1.4144294
C	2.3110734	-0.5692829	1.5177702
C	1.9941566	-2.7734345	2.6380594
C	0.5628140	-0.7964360	3.3096513
H	-1.7419689	-0.5548862	-3.8178848
H	-1.2951144	-2.1864819	-3.2813745
H	-0.1534347	-0.8397002	-3.0660357
H	-2.2145323	1.2554680	-2.1942951
H	-0.6005331	1.0258570	-1.4517368
H	-2.0462761	1.0096911	-0.4317526

H	2.8332103	-1.0632770	0.6866262
H	3.0522891	-0.2958833	2.2822747
H	1.8330071	0.3361719	1.1297391
H	2.4171375	-3.3460128	1.8022713
H	1.3477828	-3.4376293	3.2253990
H	2.8196261	-2.4691267	3.2958494
H	-0.1894373	-1.4426392	3.7834200
H	0.0602136	0.1079334	2.9417082
H	1.2929555	-0.5053127	4.0777750
H	-3.8563814	-0.5285094	-2.3065457
H	-3.6974896	-0.9051154	-0.5750819
H	-3.5195251	-2.1866482	-1.7922844
C	-0.3658375	-4.3347863	1.7173097
C	-2.1039982	-3.9903870	-0.6940634
O	0.2295828	-5.2909592	1.2463479
C	-1.1290937	-4.4128433	3.0189270
O	-2.7950916	-4.6370708	0.0890903
C	-1.9817654	-4.4303083	-2.1420426
H	-1.0802239	-3.4782280	3.5931222
H	-0.7772658	-5.2609456	3.6184010
H	-2.1863951	-4.5718137	2.7509018
H	-2.6867802	-3.8869271	-2.7876943
H	-2.2386498	-5.4952750	-2.1875779
H	-0.9685428	-4.2692352	-2.5328301

NHC R_1=C(CH$_3$)$_3$ R_2=OCH$_3$

41

Energy = -770.0251475299

C	-0.1086653	-0.7616589	0.1881485
N	0.2307285	-1.7111871	1.1144061
C	-0.3077277	-2.9648962	0.7920455
C	-1.0135701	-2.7914102	-0.3745803
N	-0.8842554	-1.4387392	-0.7144573
C	1.1413062	-1.4189243	2.2665441
C	-1.4209348	-0.7950874	-1.9552589
C	-2.9476065	-0.9795072	-2.0202157
C	-0.7380459	-1.4327078	-3.1789318
C	-1.1058579	0.7051580	-1.9168129
C	1.5310020	0.0635820	2.2289623
C	2.4125033	-2.2794832	2.1385728
C	0.4128129	-1.7107892	3.5902478
H	-1.1095657	-0.9639757	-4.1013663
H	-0.9367374	-2.5107632	-3.2329118
H	0.3491020	-1.2783275	-3.1283673
H	-1.4989234	1.1598990	-2.8381245
H	-0.0274127	0.8879243	-1.8526451
H	-1.5717755	1.1898995	-1.0498907
H	2.0515253	0.3153933	1.2977054
H	2.1955197	0.2645884	3.0820641
H	0.6504942	0.7135977	2.2949136
H	2.9286738	-2.0554962	1.1945553
H	2.1805250	-3.3510017	2.1641086

```
H     3.0983414   -2.0512407    2.9664486
H     0.1898390   -2.7778234    3.7101601
H    -0.5266131   -1.1432976    3.6457627
H     1.0457401   -1.4056046    4.4353490
H    -3.3483267   -0.4179974   -2.8760880
H    -3.4217874   -0.5916327   -1.1071728
H    -3.2284665   -2.0312801   -2.1498389
O    -0.0304056   -4.1075570    1.4825154
O    -1.6178624   -3.7110156   -1.1808143
C    -1.0695680   -4.6429942    2.3255446
C    -2.8657201   -4.2682846   -0.7268029
H    -1.7009808   -3.8417367    2.7359648
H    -0.5713233   -5.1792584    3.1436285
H    -1.6965640   -5.3528471    1.7657166
H    -3.3661036   -4.6742276   -1.6150022
H    -3.4987966   -3.4979642   -0.2613644
H    -2.6941470   -5.0848649   -0.0101386
```

NHC R_1=C(CH_3)$_3$ R_2=NH_2

```
37
 Energy =    -651.6541930033
C    -0.1293606   -0.8784824    0.1706803
N     0.0952762   -1.7863836    1.1780280
C    -0.6296663   -2.9652503    0.9799445
C    -1.3313690   -2.8016051   -0.1876656
N    -1.0105265   -1.5111673   -0.6544679
C     0.9997296   -1.4948972    2.3328577
C    -1.5374535   -0.8808299   -1.9051111
C    -3.0752331   -0.8315079   -1.8463090
C    -1.0605960   -1.6996083   -3.1190427
C    -0.9971387    0.5498055   -2.0159670
C     1.6472869   -0.1190788    2.1315300
C     2.1153684   -2.5559385    2.3994645
C     0.1730143   -1.4838454    3.6318540
H    -1.4048994   -1.2234570   -4.0485103
H    -1.4525338   -2.7234455   -3.0842602
H     0.0377931   -1.7388720   -3.1399590
H    -1.3881052    0.9924755   -2.9444840
H     0.0985691    0.5631763   -2.0409952
H    -1.3113865    1.1650087   -1.1638190
H     2.2406463   -0.0849239    1.2098175
H     2.3030759    0.0803689    2.9922982
H     0.8911141    0.6709058    2.0612284
H     2.6402877   -2.6252047    1.4365751
H     1.7355767   -3.5502621    2.6694303
H     2.8478144   -2.2735648    3.1681297
H    -0.3260980   -2.4465371    3.7980171
H    -0.5918270   -0.6955611    3.5845572
H     0.8287553   -1.2739857    4.4890283
H    -3.4612971   -0.2954886   -2.7253829
H    -3.4085164   -0.2959047   -0.9458755
H    -3.5125602   -1.8377216   -1.8480063
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N	-0.7082556	-4.0404881	1.8873810
N	-2.1590909	-3.7267453	-0.8643727
H	-1.4929848	-4.6487217	1.6464250
H	0.1404624	-4.6079541	1.9306788
H	-3.1140410	-3.7793776	-0.5049843
H	-1.7595105	-4.6658304	-0.8926530

NHC R_1=C(CH_3)$_3$ R_2=OH

35
Energy = -691.4095511586

C	-0.1411860	-0.9094244	0.1726284
N	0.1096269	-1.8210831	1.1765713
C	-0.5672314	-3.0097869	0.9549344
C	-1.2691770	-2.8628924	-0.2044288
N	-0.9804341	-1.5729413	-0.6775627
C	0.9962680	-1.5365893	2.3473756
C	-1.5221368	-0.9756050	-1.9330744
C	-3.0580518	-0.9076062	-1.8385901
C	-1.0819159	-1.8381549	-3.1304827
C	-0.9692872	0.4440744	-2.0960703
C	1.5325120	-0.1058272	2.2330971
C	2.1748655	-2.5278550	2.3351906
C	0.1734171	-1.6736444	3.6416935
H	-1.4698965	-1.4045855	-4.0631010
H	-1.4515069	-2.8679030	-3.0468503
H	0.0146879	-1.8662307	-3.1951889
H	-1.3494145	0.8547188	-3.0431507
H	0.1266803	0.4427594	-2.1155029
H	-1.2801877	1.0943582	-1.2695294
H	2.1082381	0.0347914	1.3106321
H	2.1826089	0.0869449	3.0991026
H	0.7173068	0.6279233	2.2244241
H	2.7547637	-2.4181407	1.4081949
H	1.8313587	-3.5669347	2.4135580
H	2.8416343	-2.3218896	3.1837411
H	-0.2133539	-2.6919861	3.7727914
H	-0.6736869	-0.9732372	3.6294734
H	0.8044812	-1.4321300	4.5085392
H	-3.4646951	-0.4013689	-2.7253772
H	-3.3637293	-0.3413672	-0.9478886
H	-3.5167363	-1.9062834	-1.7978472
O	-0.4949951	-4.0970116	1.7804200
O	-1.9965104	-3.8542827	-0.8312900
H	-0.9683811	-4.8225944	1.3280494
H	-2.9502553	-3.6978547	-0.6940818

NHC R_1=C(CH_3)$_3$ R_2=SH

35
Energy = -1337.4001517210

C	-0.1579684	-0.9213556	0.1645928

N	0.0837160	-1.8332958	1.1681889
C	-0.5907202	-3.0280999	0.9453375
C	-1.2961491	-2.8708114	-0.2341031
N	-0.9994537	-1.5641880	-0.6852950
C	0.9924819	-1.5215537	2.3222639
C	-1.4873946	-0.9224487	-1.9517887
C	-3.0248370	-0.8573578	-1.9374757
C	-0.9725607	-1.7297219	-3.1572078
C	-0.9324306	0.5051944	-2.0342697
C	1.4957329	-0.0788673	2.1892976
C	2.1987462	-2.4771606	2.2860366
C	0.2078447	-1.6544704	3.6392374
H	-1.2648945	-1.2254931	-4.0890611
H	-1.3856038	-2.7455857	-3.1785680
H	0.1240431	-1.7941337	-3.1313481
H	-1.3018330	0.9582012	-2.9662056
H	0.1636766	0.5132506	-2.0394235
H	-1.2611975	1.1144053	-1.1838295
H	2.0517098	0.0696249	1.2566059
H	2.1574987	0.1299927	3.0426243
H	0.6659998	0.6381950	2.1946366
H	2.7465340	-2.3623459	1.3405687
H	1.9013375	-3.5294229	2.3863185
H	2.8824852	-2.2391933	3.1121433
H	-0.1677197	-2.6725881	3.8077817
H	-0.6487737	-0.9662658	3.6450544
H	0.8627646	-1.3966570	4.4829423
H	-3.3772196	-0.3331103	-2.8370575
H	-3.3773246	-0.3015887	-1.0571697
H	-3.4772016	-1.8565259	-1.9313731
S	-0.5699372	-4.4638666	1.9650251
S	-2.2544900	-4.1276854	-0.9975316
H	-1.3286632	-5.1584410	1.0665562
H	-3.4457284	-3.9047797	-0.3749738

(NHC)Ni(CO)$_3$ complex R_1=CH$_3$ R_2=H

22

Energy = -2153.8438617750

C	0.5566346	8.7362571	24.0069889
N	0.7659499	7.9055600	25.0791164
C	0.2345361	6.6416288	24.8670836
C	-0.3285758	6.6629153	23.6292761
N	-0.1239505	7.9383572	23.1223355
C	1.4589634	8.2851289	26.3024618
C	-0.5855043	8.3660008	21.8073697
H	1.7517154	9.3355253	26.2141506
H	2.3563964	7.6667571	26.4410278
H	0.7948308	8.1626124	27.1686340
H	-1.0842120	7.5209059	21.3191101
H	0.2626937	8.6906122	21.1928244

H	-1.2928015	9.1984772	21.9032439
Ni	1.1251608	10.6333084	23.8180209
C	0.6356067	11.3391624	22.2346531
C	2.9235528	10.6590107	23.9428667
C	0.3398902	11.5716651	25.1421450
O	4.0781706	10.6896253	24.0095768
O	-0.1609640	12.1973567	25.9766766
O	0.3633583	11.8738932	21.2441781
H	-0.8497964	5.8922090	23.0747778
H	0.3005848	5.8489710	25.6026321

$(NHC)Ni(CO)_3$ complex $R_1=CH_3$ $R_2=OH$

24
Energy = -2304.3600332990

C	0.5991160	8.7224982	23.9432709
N	0.7664903	7.8910068	25.0319548
C	0.1984598	6.6506904	24.8141354
C	-0.3544578	6.6748726	23.5687410
N	-0.0763260	7.9456930	23.0437631
C	1.4488445	8.2437156	26.2690021
C	-0.4864078	8.3597857	21.7101172
H	1.8226665	9.2655187	26.1557853
H	2.2860329	7.5570036	26.4505605
H	0.7548886	8.1952182	27.1187824
H	-0.6620597	7.4628415	21.1042512
H	0.3128487	8.9547624	21.2581615
H	-1.4034830	8.9641270	21.7467174
O	0.2773609	5.6853941	25.7654103
O	-0.9219143	5.6478314	22.8641831
H	-0.0519509	4.8527223	25.3793393
H	-1.8936214	5.7381931	22.8611347
Ni	1.1517536	10.6333315	23.8112149
C	0.6451696	11.4028107	22.2640089
C	2.9488487	10.7050701	23.9504177
C	0.3228202	11.4911273	25.1609919
O	4.1006631	10.7805473	24.0281805
O	-0.2204135	12.0597091	26.0098163
O	0.3511608	11.9900595	21.3098692

$(NHC)Ni(CO)_3$ complex $R_1=C(CH_3)_3$ $R_2=C_6H_5$

60
Energy = -2852.0503029310

C	0.6284688	8.6285999	24.0315708
N	0.3250788	8.0722349	25.2573930
C	-0.5929736	7.0151042	25.1077547
C	-0.7911750	6.8491991	23.7616710
N	0.0094554	7.8078540	23.1113922
C	1.0859598	8.3379663	26.5483137
C	0.3730946	7.7298942	21.6341062

C	2.3705957	9.1309068	26.2812605
C	1.5304503	6.9846504	27.1392590
C	0.2032945	9.0904107	27.5563145
C	0.6352303	6.2532483	21.2738999
C	1.6790314	8.4828617	21.3507904
C	-0.7591047	8.2921522	20.7611237
Ni	0.9177638	10.6864921	23.7299787
C	-0.1095537	11.3191040	22.3882077
C	2.6542609	11.0918875	23.4405180
C	0.2398875	11.6318176	25.1089080
O	3.7503590	11.4054130	23.2466338
O	-0.1991290	12.4063612	25.8507864
O	-0.7298303	11.9369320	21.6286196
C	-1.8333347	5.9782908	23.1619894
C	-1.3934193	6.3462353	26.1654853
H	-0.4496593	8.2671437	19.7064416
H	-0.9853435	9.3318718	21.0231636
H	-1.6749443	7.6966250	20.8563989
H	1.0412510	6.2129199	20.2540953
H	-0.2702383	5.6403038	21.2944385
H	1.3794979	5.8114783	21.9518591
H	2.9982804	8.6333082	25.5304715
H	2.9317555	9.1825057	27.2247497
H	2.1756572	10.1497173	25.9381576
H	-0.1675946	10.0317070	27.1350366
H	0.7962840	9.3294393	28.4505622
H	-0.6532395	8.4835965	27.8741731
H	2.1129425	6.4104401	26.4048748
H	0.6913781	6.3731386	27.4843996
H	2.1770342	7.1804055	28.0053088
H	1.9558808	8.2889022	20.3049134
H	2.4921270	8.1275754	21.9972551
H	1.5830779	9.5620555	21.4895111
C	-2.4579886	7.0325088	26.7769322
C	-3.0324401	6.5438318	22.6935921
C	-1.7028442	4.5795691	23.1418917
C	-1.1885516	4.9977678	26.5022465
C	-4.0598030	5.7363501	22.2010045
H	-3.1633192	7.6260148	22.7347189
C	-2.7300785	3.7713805	22.6514378
C	-3.9105604	4.3475070	22.1754945
H	-4.9837413	6.1949378	21.8456675
H	-4.7137099	3.7165211	21.7924357
H	-2.6067897	2.6873980	22.6411933
H	-0.7793505	4.1262459	23.5032293
C	-3.2785495	6.3947046	27.7099645

H	-2.6505420	8.0707448	26.5032275
C	-2.0096976	4.3585093	27.4330624
C	-3.0551526	5.0563467	28.0430261
H	-0.3685966	4.4509603	26.0350211
H	-1.8315735	3.3111386	27.6814049
H	-3.6971880	4.5572120	28.7701040
H	-4.1014107	6.9439310	28.1697890

(NHC)Ni(CO)$_3$ complex R_1=C(CH$_3$)$_3$ R_2=COCH$_3$

50

Energy = -2695.1862008350

C	0.6513715	8.6255383	24.1367238
N	0.7000170	7.7873646	25.2380599
C	-0.0069410	6.6030241	24.9973775
C	-0.4723556	6.6718094	23.7086325
N	-0.0495655	7.9004864	23.1876910
C	1.6557841	7.9449070	26.4200828
C	-0.2578836	8.2604692	21.7181510
C	2.9933635	8.5118094	25.9158931
C	1.9729493	6.5660617	27.0231645
C	1.0303369	8.8366231	27.5048851
C	-0.1822645	6.9762775	20.8676052
C	0.8632348	9.1694700	21.2036077
C	-1.6281236	8.9335019	21.5507715
Ni	1.0538899	10.6707139	24.1343486
C	-0.3708831	11.5735289	23.4836974
C	2.5878283	11.0348960	23.2490816
C	1.2431189	11.5223745	25.7208249
O	3.5713193	11.3362817	22.7218037
O	1.3911163	12.2952522	26.5707230
O	-1.2094194	12.3101026	23.1776543
C	-1.5323497	5.7517602	23.1308849
C	-0.5385414	5.6124656	25.9969241
H	-1.7821585	9.1847708	20.4915113
H	-1.6817424	9.8617300	22.1296797
H	-2.4382440	8.2709814	21.8777309
H	-0.1535586	7.2741671	19.8117007
H	-1.0506487	6.3199262	20.9782553
H	0.7363118	6.4112013	21.0792480
H	3.4229099	7.8568389	25.1448351
H	3.6936876	8.5550867	26.7616780
H	2.8882660	9.5154118	25.4962450
H	0.5771991	9.7322694	27.0712359
H	1.8055742	9.1543447	28.2151700
H	0.2612876	8.2983348	28.0738517

H	2.3442105	5.8591829	26.2694199
H	1.1237784	6.1127967	27.5483665
H	2.7623855	6.7061606	27.7740423
H	0.7375836	9.2744438	20.1171276
H	1.8539100	8.7345223	21.3947135
H	0.8311618	10.1650691	21.6484361
O	-0.3784916	4.4084402	25.8476406
O	-2.6665302	6.1798061	22.9670327
C	-1.1489719	4.3248515	22.8449661
C	-1.4529382	6.1483404	27.0815644
H	-0.2507361	4.2856890	22.2121953
H	-1.9845647	3.8037892	22.3641722
H	-0.8777249	3.8296733	23.7899712
H	-1.2702505	7.1987821	27.3303543
H	-1.3979945	5.5131535	27.9740777
H	-2.4796238	6.0826086	26.6846623

(NHC)Ni(CO)$_3$ complex R_1=C(CH$_3$)$_3$ R_2=OCH$_3$

48

Energy = -2618.9146779010

C	0.6566611	8.6738832	23.9531761
N	0.7542368	7.7715363	24.9956625
C	-0.0416434	6.6483653	24.7426044
C	-0.5466811	6.7895408	23.4823156
N	-0.0825198	8.0112275	22.9868936
C	1.7920204	7.7671366	26.1019151
C	-0.2389137	8.3998537	21.5321264
C	2.8186485	8.8869297	25.9115353
C	2.5642627	6.4322724	26.0080529
C	1.1022978	7.9009351	27.4686622
C	0.1928331	7.2005141	20.6588979
C	0.6923768	9.5597838	21.1672471
C	-1.7052383	8.7683892	21.2574425
Ni	0.5461431	10.7438901	24.3009195
C	-0.9279528	11.4446440	23.5337843
C	2.0463785	11.5932232	23.7628607
C	0.1830829	11.0743875	26.0365499
O	2.9844477	12.1880122	23.4407673
O	-0.1234597	11.4723104	27.0812097
O	-1.8505425	12.0536074	23.1861073
O	-1.4287060	6.0014675	22.8140076
O	-0.2803971	5.6492897	25.6400218
H	-1.8239323	9.0464570	20.2006476
H	-2.0160301	9.6227457	21.8710141
H	-2.3721159	7.9224765	21.4671863

H	0.2081119	7.5220830	19.6087327
H	-0.4945262	6.3531577	20.7384809
H	1.2077640	6.8724615	20.9242709
H	3.2792804	8.8398558	24.9166261
H	3.6048653	8.7466935	26.6671123
H	2.3889217	9.8838513	26.0375854
H	0.5055995	8.8196469	27.5208380
H	1.8651147	7.9457456	28.2591458
H	0.4544286	7.0409885	27.6772964
H	3.0536040	6.3404274	25.0280891
H	1.9190113	5.5620690	26.1679524
H	3.3472331	6.4250613	26.7794435
H	0.5859561	9.7461464	20.0893353
H	1.7411385	9.3083870	21.3746362
H	0.4530852	10.4803678	21.7049561
C	-1.0721557	4.6015932	22.7369657
C	-1.5992838	5.7099530	26.2392306
H	-0.9851872	4.1585949	23.7384711
H	-0.1202826	4.4784282	22.1982079
H	-1.8824478	4.1178148	22.1804929
H	-1.6496215	4.8724188	26.9445373
H	-2.3811134	5.6028925	25.4727805
H	-1.7381029	6.6610629	26.7742348

(NHC)Ni(CO)$_3$ complex R$_1$=C(CH$_3$)$_3$ R$_2$=COOCH$_3$

52

Energy = -2845.7262550740

C	0.5436940	8.7406612	24.0572826
N	0.8755820	7.8555920	25.0644192
C	0.2678709	6.6115504	24.8453573
C	-0.3633786	6.6826981	23.6289300
N	-0.1733268	7.9743813	23.1446878
C	2.0360618	8.0313467	26.0501284
C	-0.6450163	8.4153447	21.7605395
C	3.0698825	9.0114630	25.4777401
C	2.7642326	6.6798414	26.1980845
C	1.5288055	8.5170741	27.4139112
C	-0.5172251	7.2399944	20.7728256
C	0.2559572	9.5288739	21.2140518
C	-2.1111144	8.8655265	21.8473152
Ni	0.5053982	10.8101837	24.2683294
C	-1.0651520	11.5321918	23.7384043
C	1.8782011	11.5968449	23.3960330
C	0.5073463	11.4054299	25.9783510

O	2.7368304	12.1553171	22.8605131
O	0.4435503	12.0275998	26.9530154
O	-1.9941874	12.1862168	23.5178721
C	-1.3489663	5.6650025	23.1070110
C	0.0070595	5.4929421	25.7813844
H	-2.4500288	9.1917108	20.8540182
H	-2.2257424	9.7062147	22.5390942
H	-2.7555820	8.0445127	22.1857470
H	-0.7162395	7.6306083	19.7663624
H	-1.2399688	6.4360230	20.9404881
H	0.5012520	6.8273198	20.7680941
H	3.4235123	8.6867413	24.4898596
H	3.9285973	9.0326221	26.1628903
H	2.6757004	10.0262028	25.3850305
H	1.0241200	9.4839616	27.3257029
H	2.3851353	8.6415309	28.0921030
H	0.8320268	7.7989865	27.8579262
H	3.0668604	6.2786542	25.2211173
H	2.1791834	5.9234378	26.7307207
H	3.6753361	6.8503343	26.7872757
H	-0.0442475	9.7253997	20.1755059
H	1.3119372	9.2243841	21.2158604
H	0.1667954	10.4582908	21.7794353
O	-0.8976914	4.5369009	22.5216156
O	-0.0895110	4.3280618	25.4314332
O	-2.5438165	5.8496300	23.2174740
C	0.5123855	4.2417203	22.4115777
O	-0.2231974	5.9082284	27.0513374
C	-0.5693878	4.8531761	27.9829152

(NHC)Ni(CO)$_3$ complex R$_1$=C(CH$_3$)$_3$ R$_2$=COCH$_3$

44

Energy = -2616.5246380680

C	0.6116351	8.6987361	24.0348390
N	0.5364047	7.9154089	25.1794085
C	-0.4087765	6.9098195	25.0213332
C	-0.8709670	6.9834521	23.7095079
N	-0.1710935	8.0355128	23.1073005
C	1.5478043	7.9273823	26.3215789
C	-0.0826673	8.2290900	21.5898415
C	2.8118667	8.6958427	25.9192629
C	1.9932064	6.4727830	26.5815018
C	0.9331976	8.5539888	27.5835220
C	0.1341712	6.8358758	20.9663240

C	1.1435012	9.0703821	21.2184195
C	-1.3600020	8.8941137	21.0609748
Ni	0.9211367	10.7412771	24.0750646
C	-0.3844642	11.5826533	23.1476804
C	2.5514066	11.2585056	23.4782853
C	0.6247545	11.4536021	25.7093526
O	3.5743151	11.6456083	23.1084508
O	0.4043418	12.1163041	26.6327449
O	-1.1633261	12.2980047	22.6803313
C	-2.0784383	6.2505979	23.2722586
C	-0.9404864	6.0547495	26.0999849
H	-1.2710256	9.0140222	19.9721824
H	-1.4939906	9.8898266	21.4990063
H	-2.2456569	8.2834814	21.2638746
H	0.2697750	6.9631287	19.8840062
H	-0.7190032	6.1695218	21.1160554
H	1.0468741	6.3710069	21.3657734
H	3.2510699	8.2882383	24.9991106
H	3.5427895	8.5835986	26.7322832
H	2.6242976	9.7611994	25.7642384
H	0.6069122	9.5819352	27.3939836
H	1.6908768	8.5776246	28.3790849
H	0.0731293	7.9869146	27.9628369
H	2.3835544	6.0121966	25.6637242
H	1.2010009	5.8290860	26.9834262
H	2.8005653	6.4862575	27.3257244
H	1.2267327	9.0539497	20.1227964
H	2.0668982	8.6506241	21.6384744
H	1.0596213	10.1105474	21.5408245
O	-1.5219426	4.9942540	25.9215844
O	-2.6163367	6.2751864	22.1741113
H	-2.5051527	5.6500154	24.1001539
H	-0.8235597	6.4632038	27.1277962

HEP complex R_1=CH_3 R_2=COH

55
Energy = -6424.8011267490

H	-2.5375169	-5.4719844	3.0378475
C	-2.8356150	-5.7873865	2.0385777
C	-4.0534397	-5.3767305	1.4952484
H	-4.7112113	-4.7362750	2.0833494
C	-4.4460522	-5.7729418	0.2052778
H	-5.4049521	-5.4365535	-0.1896312
C	-3.6343924	-6.5886554	-0.5838186
H	-3.9541446	-6.8872611	-1.5799486
C	-2.4093753	-6.9989078	-0.0464326

C	-2.0229352	-6.6061683	1.2503714
N	-1.3669573	-7.7884563	-0.5327397
N	-0.7761023	-7.1879483	1.4883197
C	-1.3005486	-8.4370827	-1.8615411
C	-1.2939739	-7.4018358	-2.9885020
H	-2.2381103	-6.8440089	-3.0510492
H	-0.4720548	-6.6872035	-2.8499340
H	-1.1452686	-7.9142107	-3.9491360
C	-2.3759984	-9.5162011	-2.0041060
H	-3.3910215	-9.0966312	-1.9800767
H	-2.2509608	-10.0330200	-2.9658497
H	-2.2819166	-10.2569025	-1.1985722
C	-0.0239630	-6.9358243	2.7431948
C	0.9336567	-5.7537846	2.5646118
H	1.6948392	-5.9823577	1.8061140
H	0.3948196	-4.8513482	2.2440093
H	1.4341750	-5.5331075	3.5181183
C	0.6634185	-8.1881736	3.2773163
H	-0.8031620	-6.6543238	3.4670011
H	1.4759886	-8.5107599	2.6111557
H	1.0897384	-7.9642561	4.2655017
H	-0.0364672	-9.0275906	3.3735409
C	-0.3707497	-7.9015770	0.3965323
H	-0.3142524	-8.9268340	-1.8455109
Pd	1.3461819	-8.9587744	0.0660867
Br	2.4302327	-6.9374627	-0.8900299
Br	0.2438429	-11.0621227	0.8193553
C	3.0455566	-9.9999724	-0.3003793
N	3.2884871	-10.8641292	-1.3293690
N	4.2057737	-9.9838011	0.4259910
C	4.5739110	-11.3813571	-1.2613707
C	2.2943088	-11.1830484	-2.3527124
C	5.1580519	-10.8217779	-0.1249555
C	4.3677139	-9.1630091	1.6300584
H	5.4252747	-8.9268486	1.7647109
H	4.0099581	-9.7193558	2.5066402
H	3.7710239	-8.2553520	1.4885051
H	2.2380441	-12.2675479	-2.5004036
H	2.5427030	-10.6834917	-3.2986312
H	1.3282132	-10.8269356	-1.9814209
C	6.5148962	-11.0670948	0.3860073
C	5.1224299	-12.3094267	-2.2519160
O	6.2334671	-12.8169357	-2.1913135
H	4.4419615	-12.5339360	-3.1066549
O	6.9604687	-10.5935504	1.4232726
H	7.1127347	-11.7381959	-0.2647903

HEP complex R_1=CH_3 R_2=C_6H_5

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Energy = -6660.3324449980

H	-2.7042101	-5.5409402	3.0211505
C	-2.9886261	-5.9436129	2.0494550

C	-4.2665573	-5.7254356	1.5325155
H	-4.9864377	-5.1489443	2.1139896
C	-4.6389889	-6.2315326	0.2759590
H	-5.6445006	-6.0425944	-0.1010459
C	-3.7481573	-6.9705098	-0.5042298
H	-4.0521025	-7.3529506	-1.4764411
C	-2.4661453	-7.1935243	0.0094358
C	-2.0975420	-6.6868757	1.2716542
N	-1.3435212	-7.8650043	-0.4739822
N	-0.7766769	-7.0823886	1.4898505
C	-1.2258167	-8.5585931	-1.7756977
C	-1.3180664	-7.5671546	-2.9382014
H	-2.3049741	-7.0881173	-3.0003939
H	-0.5542373	-6.7844064	-2.8355710
H	-1.1445494	-8.0976503	-3.8849686
C	-2.1978724	-9.7366566	-1.8758218
H	-3.2488206	-9.4162334	-1.8771061
H	-2.0139613	-10.2788866	-2.8139396
H	-2.0412330	-10.4324622	-1.0408746
C	-0.0303808	-6.6579152	2.6990462
C	0.6753157	-5.3209688	2.4506012
H	1.4385974	-5.4310957	1.6672709
H	-0.0360226	-4.5467085	2.1316610
H	1.1612761	-4.9796925	3.3757885
C	0.9168409	-7.7353680	3.2154849
H	-0.8145634	-6.5130331	3.4579723
H	1.7543500	-7.8828484	2.5187780
H	1.3210517	-7.4148395	4.1861565
H	0.4084435	-8.6996692	3.3404526
C	-0.3091984	-7.7936639	0.4204760
H	-0.2024086	-8.9658795	-1.7449680
Pd	1.5112951	-8.6461517	0.0436209
Br	2.3729461	-6.5065622	-0.8846771
Br	0.6855423	-10.8399839	0.8750138
C	3.2809459	-9.5217718	-0.4320564
N	3.6529373	-9.9831430	-1.6563088
N	4.3440590	-9.7759004	0.3762517
C	4.9407957	-10.5296642	-1.6258571
C	2.8193982	-9.8341948	-2.8451851
C	5.3874839	-10.3860516	-0.3293419
C	4.3251885	-9.5231614	1.8131938
H	5.0251030	-10.2035685	2.3096296
H	3.3088022	-9.7102072	2.1774026
H	4.6086768	-8.4843366	2.0302071
H	3.4537132	-9.8625858	-3.7373625
H	2.3107470	-8.8652075	-2.7845272
H	2.0751525	-10.6407185	-2.8989601
C	5.6238187	-11.1023204	-2.7954191
C	6.6707332	-10.7773798	0.2727722
C	7.1534397	-12.0910862	0.1316958
C	5.0178977	-12.1076032	-3.5727008
C	6.9132067	-10.6640238	-3.1493850
C	7.5765932	-11.2173315	-4.2449540
C	5.6807441	-12.6530089	-4.6730924

C	6.9625387	-12.2110336	-5.0125323
H	7.4802574	-12.6389802	-5.8719493
H	8.5749403	-10.8632723	-4.5058786
H	7.3889277	-9.8790071	-2.5610321
H	4.0287446	-12.4775049	-3.2987495
H	5.1966026	-13.4331753	-5.2622602
C	7.4507898	-9.8460804	0.9843056
C	8.6743761	-10.2202412	1.5409487
C	8.3809024	-12.4602547	0.6830584
C	9.1442239	-11.5281035	1.3917540
H	6.5533473	-12.8237169	-0.4089448
H	8.7385993	-13.4841586	0.5657044
H	9.2668686	-9.4839182	2.0859957
H	10.1009198	-11.8197499	1.8271195
H	7.1025972	-8.8168248	1.0833641

HEP complex R_1=CH_3 R_2=Br

51

Energy = -11345.7239381400

H	-2.6416238	-5.4956898	3.0113452
C	-2.9067491	-5.8186176	2.0051840
C	-4.1212263	-5.4394184	1.4317188
H	-4.8094882	-4.8158910	2.0029085
C	-4.4710978	-5.8455558	0.1329353
H	-5.4279693	-5.5334074	-0.2860255
C	-3.6192991	-6.6401693	-0.6351706
H	-3.9062684	-6.9469510	-1.6388543
C	-2.3983992	-7.0196415	-0.0671235
C	-2.0542702	-6.6170491	1.2385029
N	-1.3265766	-7.7848954	-0.5258472
N	-0.8006590	-7.1697878	1.5087956
C	-1.2102767	-8.4284517	-1.8537172
C	-1.2011252	-7.3894225	-2.9774700
H	-2.1551939	-6.8513677	-3.0601460
H	-0.3978797	-6.6582271	-2.8175762
H	-1.0190520	-7.8950312	-3.9359460
C	-2.2539832	-9.5343031	-2.0255189
H	-3.2807058	-9.1431337	-2.0177632
H	-2.0962099	-10.0399786	-2.9884903
H	-2.1541059	-10.2782921	-1.2235349
C	-0.0847340	-6.8973870	2.7797026
C	0.8481994	-5.6926771	2.6219038
H	1.6312197	-5.9027796	1.8802374
H	0.2952242	-4.8030687	2.2895716
H	1.3212668	-5.4605777	3.5867926
C	0.6203921	-8.1312161	3.3341580
H	-0.8873521	-6.6331985	3.4843244
H	1.4548694	-8.4375378	2.6872096
H	1.0179622	-7.8932921	4.3309998
H	-0.0606639	-8.9873930	3.4167331
C	-0.3519566	-7.8764954	0.4291549
H	-0.2125163	-8.8942751	-1.8146979

Pd	1.3804567	-8.9065730	0.1263372
Br	2.4486243	-6.8524241	-0.7758074
Br	0.2737421	-11.0134936	0.8681526
C	3.0958330	-9.9379845	-0.2591937
N	3.3180806	-10.7948102	-1.2994037
N	4.2761229	-9.8966298	0.4261829
C	4.6219926	-11.2743489	-1.2701360
C	2.3220905	-11.1307110	-2.3108369
C	5.2225694	-10.7166508	-0.1757577
Br	5.3369846	-12.4587352	-2.5220174
Br	6.9600163	-10.9520938	0.4615898
C	4.5021437	-9.1032659	1.6277707
H	5.4583943	-8.5732722	1.5466790
H	4.5101271	-9.7473070	2.5173577
H	3.6873608	-8.3748541	1.6923224
H	2.4493729	-12.1769862	-2.6106352
H	2.4324022	-10.4797109	-3.1882709
H	1.3351346	-10.9988387	-1.8546896

HEP complex R_1=CH_3 R_2=H

51

Energy = -6198.0450219130

H	-2.6361040	-5.5456520	3.0470060
C	-2.9040076	-5.8460041	2.0345085
C	-4.1155662	-5.4460729	1.4685089
H	-4.7984547	-4.8276834	2.0516698
C	-4.4684190	-5.8241980	0.1619824
H	-5.4225143	-5.4961825	-0.2513383
C	-3.6231289	-6.6116989	-0.6211812
H	-3.9110789	-6.8959860	-1.6311704
C	-2.4061826	-7.0129007	-0.0602007
C	-2.0582001	-6.6362823	1.2526610
N	-1.3400179	-7.7773815	-0.5330969
N	-0.8077109	-7.2007123	1.5106817
C	-1.2259710	-8.4031469	-1.8695529
C	-1.2022502	-7.3484978	-2.9783181
H	-2.1510836	-6.8004418	-3.0577687
H	-0.3929201	-6.6274205	-2.8037222
H	-1.0199848	-7.8419217	-3.9432092
C	-2.2794716	-9.4963242	-2.0611307
H	-3.3025803	-9.0957850	-2.0547519
H	-2.1199231	-9.9913359	-3.0294280
H	-2.1908886	-10.2514017	-1.2681927
C	-0.0830780	-6.9484722	2.7804852
C	0.8325765	-5.7285382	2.6382893
H	1.6026142	-5.9113983	1.8759087
H	0.2641154	-4.8362692	2.3407674
H	1.3230580	-5.5173198	3.5992326
C	0.6488654	-8.1832062	3.2969434
H	-0.8813044	-6.7124883	3.5002925
H	1.4862643	-8.4543992	2.6379451
H	1.0462267	-7.9643061	4.2984726

H	-0.0149504	-9.0544614	3.3591439
C	-0.3635463	-7.8900587	0.4176754
H	-0.2332901	-8.8807725	-1.8326149
Pd	1.3703612	-8.9150136	0.0987175
Br	2.4231241	-6.8429719	-0.7900147
Br	0.2646416	-11.0299098	0.8286657
C	3.0921611	-9.9316128	-0.2767241
N	3.3239701	-10.8515870	-1.2558222
N	4.2823148	-9.8312056	0.3814189
C	4.6306170	-11.3131214	-1.2110686
C	2.3378656	-11.2628041	-2.2491470
C	5.2348697	-10.6729052	-0.1724958
C	4.5115931	-8.9725991	1.5379587
H	5.5863979	-8.7753762	1.6268471
H	4.1518633	-9.4575657	2.4554234
H	3.9797779	-8.0268614	1.3807849
H	2.6285117	-12.2393626	-2.6537782
H	2.2862906	-10.5292036	-3.0649302
H	1.3618500	-11.3468499	-1.7564299
H	6.2438368	-10.7433350	0.2144994
H	5.0120204	-12.0454947	-1.9116124

HEP complex R_1=CH_3 R_2=CH_3

57

Energy = -6276.7114175010

H	-2.6425581	-5.5067562	3.0327067
C	-2.9140259	-5.8185384	2.0247033
C	-4.1324379	-5.4335019	1.4631834
H	-4.8172123	-4.8166810	2.0457108
C	-4.4904116	-5.8257027	0.1624412
H	-5.4504726	-5.5105688	-0.2471760
C	-3.6422407	-6.6110635	-0.6197427
H	-3.9348857	-6.9071349	-1.6249742
C	-2.4175947	-6.9961154	-0.0640345
C	-2.0659888	-6.6086285	1.2447998
N	-1.3479103	-7.7543801	-0.5379523
N	-0.8112067	-7.1646440	1.5003751
C	-1.2380453	-8.3840617	-1.8725208
C	-1.2401673	-7.3342758	-2.9860446
H	-2.1977081	-6.8008940	-3.0594979
H	-0.4406379	-6.5995364	-2.8231566
H	-1.0594862	-7.8296297	-3.9501333
C	-2.2788860	-9.4919600	-2.0486454
H	-3.3071090	-9.1047178	-2.0296263
H	-2.1255050	-9.9873911	-3.0177783
H	-2.1698190	-10.2427993	-1.2540793
C	-0.0875124	-6.9108828	2.7703493
C	0.8616585	-5.7184410	2.6169003
H	1.6360976	-5.9333544	1.8674576
H	0.3188381	-4.8183063	2.2959580
H	1.3454455	-5.5019273	3.5801498
C	0.6024458	-8.1583902	3.3141053

H	-0.8838344	-6.6399215	3.4796782
H	1.4328112	-8.4692236	2.6641134
H	1.0023857	-7.9341074	4.3134296
H	-0.0897621	-9.0065345	3.3887720
C	-0.3670735	-7.8598770	0.4101080
H	-0.2384316	-8.8471429	-1.8438259
Pd	1.3546939	-8.9151563	0.1072691
Br	2.4814883	-6.8785708	-0.7707649
Br	0.1784282	-10.9994527	0.8151682
C	3.0547429	-9.9868205	-0.2360805
N	3.2801995	-10.8930321	-1.2265056
N	4.2204946	-9.9570262	0.4661397
C	4.5703216	-11.4263128	-1.1516918
C	2.3065109	-11.2319890	-2.2549775
C	5.1665364	-10.8363953	-0.0690849
C	4.4462203	-9.1270093	1.6400245
H	5.4283621	-8.6421223	1.5745173
H	4.3949354	-9.7272768	2.5599781
H	3.6719391	-8.3527603	1.6571878
H	2.3831326	-12.2977508	-2.5016815
H	2.4726970	-10.6337637	-3.1624811
H	1.3077049	-11.0340969	-1.8521652
C	6.5234776	-11.0182261	0.5167348
C	5.0840030	-12.4448061	-2.1090817
H	7.0803178	-11.7761310	-0.0475797
H	6.4780474	-11.3528212	1.5647314
H	7.1124718	-10.0880519	0.4932140
H	5.0387664	-12.0914352	-3.1507230
H	4.5158797	-13.3870765	-2.0544533
H	6.1320495	-12.6784761	-1.8847280

HEP complex R_1=CH_3 R_2=NH_2

55

Energy = -6308.8117259440

H	-2.6532284	-5.4943647	3.0257588
C	-2.9517386	-5.8945027	2.0572999
C	-4.2342070	-5.6674935	1.5549296
H	-4.9441763	-5.0872289	2.1449152
C	-4.6239598	-6.1700992	0.3022542
H	-5.6326335	-5.9750482	-0.0630405
C	-3.7464171	-6.9138718	-0.4885076
H	-4.0635387	-7.2934600	-1.4575173
C	-2.4607261	-7.1469890	0.0111356
C	-2.0745531	-6.6438459	1.2694866
N	-1.3492286	-7.8282711	-0.4842472
N	-0.7553466	-7.0519913	1.4741856
C	-1.2524627	-8.5243119	-1.7863832
C	-1.3472705	-7.5338801	-2.9498140
H	-2.3315071	-7.0485049	-3.0055342
H	-0.5781083	-6.7555777	-2.8545357
H	-1.1839532	-8.0668792	-3.8970748
C	-2.2402478	-9.6902034	-1.8722573

H	-3.2866018	-9.3550594	-1.8619703
H	-2.0746355	-10.2387770	-2.8099570
H	-2.0823691	-10.3839136	-1.0358917
C	0.0091620	-6.6238934	2.6706139
C	0.6794814	-5.2695463	2.4158029
H	1.4339555	-5.3619499	1.6214693
H	-0.0549204	-4.5120716	2.1089753
H	1.1704916	-4.9180162	3.3344510
C	0.9911808	-7.6836385	3.1580830
H	-0.7606814	-6.5017076	3.4484736
H	1.8190896	-7.8088617	2.4451534
H	1.4075669	-7.3600484	4.1227808
H	0.5055111	-8.6591987	3.2875544
C	-0.3062074	-7.7697198	0.4011178
H	-0.2333862	-8.9431234	-1.7671808
Pd	1.4934922	-8.6618888	0.0292328
Br	2.3917113	-6.5290863	-0.8836424
Br	0.5958421	-10.8308148	0.8596306
C	3.2423541	-9.5970542	-0.4235508
N	3.6766404	-9.9527285	-1.6672838
N	4.2088470	-10.0354880	0.4224897
C	4.9011900	-10.6163512	-1.6025574
C	2.9595226	-9.6783478	-2.9044991
C	5.2476531	-10.6705999	-0.2758144
C	4.1673870	-9.8901107	1.8709077
H	4.8379932	-10.6376342	2.3093461
H	3.1383740	-10.0624257	2.2065690
H	4.4941088	-8.8844338	2.1698468
H	3.6872526	-9.6254578	-3.7231916
H	2.4477584	-8.7152011	-2.7973688
H	2.2257806	-10.4696331	-3.1143486
N	5.5895852	-11.0070099	-2.7585690
N	6.3306558	-11.2645300	0.3890119
H	6.5925535	-12.1719037	0.0072450
H	7.1572925	-10.6731365	0.4815486
H	5.2258476	-11.8542166	-3.1987791
H	6.5882044	-11.1173884	-2.5885219

HEP complex R_1=CH_3 R_2=NO_2

55
Energy = -6607.2663717840

H	-2.6492781	-5.4905864	3.0156485
C	-2.9466242	-5.9036405	2.0524824
C	-4.2332927	-5.6975384	1.5542591
H	-4.9468365	-5.1201462	2.1424023
C	-4.6232523	-6.2163148	0.3079152
H	-5.6350655	-6.0343319	-0.0549222
C	-3.7431550	-6.9597993	-0.4789888
H	-4.0614383	-7.3525239	-1.4422399
C	-2.4529482	-7.1739735	0.0180314
C	-2.0650964	-6.6497851	1.2661758
N	-1.3372762	-7.8509091	-0.4756421

N	-0.7374048	-7.0352313	1.4676196
C	-1.2451901	-8.5648389	-1.7700268
C	-1.3386727	-7.5857081	-2.9429203
H	-2.3179292	-7.0902290	-2.9919485
H	-0.5614934	-6.8134350	-2.8629743
H	-1.1923030	-8.1294524	-3.8865889
C	-2.2358897	-9.7289883	-1.8437274
H	-3.2811178	-9.3918588	-1.8584320
H	-2.0564164	-10.2975754	-2.7665718
H	-2.0945922	-10.4064336	-0.9914996
C	0.0214368	-6.5725279	2.6564328
C	0.6143941	-5.1824067	2.4010928
H	1.3732327	-5.2322350	1.6071987
H	-0.1604029	-4.4656076	2.0965070
H	1.0865649	-4.8061536	3.3195631
C	1.0674684	-7.5762814	3.1274682
H	-0.7439379	-6.4962252	3.4447006
H	1.8992129	-7.6367822	2.4108107
H	1.4688334	-7.2369964	4.0927735
H	0.6419932	-8.5802290	3.2514700
C	-0.2920814	-7.7618673	0.4013333
H	-0.2288037	-8.9891475	-1.7469698
Pd	1.5136473	-8.6289704	0.0221229
Br	2.3732512	-6.4819113	-0.8818062
Br	0.6427958	-10.7958252	0.8692677
C	3.2722280	-9.5304661	-0.4436550
N	3.7217001	-9.8528425	-1.6988345
N	4.2545617	-9.9583851	0.4104240
C	4.9522054	-10.4688455	-1.6272752
C	2.9947340	-9.5226664	-2.9284987
C	5.2955030	-10.5245515	-0.2951768
C	4.1438066	-9.8767673	1.8700270
H	4.4788184	-10.8160085	2.3215485
H	3.0839538	-9.7194315	2.0927894
H	4.7577768	-9.0508494	2.2458576
H	3.6801454	-9.0830525	-3.6608291
H	2.2344675	-8.7861136	-2.6510054
H	2.5419975	-10.4279127	-3.3474127
N	5.6933960	-10.9137589	-2.7889848
N	6.4782811	-11.0799740	0.3255829
O	6.8857515	-10.5060195	1.3430313
O	6.9739888	-12.0750105	-0.2009363
O	6.9144923	-10.7724106	-2.7641824
O	5.0263600	-11.3915578	-3.7145766

HEP complex R_1=CH_3 R_2=OH

53
Energy = -6348.5608491550

H	-2.6119328	-5.4538766	3.0099753
C	-2.9238119	-5.8727446	2.0536262
C	-4.2131739	-5.6556783	1.5652103
H	-4.9144281	-5.0637654	2.1539990

C	-4.6205179	-6.1825547	0.3281545
H	-5.6342655	-5.9941484	-0.0262184
C	-3.7545519	-6.9420130	-0.4603765
H	-4.0857978	-7.3405895	-1.4169794
C	-2.4613259	-7.1642769	0.0249992
C	-2.0575090	-6.6360500	1.2673375
N	-1.3547072	-7.8508344	-0.4745403
N	-0.7335055	-7.0349471	1.4596081
C	-1.2702578	-8.5607403	-1.7701968
C	-1.3791580	-7.5801437	-2.9407513
H	-2.3628467	-7.0927200	-2.9855411
H	-0.6067116	-6.8030213	-2.8623246
H	-1.2313177	-8.1211832	-3.8858507
C	-2.2554966	-9.7298585	-1.8369509
H	-3.3028427	-9.3985276	-1.8141658
H	-2.1004814	-10.2811966	-2.7748391
H	-2.0844367	-10.4202720	-1.0005856
C	0.0451804	-6.5830434	2.6382560
C	0.6999831	-5.2268673	2.3549089
H	1.4414954	-5.3235034	1.5490241
H	-0.0454558	-4.4786818	2.0520793
H	1.2045394	-4.8608337	3.2603904
C	1.0434836	-7.6273180	3.1258372
H	-0.7140972	-6.4566459	3.4257909
H	1.8643860	-7.7515942	2.4046369
H	1.4682118	-7.2886269	4.0816152
H	0.5680611	-8.6055699	3.2724051
C	-0.2987236	-7.7700979	0.3928213
H	-0.2495815	-8.9760990	-1.7569887
Pd	1.4982294	-8.6573787	0.0034593
Br	2.3760446	-6.5230928	-0.9331972
Br	0.6110691	-10.8159098	0.8630321
C	3.2518925	-9.5723783	-0.4744824
N	3.7095660	-9.8446664	-1.7243349
N	4.2302389	-10.0301275	0.3682870
C	4.9768040	-10.4401118	-1.6722069
C	2.9747037	-9.5764421	-2.9544647
C	5.2873873	-10.5600802	-0.3492735
C	4.1843445	-9.9606003	1.8237410
H	4.7209305	-10.8203337	2.2405501
H	3.1326010	-9.9994936	2.1271949
H	4.6500512	-9.0324204	2.1824686
H	3.6250996	-9.8007207	-3.8072195
H	2.6740036	-8.5212999	-2.9699367
H	2.0858483	-10.2177353	-3.0069026
O	5.6585627	-10.9102722	-2.7605891
O	6.3685089	-11.0713182	0.2937074
H	6.1617786	-10.1849348	-3.1773112
H	6.8925795	-11.5775894	-0.3540079

HEP complex R_1=CH_3 R_2=SH

53

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 Energy =   -6994.5532303590
 H    -2.6904063   -5.6428682    3.1152194
 C    -2.9789080   -5.9997920    2.1271315
 C    -4.2680190   -5.7812890    1.6392858
 H    -4.9904251   -5.2510215    2.2601543
 C    -4.6491484   -6.2293406    0.3632754
 H    -5.6639157   -6.0427100    0.0107871
 C    -3.7547631   -6.9074523   -0.4662301
 H    -4.0646178   -7.2456799   -1.4527055
 C    -2.4610286   -7.1295417    0.0178432
 C    -2.0839925   -6.6832388    1.3000878
 N    -1.3328802   -7.7515826   -0.5163916
 N    -0.7532992   -7.0650420    1.4792720
 C    -1.2212025   -8.3676767   -1.8571621
 C    -1.3699392   -7.3167504   -2.9602762
 H    -2.3778884   -6.8807044   -2.9896081
 H    -0.6417357   -6.5070701   -2.8181858
 H    -1.1800830   -7.7842196   -3.9365663
 C    -2.1584578   -9.5687478   -2.0011645
 H    -3.2178937   -9.2822328   -1.9484580
 H    -1.9897588  -10.0462002   -2.9767539
 H    -1.9538276  -10.3079339   -1.2153279
 C     0.0117488   -6.6842059    2.6918163
 C     0.7825470   -5.3827449    2.4515542
 H     1.5381882   -5.5192056    1.6655232
 H     0.1072151   -4.5744790    2.1384298
 H     1.2839956   -5.0701684    3.3785725
 C     0.8969382   -7.8163402    3.2013757
 H    -0.7640849   -6.5026446    3.4502823
 H     1.6990087   -8.0361913    2.4832114
 H     1.3489056   -7.5134549    4.1564788
 H     0.3267122   -8.7414768    3.3529834
 C    -0.2894034   -7.7112135    0.3677760
 H    -0.1845424   -8.7405467   -1.8706925
Pd     1.5318420   -8.5411771   -0.0516124
Br     2.3762381   -6.3916644   -0.9628516
Br     0.7234079  -10.7646554    0.7232409
 C     3.2945144   -9.4236162   -0.5373804
 N     3.6851617   -9.8724018   -1.7516605
 N     4.3147868   -9.7618675    0.3140641
 C     4.9322985  -10.5221235   -1.6764804
 C     2.8871056   -9.7346263   -2.9637664
 C     5.3196566  -10.4363181   -0.3562279
 C     4.2973502   -9.4797276    1.7444447
 H     5.3209317   -9.5298519    2.1355243
 H     3.6569947  -10.2035291    2.2656098
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H	3.9041285	-8.4688110	1.8961884
H	3.5538891	-9.7767459	-3.8324480
H	2.3762163	-8.7659583	-2.9280267
H	2.1491836	-10.5461184	-3.0281292
S	5.8493791	-11.1404009	-3.0221709
S	6.7659505	-11.0186710	0.4381817
H	7.3073664	-11.4323936	-0.7382567
H	5.3064796	-12.3876052	-3.0919403

HEP complex R_1=CH_3 R_2=F

51

Energy = -6396.5977400020

H	-2.6353822	-5.5654017	3.0548154
C	-2.9049658	-5.8625185	2.0419185
C	-4.1212533	-5.4683644	1.4825343
H	-4.8064465	-4.8578883	2.0711555
C	-4.4766857	-5.8423370	0.1755052
H	-5.4346370	-5.5186140	-0.2322422
C	-3.6288919	-6.6193949	-0.6150839
H	-3.9194025	-6.9010752	-1.6250980
C	-2.4064686	-7.0140022	-0.0610851
C	-2.0565975	-6.6425060	1.2524940
N	-1.3366066	-7.7679563	-0.5428366
N	-0.8012179	-7.2001607	1.5033759
C	-1.2237546	-8.3830312	-1.8846587
C	-1.2155732	-7.3200210	-2.9855382
H	-2.1716503	-6.7840687	-3.0590860
H	-0.4155290	-6.5893645	-2.8080815
H	-1.0291087	-7.8041632	-3.9542230
C	-2.2697014	-9.4831270	-2.0782505
H	-3.2955135	-9.0898408	-2.0625088
H	-2.1128045	-9.9697676	-3.0512040
H	-2.1711278	-10.2430083	-1.2910228
C	-0.0739410	-6.9495867	2.7724505
C	0.8401977	-5.7284786	2.6317709
H	1.6138324	-5.9099117	1.8727417
H	0.2709134	-4.8378840	2.3309934
H	1.3261139	-5.5151719	3.5945511
C	0.6583362	-8.1849023	3.2870342
H	-0.8708753	-6.7149075	3.4938459
H	1.4934550	-8.4579556	2.6259697
H	1.0595036	-7.9658880	4.2869078
H	-0.0062536	-9.0553015	3.3523095
C	-0.3578945	-7.8806231	0.4048660

H	-0.2267206	-8.8519243	-1.8571774
Pd	1.3714649	-8.9070359	0.0887310
Br	2.4434229	-6.8378042	-0.7795668
Br	0.2355504	-11.0133795	0.7925799
C	3.0921925	-9.9360495	-0.2714176
N	3.3213206	-10.8627505	-1.2500033
N	4.2772239	-9.8380963	0.4040801
C	4.6234766	-11.3261193	-1.1840442
C	2.3512221	-11.2887477	-2.2544445
C	5.2200739	-10.6903804	-0.1430822
F	5.1005383	-12.2293527	-2.0366401
F	6.4537211	-10.7927945	0.3457526
C	4.5256701	-8.9738842	1.5536653
H	5.5749385	-8.6577495	1.5472612
H	4.3076130	-9.5056254	2.4896244
H	3.8783423	-8.0959371	1.4514492
H	2.5708686	-12.3206816	-2.5504460
H	2.4005992	-10.6353024	-3.1354136
H	1.3576026	-11.2422725	-1.7945485

HEP complex R_1=CH_3 R_2=Cl

51

Energy = -7117.3663752980

H	-2.6392304	-5.5249553	3.0319952
C	-2.9035242	-5.8327239	2.0208361
C	-4.1128270	-5.4353908	1.4487007
H	-4.7966073	-4.8125558	2.0258910
C	-4.4623617	-5.8209809	0.1435107
H	-5.4148858	-5.4943519	-0.2745383
C	-3.6147821	-6.6124359	-0.6327278
H	-3.8999919	-6.9020117	-1.6419289
C	-2.3992221	-7.0100737	-0.0659226
C	-2.0556470	-6.6284127	1.2463399
N	-1.3315308	-7.7760045	-0.5331071
N	-0.8064345	-7.1937271	1.5115517
C	-1.2141727	-8.4016325	-1.8693590
C	-1.1953010	-7.3474819	-2.9787334
H	-2.1487088	-6.8085910	-3.0635336
H	-0.3935167	-6.6186528	-2.8015370
H	-1.0040627	-7.8404324	-3.9420484
C	-2.2626216	-9.4999122	-2.0597300
H	-3.2871082	-9.1030929	-2.0530329
H	-2.1022702	-9.9949829	-3.0278125
H	-2.1714163	-10.2537468	-1.2658729

C	-0.0896549	-6.9421480	2.7866143
C	0.8488925	-5.7400191	2.6442172
H	1.6295237	-5.9441263	1.8983545
H	0.3002802	-4.8431937	2.3241480
H	1.3249150	-5.5232034	3.6111582
C	0.6099133	-8.1863487	3.3250103
H	-0.8914134	-6.6833621	3.4943379
H	1.4465381	-8.4857652	2.6775035
H	1.0042423	-7.9649463	4.3270456
H	-0.0739045	-9.0416099	3.3919922
C	-0.3596092	-7.8864001	0.4220391
H	-0.2186151	-8.8728717	-1.8331380
Pd	1.3706672	-8.9153464	0.1099433
Br	2.4261181	-6.8496428	-0.7832474
Br	0.2534846	-11.0214184	0.8397915
C	3.0943454	-9.9386835	-0.2680506
N	3.3181304	-10.8444077	-1.2656878
N	4.2836403	-9.8430906	0.3964334
C	4.6299334	-11.3029477	-1.2293062
C	2.3256329	-11.2478622	-2.2556134
C	5.2366931	-10.6763441	-0.1763939
Cl	5.2764302	-12.4323505	-2.3272644
Cl	6.8309390	-10.8312995	0.4007499
C	4.5203792	-8.9939531	1.5574128
H	5.4714690	-8.4620759	1.4386701
H	4.5458366	-9.5967103	2.4751357
H	3.7021697	-8.2678997	1.5996220
H	2.4571378	-12.3105345	-2.4883795
H	2.4359750	-10.6538513	-3.1726703
H	1.3371931	-11.0921476	-1.8110488

HEP complex R_1=CH_3 R_2=I

51

Energy = -6792.5488970260

H	-2.6273413	-5.5092399	3.0266570
C	-2.8981124	-5.8192217	2.0179389
C	-4.1072196	-5.4167175	1.4491016
H	-4.7855457	-4.7883663	2.0268057
C	-4.4641786	-5.8054135	0.1468107
H	-5.4166758	-5.4753069	-0.2686423
C	-3.6245769	-6.6054110	-0.6294360
H	-3.9166651	-6.8983349	-1.6357155
C	-2.4082949	-7.0069299	-0.0665512
C	-2.0575019	-6.6218328	1.2427392

N	-1.3450817	-7.7785605	-0.5354009
N	-0.8096391	-7.1907743	1.5051089
C	-1.2335321	-8.4043002	-1.8721866
C	-1.2121557	-7.3484012	-2.9798384
H	-2.1621597	-6.8020900	-3.0563242
H	-0.4035883	-6.6263206	-2.8058147
H	-1.0315460	-7.8406777	-3.9455100
C	-2.2889552	-9.4957228	-2.0632118
H	-3.3110785	-9.0928066	-2.0547089
H	-2.1322953	-9.9885711	-3.0330013
H	-2.2018981	-10.2526543	-1.2719299
C	-0.0888772	-6.9399743	2.7780844
C	0.8627376	-5.7486813	2.6302093
H	1.6412988	-5.9636486	1.8853281
H	0.3242091	-4.8472055	2.3062668
H	1.3411074	-5.5334199	3.5963925
C	0.5970310	-8.1891153	3.3223320
H	-0.8871727	-6.6692537	3.4852540
H	1.4272810	-8.5031489	2.6735197
H	0.9975242	-7.9660868	4.3215231
H	-0.0968212	-9.0356425	3.3972776
C	-0.3691613	-7.8882029	0.4159041
H	-0.2409255	-8.8816299	-1.8379123
Pd	1.3637249	-8.9139385	0.1069859
Br	2.4069927	-6.8530915	-0.8108316
Br	0.2583875	-11.0216480	0.8492304
C	3.0967408	-9.9283729	-0.2611595
N	3.3321038	-10.8263470	-1.2625661
N	4.2803207	-9.8281202	0.4122396
C	4.6480940	-11.2779602	-1.2222946
C	2.3355270	-11.2143783	-2.2544137
C	5.2458503	-10.6510419	-0.1591169
I	5.4733910	-12.6312584	-2.5529934
I	7.1829763	-10.8439750	0.5417816
C	4.4848831	-8.9799282	1.5798168
H	5.4185966	-8.4156753	1.4691802
H	4.5262391	-9.5879719	2.4936571
H	3.6433726	-8.2807394	1.6250363
H	2.4616602	-12.2751809	-2.4998988
H	2.4462107	-10.6100869	-3.1648688
H	1.3480192	-11.0598621	-1.8065742

HEP complex R_1=CH_3 R_2=$COCH_3$

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 Energy =   -6503.4658051510
 H    -2.5768389   -5.4768675    3.0427515
 C    -2.8817314   -5.8312404    2.0587013
 C    -4.1355701   -5.5044614    1.5407041
 H    -4.8143866   -4.8910287    2.1336376
 C    -4.5362539   -5.9481201    0.2689955
 H    -5.5218536   -5.6740583   -0.1080196
 C    -3.6981277   -6.7313522   -0.5254647
 H    -4.0233383   -7.0648348   -1.5087146
 C    -2.4394358   -7.0617061   -0.0112651
 C    -2.0422776   -6.6172268    1.2652583
 N    -1.3662202   -7.8011722   -0.5084574
 N    -0.7557717   -7.1158156    1.4785647
 C    -1.3015276   -8.4738056   -1.8243803
 C    -1.3385073   -7.4574031   -2.9681392
 H    -2.2951897   -6.9196237   -3.0172011
 H    -0.5293547   -6.7235494   -2.8553858
 H    -1.2003046   -7.9794731   -3.9253054
 C    -2.3487307   -9.5845559   -1.9354369
 H    -3.3757923   -9.1958451   -1.9087793
 H    -2.2177054  -10.1144558   -2.8892367
 H    -2.2248053  -10.3084852   -1.1190889
 C     0.0132872   -6.7881133    2.7050751
 C     0.8992225   -5.5609579    2.4706736
 H     1.6535383   -5.7676495    1.6991790
 H     0.3027952   -4.6984284    2.1420054
 H     1.4098121   -5.2874931    3.4049482
 C     0.7829061   -7.9867960    3.2492777
 H    -0.7611240   -6.5306680    3.4427911
 H     1.5809450   -8.2898293    2.5577782
 H     1.2372581   -7.7108990    4.2113587
 H     0.1295920   -8.8554696    3.3996202
 C    -0.3355812   -7.8291783    0.3915810
 H    -0.3060823   -8.9445742   -1.8103542
Pd     1.4275509   -8.7990770    0.0212722
Br     2.4069307   -6.7439075   -0.9629210
Br     0.4756199  -10.9538474    0.8339555
 C     3.1288845   -9.8246846   -0.3905717
 N     3.3653854  -10.5881022   -1.4945777
 N     4.2239988   -9.9948575    0.4001798
 C     4.5810736  -11.2590267   -1.3921883
 C     2.4800556  -10.5516340   -2.6562510
 C     5.1354501  -10.8754848   -0.1756302
 C     4.3129997   -9.3871394    1.7314310
 H     5.3636003   -9.2441521    1.9910383
 H     3.8158056  -10.0328124    2.4676372
```

H	3.7957082	-8.4234461	1.6819121
H	3.0714795	-10.5018264	-3.5773397
H	1.8752735	-9.6429770	-2.5679538
H	1.8195566	-11.4277701	-2.6728376
C	6.4264748	-11.2484295	0.4794625
C	5.1498037	-12.1826096	-2.4057491
O	6.3649750	-12.2522990	-2.5553892
C	4.2187721	-13.0782799	-3.2032017
O	7.0033970	-10.4253752	1.1828274
C	6.9821822	-12.6434391	0.3082530
H	6.2067022	-13.3912849	0.1031751
H	7.5265564	-12.9003076	1.2253323
H	7.6900808	-12.6518170	-0.5310489
H	3.2874097	-13.3119294	-2.6720467
H	4.7625164	-14.0014354	-3.4372406
H	3.9591710	-12.5993903	-4.1594415

HEP complex R_1=CH_3 R_2=$COOCH_3$

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Energy = -6654.0127941410

H	-2.5937034	-5.5422831	3.0861995
C	-2.8922328	-5.8790068	2.0939987
C	-4.1433913	-5.5449402	1.5739059
H	-4.8266047	-4.9430139	2.1734693
C	-4.5360716	-5.9678117	0.2926126
H	-5.5202385	-5.6894475	-0.0851466
C	-3.6920108	-6.7364245	-0.5100918
H	-4.0111753	-7.0561151	-1.4999405
C	-2.4355377	-7.0724465	0.0053232
C	-2.0471853	-6.6501712	1.2923751
N	-1.3586344	-7.8013318	-0.4982065
N	-0.7621214	-7.1524769	1.5053121
C	-1.2777771	-8.4444194	-1.8281786
C	-1.3262347	-7.4047557	-2.9502874
H	-2.2923748	-6.8839547	-2.9969279
H	-0.5314514	-6.6591415	-2.8156137
H	-1.1697848	-7.9046403	-3.9164389
C	-2.3061087	-9.5692074	-1.9678107
H	-3.3396542	-9.1982893	-1.9307422
H	-2.1665357	-10.0716317	-2.9353912
H	-2.1693993	-10.3119654	-1.1704944
C	0.0020814	-6.8447790	2.7395319
C	0.8862556	-5.6116875	2.5305815

H	1.6474318	-5.8046037	1.7622133
H	0.2905049	-4.7457978	2.2095788
H	1.3880389	-5.3512271	3.4733888
C	0.7741337	-8.0503714	3.2650459
H	-0.7751553	-6.6022548	3.4793816
H	1.5743676	-8.3415672	2.5706002
H	1.2252981	-7.7876515	4.2323967
H	0.1226387	-8.9227674	3.4007341
C	-0.3351546	-7.8469112	0.4088705
H	-0.2732076	-8.8963165	-1.8208013
Pd	1.4271115	-8.8070377	0.0263244
Br	2.3992958	-6.7277807	-0.9170656
Br	0.4744364	-10.9761019	0.7958012
C	3.1405278	-9.7898199	-0.4269083
N	3.3674695	-10.5383222	-1.5450577
N	4.2838008	-9.8818689	0.3025830
C	4.6346531	-11.1054227	-1.5159777
C	2.3808787	-10.6160198	-2.6234936
C	5.2185102	-10.6911888	-0.3329044
C	4.4288959	-9.2536075	1.6174668
H	5.4889228	-9.0718804	1.8112331
H	4.0048708	-9.9067909	2.3919551
H	3.8764090	-8.3086371	1.5904309
H	2.8106138	-11.1433048	-3.4771774
H	2.0962801	-9.5960622	-2.9073355
H	1.4987659	-11.1574260	-2.2587095
C	6.5552526	-10.9870433	0.2265472
C	5.2562997	-11.9064525	-2.6013296
O	6.4011586	-11.7708324	-2.9825995
O	4.3843423	-12.8148994	-3.1138334
O	7.1954511	-10.2272348	0.9341638
O	6.9715134	-12.2201731	-0.1363087
C	8.3214351	-12.5536719	0.2645132
H	8.5004169	-13.5553445	-0.1367755
H	8.4062359	-12.5503763	1.3585453
H	9.0323334	-11.8326309	-0.1581225
C	4.9203721	-13.6329701	-4.1824842
H	4.0944622	-14.2793748	-4.4933816
H	5.7631767	-14.2303639	-3.8131126
H	5.2624724	-13.0038307	-5.0141247

HEP complex R_1=CH_3 R_2=OCH_3

59
 Energy = -6427.1842876040

H	-2.4749782	-5.4594771	3.0472620
C	-2.7899982	-5.7696341	2.0515004
C	-4.0085388	-5.3400406	1.5233590
H	-4.6496007	-4.6902048	2.1197011
C	-4.4217887	-5.7283109	0.2377139
H	-5.3795650	-5.3762673	-0.1464463
C	-3.6313089	-6.5561568	-0.5612088
H	-3.9660474	-6.8483262	-1.5544404
C	-2.4073974	-6.9872961	-0.0381688
C	-1.9987727	-6.5997331	1.2538562
N	-1.3845965	-7.7952950	-0.5346626
N	-0.7584214	-7.1995156	1.4764372
C	-1.3414849	-8.4468012	-1.8626388
C	-1.3205902	-7.4109751	-2.9890930
H	-2.2514272	-6.8294697	-3.0408909
H	-0.4793595	-6.7179282	-2.8558339
H	-1.1937597	-7.9247337	-3.9522456
C	-2.4417278	-9.5016920	-1.9985151
H	-3.4479078	-9.0609868	-1.9730740
H	-2.3296782	-10.0241550	-2.9588798
H	-2.3604417	-10.2418545	-1.1910444
C	0.0195285	-6.9441023	2.7138859
C	0.9755310	-5.7647978	2.5061367
H	1.7091985	-5.9972381	1.7218362
H	0.4301460	-4.8597706	2.2038628
H	1.5086107	-5.5470413	3.4426585
C	0.7189928	-8.1917656	3.2438369
H	-0.7435799	-6.6568730	3.4527729
H	1.5371642	-8.5039975	2.5795274
H	1.1388962	-7.9655552	4.2345950
H	0.0289522	-9.0400361	3.3339327
C	-0.3766096	-7.9233106	0.3815562
H	-0.3664371	-8.9601637	-1.8523455
Pd	1.3190689	-9.0025418	0.0322508
Br	2.3898648	-6.9951481	-0.9753951
Br	0.1828018	-11.0647150	0.8637292
C	3.0116228	-10.0669959	-0.3629855
N	3.1949707	-11.0109009	-1.3201937
N	4.2247355	-9.9609052	0.2591779
C	4.5168166	-11.4903033	-1.3175275
C	2.1632770	-11.4858309	-2.2326113
C	5.1553330	-10.8262714	-0.3005701
C	4.5219416	-9.0738853	1.3763513
H	5.5162880	-8.6330264	1.2413713
H	4.4941468	-9.6246455	2.3267729
H	3.7684235	-8.2791213	1.3743495

H	2.4307420	-12.4941281	-2.5692525
H	2.0730314	-10.8181228	-3.1011343
H	1.2128911	-11.5203576	-1.6867581
O	4.9409513	-12.4704638	-2.1564477
O	6.4013769	-10.8466281	0.2204977
C	7.2136068	-11.9863561	-0.1116015
H	6.6897962	-12.9213642	0.1340724
H	8.1189297	-11.8881820	0.4963050
H	7.4821403	-11.9851995	-1.1781587
C	5.3784713	-12.0061654	-3.4562301
H	4.5589841	-11.5065037	-3.9941986
H	5.6927803	-12.8997067	-4.0075426
H	6.2241048	-11.3086663	-3.3528738

HEP complex R_1=C(CH_3)$_3$ R_2=H

69

Energy = -6433.9927073880

H	-2.7183305	-5.3449096	2.9724543
C	-2.9852350	-5.7320501	1.9897118
C	-4.2376222	-5.4598221	1.4384952
H	-4.9486239	-4.8560356	2.0029676
C	-4.5966265	-5.9486138	0.1713832
H	-5.5832126	-5.7194448	-0.2322818
C	-3.7153313	-6.7223518	-0.5842436
H	-4.0085443	-7.0923412	-1.5642861
C	-2.4578764	-6.9980587	-0.0354963
C	-2.1019052	-6.5105631	1.2364076
N	-1.3544743	-7.7174610	-0.4907309
N	-0.8047196	-6.9631451	1.4894018
C	-1.2514080	-8.4039266	-1.7962864
C	-1.2988313	-7.4009002	-2.9517152
H	-2.2633993	-6.8788163	-3.0136591
H	-0.5013428	-6.6537949	-2.8407646
H	-1.1445378	-7.9318574	-3.9013802
C	-2.2662850	-9.5439238	-1.9093905
H	-3.3040232	-9.1836052	-1.9081404
H	-2.1026147	-10.0839436	-2.8522643
H	-2.1405526	-10.2520978	-1.0791539
C	-0.0882244	-6.5900017	2.7356969
C	1.0005822	-5.5514022	2.4535332
H	1.7518817	-5.9356873	1.7524995
H	0.5671047	-4.6449019	2.0090294
H	1.4955733	-5.2712538	3.3944072

C	0.3903939	-7.8105208	3.5183124
H	-0.8633488	-6.1045999	3.3447089
H	1.1397695	-8.3855933	2.9627759
H	0.8332869	-7.4751666	4.4670355
H	-0.4434491	-8.4891208	3.7400256
C	-0.3416439	-7.7017832	0.4326348
H	-0.2432714	-8.8434979	-1.7666940
Pd	1.4156436	-8.7009885	0.0992102
Br	2.3132712	-6.6166562	-0.9674346
Br	0.3475579	-10.6893445	1.1788378
C	3.1657436	-9.7632702	-0.3428920
N	3.4587601	-10.4903070	-1.4806026
N	4.2962582	-9.8840215	0.4367494
C	4.7275446	-11.0420331	-1.3907928
C	2.5858529	-10.7123040	-2.6977540
C	5.2466659	-10.6685544	-0.1981367
C	4.5122061	-9.4035900	1.8531759
C	6.0193195	-9.3920675	2.1649670
C	3.7973498	-10.3799448	2.8011323
C	3.9903577	-7.9776290	2.0178226
C	3.3226402	-11.6068044	-3.7095976
C	2.2980729	-9.3668460	-3.3734306
C	1.3004597	-11.4337831	-2.2759158
H	0.6588876	-11.5800419	-3.1566743
H	0.7470154	-10.8702539	-1.5166905
H	1.5293796	-12.4190913	-1.8461758
H	2.6542456	-11.7531592	-4.5677971
H	3.5536816	-12.6003409	-3.3003228
H	4.2449372	-11.1434961	-4.0866987
H	1.6474872	-9.5288294	-4.2445955
H	3.2291255	-8.8966010	-3.7193207
H	1.8146666	-8.6613137	-2.6880564
H	4.5053292	-7.2807093	1.3433931
H	4.1485259	-7.6559112	3.0565703
H	2.9183487	-7.9162382	1.7900264
H	4.2190692	-11.3909446	2.7034722
H	2.7237860	-10.4364507	2.5782605
H	3.9306781	-10.0528729	3.8424014
H	6.5833556	-8.8001644	1.4303725
H	6.4501496	-10.4010748	2.2249065
H	6.1575311	-8.9257977	3.1492658
H	5.1723622	-11.6439969	-2.1681585
H	6.2109061	-10.8971561	0.2295097

HEP complex R_1=C(CH_3)$_3$ R_2=NO_2

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73
 Energy =   -6843.1907857360
 H    -2.6393139   -5.4207243    3.0024043
 C    -2.9184327   -5.8062507    2.0226230
 C    -4.1900924   -5.5635708    1.5040162
 H    -4.9038469   -4.9857599    2.0916450
 C    -4.5651709   -6.0471137    0.2392191
 H    -5.5661447   -5.8390918   -0.1391752
 C    -3.6824704   -6.7887117   -0.5454627
 H    -3.9873163   -7.1515412   -1.5243923
 C    -2.4069799   -7.0397535   -0.0267235
 C    -2.0335838   -6.5537269    1.2397344
 N    -1.2979392   -7.7298762   -0.5144879
 N    -0.7182169   -6.9720823    1.4585807
 C    -1.2222251   -8.4215164   -1.8202928
 C    -1.2921729   -7.4221205   -2.9774655
 H    -2.2579766   -6.9005186   -3.0196940
 H    -0.4935200   -6.6737284   -2.8849513
 H    -1.1585281   -7.9556739   -3.9287355
 C    -2.2389970   -9.5621826   -1.9084964
 H    -3.2771296   -9.2045105   -1.8999540
 H    -2.0841592  -10.1114499   -2.8473386
 H    -2.1023865  -10.2624833   -1.0736189
 C     0.0092594   -6.5838042    2.6948002
 C     1.0304981   -5.4794160    2.4124749
 H     1.8095479   -5.8163737    1.7173108
 H     0.5427758   -4.6037013    1.9626964
 H     1.5004380   -5.1651080    3.3552982
 C     0.5745783   -7.7895378    3.4397946
 H    -0.7774952   -6.1561331    3.3312961
 H     1.3377124   -8.3085106    2.8497565
 H     1.0275810   -7.4485370    4.3814350
 H    -0.2129505   -8.5180313    3.6718395
 C    -0.2649004   -7.6873489    0.3830877
 H    -0.2174618   -8.8676806   -1.8081459
Pd     1.5067067   -8.6261658    0.0178491
Br     2.2939296   -6.4704027   -1.0091792
Br     0.4897659  -10.6679329    1.0248901
 C     3.2025149   -9.8383321   -0.3469679
 N     3.2728483  -10.8221907   -1.3083809
 N     4.2422466  -10.1076046    0.5465027
 C     4.2613044  -11.7388503   -0.9644526
 C     2.6008109  -10.7867640   -2.6963405
 C     4.8765479  -11.2635703    0.1588869
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C	4.5729800	-9.3499051	1.8376064
C	6.0956923	-9.3350432	2.0752612
C	3.8435634	-10.0600969	2.9881181
C	4.1285037	-7.8962887	1.7113010
C	3.5374270	-11.4319107	-3.7380222
C	2.4241112	-9.3283681	-3.1222303
C	1.2530301	-11.5140321	-2.6285801
H	0.7534267	-11.4235704	-3.6034971
H	0.6117645	-11.0766675	-1.8528090
H	1.3867148	-12.5769931	-2.4008524
H	3.1490606	-11.1703386	-4.7307685
H	3.5696555	-12.5228281	-3.6837239
H	4.5563875	-11.0251352	-3.6710427
H	1.9720022	-9.3235578	-4.1233227
H	3.3862670	-8.8017651	-3.1735459
H	1.7810301	-8.7565255	-2.4476422
H	4.6100791	-7.3899129	0.8650947
H	4.4052290	-7.3773867	2.6388458
H	3.0443994	-7.7991719	1.5740426
H	4.2099915	-11.0867423	3.1195364
H	2.7629766	-10.1034849	2.7989274
H	4.0222248	-9.5089229	3.9217063
H	6.6494200	-9.0452971	1.1724767
H	6.4928369	-10.2796038	2.4596997
H	6.2963733	-8.5791731	2.8447468
N	4.4231603	-13.1055478	-1.4160047
N	5.9861299	-11.9417217	0.8555964
O	3.4209376	-13.7119095	-1.8058195
O	5.5569901	-13.5859546	-1.3110542
O	5.6776282	-12.6892987	1.7823343
O	7.1157618	-11.7023926	0.4460862

HEP complex R_1=$C(CH_3)_3$ R_2=CH_3

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Energy = -6512.6346281130

H	-2.5248841	-5.3051085	2.9266615
C	-2.8440486	-5.7537211	1.9867058
C	-4.1276067	-5.5207295	1.4923278
H	-4.8108659	-4.8889037	2.0603742
C	-4.5511969	-6.0802732	0.2754747
H	-5.5586312	-5.8752004	-0.0875544
C	-3.7068087	-6.8916858	-0.4827910
H	-4.0482115	-7.3122187	-1.4260240
C	-2.4198144	-7.1323779	0.0116270

C	-1.9967833	-6.5674192	1.2290601
N	-1.3371435	-7.8687734	-0.4650893
N	-0.6796162	-6.9867913	1.4276629
C	-1.3297780	-8.6741498	-1.7041343
C	-1.4127798	-7.7803354	-2.9435984
H	-2.3689979	-7.2425502	-3.0052317
H	-0.5971961	-7.0438617	-2.9365047
H	-1.3160878	-8.3971933	-3.8478529
C	-2.3792986	-9.7879285	-1.6542488
H	-3.4073279	-9.4023020	-1.6372258
H	-2.2752738	-10.4201655	-2.5467516
H	-2.2238262	-10.4174617	-0.7680554
C	0.0738062	-6.5856880	2.6431955
C	1.1413520	-5.5367394	2.3240690
H	1.8743936	-5.9102997	1.5994708
H	0.6830324	-4.6365131	1.8920666
H	1.6607137	-5.2495076	3.2496441
C	0.5809023	-7.7983063	3.4214064
H	-0.6881635	-6.1026168	3.2706048
H	1.2881697	-8.3934287	2.8327154
H	1.0802352	-7.4566159	4.3391394
H	-0.2498823	-8.4601874	3.7000462
C	-0.2634287	-7.7715930	0.3824014
H	-0.3407119	-9.1518366	-1.6829338
Pd	1.5258739	-8.6751318	-0.0132305
Br	2.2362600	-6.5253426	-1.1262698
Br	0.5998772	-10.7586189	1.0136434
C	3.2844276	-9.8183229	-0.3871553
N	3.4112173	-10.7935630	-1.3528367
N	4.2436853	-10.1263767	0.5523621
C	4.3336739	-11.7689041	-0.9467927
C	2.7049972	-10.8275767	-2.6931721
C	4.8626724	-11.3459431	0.2409431
C	4.6405300	-13.0688169	-1.6209669
C	5.8887979	-12.0846183	1.0412394
C	4.6095930	-9.3062214	1.7688017
C	6.1451205	-9.1731928	1.8682777
C	4.0118706	-9.9713349	3.0215852
C	4.0739746	-7.8814372	1.6474955
C	3.6927162	-11.2579559	-3.8023360
C	2.2320422	-9.4277969	-3.0841145
C	1.5074553	-11.7878564	-2.6108492
H	0.9801581	-11.8028608	-3.5757396
H	0.8132616	-11.4668481	-1.8225315
H	1.8175714	-12.8163281	-2.3810000
H	3.2429189	-11.0071059	-4.7720368

H	3.9060507	-12.3297696	-3.8161619
H	4.6388488	-10.7050775	-3.7222149
H	1.7803569	-9.4829132	-4.0845247
H	3.0588175	-8.7065233	-3.1083986
H	1.4850655	-9.0316015	-2.3880100
H	4.4524145	-7.3728986	0.7518072
H	4.3889376	-7.3182477	2.5370555
H	2.9778065	-7.8548261	1.5933470
H	4.4357808	-10.9658614	3.2124127
H	2.9259678	-10.0876059	2.9076312
H	4.2141739	-9.3468619	3.9029442
H	6.5682454	-8.8472129	0.9077988
H	6.6522298	-10.0876219	2.1869922
H	6.3742856	-8.3993408	2.6127800
H	3.7480331	-13.5349818	-2.0540365
H	5.0352445	-13.7713949	-0.8763280
H	5.3970945	-12.9828032	-2.4146623
H	5.8622966	-13.1454857	0.7622822
H	5.7070009	-12.0355418	2.1206736
H	6.9136625	-11.7308935	0.8545082

HEP complex R_1=C(CH$_3$)$_3$ R_2=OH

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Energy = -6584.4951749000

H	-2.4558865	-5.0784193	2.8612343
C	-2.7872670	-5.5234051	1.9237190
C	-4.0552648	-5.2386877	1.4166116
H	-4.7137335	-4.5706628	1.9724293
C	-4.4943261	-5.7919019	0.2022169
H	-5.4890849	-5.5465399	-0.1705715
C	-3.6806589	-6.6467874	-0.5414614
H	-4.0333168	-7.0620094	-1.4828924
C	-2.4089696	-6.9382443	-0.0345719
C	-1.9706867	-6.3810167	1.1804559
N	-1.3558943	-7.7257478	-0.4962701
N	-0.6751440	-6.8564548	1.3936921
C	-1.3901025	-8.5618510	-1.7142351
C	-1.4327929	-7.7002462	-2.9779497
H	-2.3672360	-7.1277979	-3.0589117
H	-0.5907266	-6.9947388	-2.9896387
H	-1.3577988	-8.3453486	-3.8643626
C	-2.4909607	-9.6233044	-1.6347605
H	-3.5002208	-9.1911753	-1.6311658
H	-2.4138591	-10.2844169	-2.5089419

H	-2.3642703	-10.2350045	-0.7319316
C	0.0618107	-6.5220376	2.6393361
C	1.2064079	-5.5407044	2.3808614
H	1.9365742	-5.9423519	1.6687682
H	0.8220064	-4.6014971	1.9597945
H	1.7127585	-5.3111849	3.3296085
C	0.4500428	-7.7818877	3.4128447
H	-0.6883495	-5.9979665	3.2476504
H	1.1333538	-8.4194010	2.8409307
H	0.9364107	-7.4936553	4.3556031
H	-0.4381404	-8.3836777	3.6481354
C	-0.2825143	-7.6655123	0.3567968
H	-0.4274303	-9.0882184	-1.6785072
Pd	1.4939866	-8.6155740	-0.0229254
Br	2.3506045	-6.4868530	-1.0381994
Br	0.5020643	-10.7172892	0.8941631
C	3.2371846	-9.7644128	-0.3860041
N	3.3997786	-10.6861313	-1.4137728
N	4.1630928	-10.1223421	0.5668160
C	4.3248198	-11.6447055	-1.0375583
C	2.7552175	-10.7164885	-2.7842871
C	4.8201610	-11.2955811	0.1746514
C	4.5001857	-9.4365431	1.8673821
C	6.0361962	-9.3313412	2.0035513
C	3.8981326	-10.2611345	3.0172441
C	3.9601424	-8.0111934	1.8793129
C	3.8538656	-10.9206818	-3.8499966
C	2.0852801	-9.3847627	-3.0969908
C	1.7276632	-11.8597698	-2.8050486
H	1.2200350	-11.8799260	-3.7798180
H	0.9784680	-11.7129527	-2.0153326
H	2.2079067	-12.8345750	-2.6500877
H	3.3876000	-10.8349868	-4.8409149
H	4.3413271	-11.8976073	-3.7874654
H	4.6170532	-10.1332788	-3.7700393
H	1.6679628	-9.4449816	-4.1119898
H	2.7884968	-8.5442408	-3.0516534
H	1.2716222	-9.1621611	-2.3980756
H	4.3822399	-7.4036551	1.0684031
H	4.2160350	-7.5518624	2.8443853
H	2.8687553	-7.9915445	1.7634754
H	4.3228877	-11.2730489	3.0443322
H	2.8102369	-10.3467176	2.8961586
H	4.1137467	-9.7705258	3.9771653
H	6.4870769	-8.9366923	1.0818887
H	6.5094942	-10.2832668	2.2728584

H	6.2665470	-8.6252958	2.8124080
O	4.6126298	-12.7580735	-1.7643602
O	5.6599389	-12.0767007	0.9287320
H	5.1489884	-13.3305925	-1.1813566
H	6.5730762	-11.7367846	0.8711816

HEP complex R_1=C(CH_3)$_3$ R_2=SH

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Energy = -7230.4804726210

H	-2.5540874	-5.3678885	3.0272473
C	-2.8652583	-5.7627606	2.0609775
C	-4.1524782	-5.5216242	1.5804301
H	-4.8459167	-4.9365893	2.1850426
C	-4.5678888	-6.0148396	0.3322411
H	-5.5794058	-5.8066619	-0.0172617
C	-3.7108522	-6.7654167	-0.4728588
H	-4.0461009	-7.1362585	-1.4388044
C	-2.4201025	-7.0142871	0.0075447
C	-2.0055323	-6.5166975	1.2567440
N	-1.3275082	-7.7070495	-0.5105295
N	-0.6829408	-6.9294030	1.4329123
C	-1.3061691	-8.4329827	-1.7980622
C	-1.4016844	-7.4651698	-2.9796177
H	-2.3674006	-6.9421109	-3.0119809
H	-0.5995149	-6.7164243	-2.9253563
H	-1.2917759	-8.0238333	-3.9194911
C	-2.3368038	-9.5648945	-1.8215041
H	-3.3712883	-9.1977601	-1.7899490
H	-2.2162001	-10.1414698	-2.7488932
H	-2.1772223	-10.2427915	-0.9724778
C	0.0669060	-6.5834828	2.6676127
C	1.1438136	-5.5311801	2.3971176
H	1.8875542	-5.8864136	1.6742839
H	0.6969867	-4.6160481	1.9850876
H	1.6491160	-5.2747650	3.3393333
C	0.5611338	-7.8305810	3.3984664
H	-0.6946481	-6.1193750	3.3094217
H	1.2675082	-8.4051152	2.7885074
H	1.0580685	-7.5302181	4.3317752
H	-0.2752870	-8.4979219	3.6451176
C	-0.2590326	-7.6502835	0.3465100
H	-0.3088533	-8.8933275	-1.8024114
Pd	1.5260205	-8.5417615	-0.0656212
Br	2.2783094	-6.3657838	-1.0710630

Br	0.5600428	-10.6560787	0.8538658
C	3.2608668	-9.7344679	-0.4359556
N	3.3463284	-10.7040456	-1.4276091
N	4.1125469	-10.1516682	0.5506817
C	4.1156499	-11.7729199	-0.9857444
C	2.7545389	-10.6317105	-2.8227683
C	4.6046869	-11.4384586	0.2576991
C	4.6006663	-9.3320575	1.7268713
C	6.1421881	-9.2774937	1.6767536
C	4.0883766	-9.9563045	3.0361772
C	4.1092506	-7.8916600	1.6231038
C	3.8545865	-10.9630788	-3.8528816
C	2.2893408	-9.2139539	-3.1398692
C	1.5739450	-11.6119294	-2.9098401
H	1.1313966	-11.5623346	-3.9147561
H	0.8089581	-11.3534699	-2.1653961
H	1.8844015	-12.6497224	-2.7281678
H	3.4438708	-10.7935410	-4.8573861
H	4.2078562	-11.9991042	-3.8138976
H	4.7181097	-10.2962371	-3.7215424
H	1.9137078	-9.2035223	-4.1723521
H	3.1008614	-8.4810470	-3.0529189
H	1.4864802	-8.8817363	-2.4724176
H	4.4227426	-7.4097013	0.6891005
H	4.5284332	-7.3303644	2.4700096
H	3.0151349	-7.8232213	1.6747416
H	4.5366226	-10.9391621	3.2242517
H	2.9965927	-10.0687560	3.0036412
H	4.3505736	-9.2998241	3.8773937
H	6.4784434	-8.8672701	0.7144547
H	6.6123196	-10.2539735	1.8342157
H	6.4930604	-8.6058556	2.4721616
S	4.3320783	-13.3250503	-1.7835800
S	5.5662696	-12.5114728	1.2565663
H	5.0318340	-13.7962783	-0.7083240
H	4.5461238	-13.1092785	1.9338572

HEP complex R_1=C(CH_3)$_3$ R_2=C_6H_5

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Energy = -6896.2529219860

H	-2.5168515	-5.3032844	2.9175201
C	-2.8387321	-5.7557056	1.9802749
C	-4.1192268	-5.5147961	1.4818099
H	-4.7977048	-4.8721979	2.0435504

C	-4.5456393	-6.0797571	0.2684176
H	-5.5511031	-5.8695979	-0.0971730
C	-3.7063838	-6.9021631	-0.4837666
H	-4.0498881	-7.3263496	-1.4245867
C	-2.4216225	-7.1487080	0.0134459
C	-1.9971911	-6.5815177	1.2294793
N	-1.3418107	-7.8929809	-0.4585368
N	-0.6844097	-7.0108257	1.4346999
C	-1.3300148	-8.6920762	-1.7019937
C	-1.4123208	-7.7910762	-2.9365038
H	-2.3694068	-7.2547013	-2.9967119
H	-0.5980887	-7.0531938	-2.9235210
H	-1.3126631	-8.4025394	-3.8441148
C	-2.3791308	-9.8067309	-1.6612779
H	-3.4073999	-9.4214472	-1.6470922
H	-2.2709080	-10.4348331	-2.5561529
H	-2.2278020	-10.4405590	-0.7774806
C	0.0672532	-6.6079184	2.6509889
C	1.1181486	-5.5407820	2.3362457
H	1.8632722	-5.9029207	1.6183222
H	0.6469221	-4.6500621	1.8984389
H	1.6254429	-5.2416291	3.2647659
C	0.5945742	-7.8169257	3.4209016
H	-0.7001325	-6.1405934	3.2837809
H	1.3102428	-8.3979742	2.8288150
H	1.0905724	-7.4717697	4.3391398
H	-0.2251231	-8.4929660	3.6980795
C	-0.2705680	-7.7997923	0.3920699
H	-0.3399638	-9.1689560	-1.6825838
Pd	1.5182888	-8.7021219	-0.0028264
Br	2.2023787	-6.5371963	-1.1059187
Br	0.6064355	-10.7901940	1.0296580
C	3.2807435	-9.8336947	-0.3795693
N	3.4332526	-10.7844853	-1.3661798
N	4.2520548	-10.1221151	0.5535406
C	4.4128959	-11.7192457	-0.9927993
C	2.7068323	-10.8122450	-2.7031563
C	4.9277088	-11.3029852	0.2052908
C	4.7538839	-13.0123294	-1.6375880
C	5.9062025	-12.0907556	0.9991980
C	4.6029218	-9.2937375	1.7761863
C	6.1339041	-9.1752471	1.9062186
C	3.9966193	-9.9524711	3.0269905
C	4.0748970	-7.8690941	1.6312726
C	3.6559699	-11.2942944	-3.8179480
C	2.2751952	-9.3994024	-3.0954580

C	1.4839661	-11.7372943	-2.6024258
H	0.9072942	-11.6801649	-3.5369247
H	0.8405194	-11.4418579	-1.7629003
H	1.7823168	-12.7834358	-2.4562332
H	3.1570897	-11.1129885	-4.7797768
H	3.8891065	-12.3604971	-3.7645207
H	4.5943732	-10.7230109	-3.8159531
H	1.8412199	-9.4399392	-4.1042789
H	3.1199586	-8.6989826	-3.1034541
H	1.5249974	-8.9859204	-2.4138841
H	4.4493278	-7.3790105	0.7238488
H	4.4018439	-7.2923075	2.5078993
H	2.9788170	-7.8339517	1.5888168
H	4.4787781	-10.9119858	3.2506636
H	2.9208504	-10.1261242	2.8900121
H	4.1425269	-9.2928159	3.8937460
H	6.5782468	-8.8035901	0.9720522
H	6.6213487	-10.1134545	2.1839065
H	6.3508360	-8.4421324	2.6947168
C	3.9047231	-14.1213032	-1.4832940
C	5.9698501	-13.1877262	-2.3185428
C	4.2477182	-15.3619043	-2.0255605
H	2.9786123	-14.0099613	-0.9180060
C	5.4505397	-15.5182060	-2.7184657
H	3.5760960	-16.2118877	-1.8955470
C	6.3145483	-14.4285790	-2.8563540
H	5.7182433	-16.4875060	-3.1412873
H	7.2613104	-14.5442218	-3.3862670
H	6.6408422	-12.3362163	-2.4388278
C	5.4593611	-12.9538378	2.0134634
C	7.2740775	-12.0864930	0.6779181
C	6.3598514	-13.7653494	2.7075666
C	8.1739156	-12.8985467	1.3694603
C	7.7199300	-13.7366262	2.3914132
H	4.3943132	-13.0000467	2.2440256
H	8.4225689	-14.3717242	2.9328237
H	5.9934635	-14.4306035	3.4909324
H	9.2329692	-12.8776708	1.1082323
H	7.6321108	-11.4276803	-0.1143059

HEP complex R_1=C(CH_3)$_3$ R_2=F

69
 Energy = -6632.5360464770
H	-2.6037962	-5.2002435	2.9076439

C	-2.9004082	-5.6178635	1.9463219
C	-4.1613315	-5.3444680	1.4164868
H	-4.8493681	-4.7117582	1.9776806
C	-4.5569802	-5.8657524	0.1733605
H	-5.5478800	-5.6310580	-0.2161754
C	-3.7054245	-6.6761404	-0.5773950
H	-4.0250836	-7.0676017	-1.5404880
C	-2.4401180	-6.9554100	-0.0484424
C	-2.0456182	-6.4308260	1.1959418
N	-1.3574268	-7.7023132	-0.5094166
N	-0.7448737	-6.8845121	1.4273040
C	-1.3320578	-8.4819222	-1.7647817
C	-1.3822930	-7.5648233	-2.9890060
H	-2.3351812	-7.0232033	-3.0652256
H	-0.5661326	-6.8303006	-2.9515886
H	-1.2662765	-8.1660509	-3.9014418
C	-2.3933782	-9.5858283	-1.7579816
H	-3.4173881	-9.1895428	-1.7485866
H	-2.2811957	-10.1989147	-2.6627625
H	-2.2593765	-10.2368696	-0.8839231
C	-0.0389907	-6.5635741	2.6944888
C	1.1305131	-5.6045565	2.4677163
H	1.8737947	-6.0234335	1.7799466
H	0.7776114	-4.6600194	2.0316167
H	1.6129776	-5.3821190	3.4303348
C	0.3052897	-7.8287936	3.4803384
H	-0.7957426	-6.0240297	3.2802356
H	1.0025531	-8.4746624	2.9356128
H	0.7585457	-7.5459673	4.4409603
H	-0.5975443	-8.4207582	3.6827152
C	-0.3113680	-7.6514567	0.3763677
H	-0.3484396	-8.9700630	-1.7341731
Pd	1.4720948	-8.5823742	0.0090323
Br	2.3207178	-6.4390306	-0.9733404
Br	0.5051071	-10.6808796	0.9576086
C	3.2110132	-9.7187450	-0.3809383
N	3.3760668	-10.6213532	-1.4201732
N	4.1646338	-10.0675835	0.5575183
C	4.3295917	-11.5607082	-1.0635472
C	2.6595818	-10.6741558	-2.7595955
C	4.8173055	-11.2167976	0.1471727
C	4.5309269	-9.3951625	1.8648708
C	6.0596438	-9.1870031	1.9014195
C	4.0509327	-10.2995971	3.0125743
C	3.8824735	-8.0215812	1.9592172
C	3.6482928	-11.1091988	-3.8639762

C	2.1674968	-9.2803674	-3.1384769
C	1.5001807	-11.6738320	-2.6422417
H	0.9558812	-11.7181500	-3.5963840
H	0.8084862	-11.3770965	-1.8426489
H	1.8687952	-12.6839070	-2.4145452
H	3.1680738	-10.9177910	-4.8327844
H	3.9057556	-12.1713350	-3.8249969
H	4.5711821	-10.5140519	-3.8278942
H	1.6550717	-9.3500877	-4.1078991
H	2.9973079	-8.5674586	-3.2270837
H	1.4713717	-8.8677029	-2.4005971
H	4.1990963	-7.3586149	1.1443536
H	4.1725972	-7.5725202	2.9196067
H	2.7869906	-8.0881676	1.9251030
H	4.5498301	-11.2769678	2.9986100
H	2.9669178	-10.4615634	2.9424968
H	4.2761800	-9.8181998	3.9743829
H	6.3897575	-8.6100129	1.0264683
H	6.6259928	-10.1219897	1.9464177
H	6.3045458	-8.6036541	2.7992182
F	4.6634759	-12.6310615	-1.7850083
F	5.7428295	-11.8652922	0.8579053

HEP complex R_1=C(CH$_3$)$_3$ R_2=NH$_2$

73

Energy = -6544.7411481060

H	-2.5728350	-5.4368653	3.0476490
C	-2.8822388	-5.8262544	2.0784943
C	-4.1728497	-5.5935029	1.6022740
H	-4.8712793	-5.0210434	2.2132663
C	-4.5849244	-6.0787157	0.3499541
H	-5.5984630	-5.8760084	0.0031071
C	-3.7215460	-6.8135454	-0.4631796
H	-4.0537992	-7.1768281	-1.4330927
C	-2.4281170	-7.0553088	0.0134851
C	-2.0162287	-6.5645358	1.2665795
N	-1.3291247	-7.7312989	-0.5124693
N	-0.6891906	-6.9642797	1.4356228
C	-1.2993585	-8.4409586	-1.8082125
C	-1.3973997	-7.4591607	-2.9779895
H	-2.3656505	-6.9403584	-3.0059757
H	-0.5985347	-6.7077758	-2.9116754
H	-1.2820747	-8.0048512	-3.9248891

C	-2.3208936	-9.5806845	-1.8491713
H	-3.3587766	-9.2231332	-1.8164105
H	-2.1926871	-10.1446235	-2.7834926
H	-2.1578152	-10.2673969	-1.0078314
C	0.0630690	-6.6193161	2.6687978
C	1.1267560	-5.5539157	2.3965509
H	1.8664550	-5.8967165	1.6636610
H	0.6657368	-4.6407076	1.9958756
H	1.6392883	-5.2988889	3.3352359
C	0.5761885	-7.8666070	3.3868396
H	-0.6990019	-6.1672182	3.3188379
H	1.2784542	-8.4325301	2.7642893
H	1.0838109	-7.5676866	4.3149016
H	-0.2519236	-8.5415103	3.6412095
C	-0.2576986	-7.6704876	0.3418630
H	-0.2984130	-8.8936017	-1.8140853
Pd	1.5413846	-8.5394595	-0.0796589
Br	2.2740237	-6.3609258	-1.0945297
Br	0.6044714	-10.6799970	0.8183908
C	3.2990805	-9.6834878	-0.4552781
N	3.3847593	-10.6718141	-1.4302076
N	4.1809066	-10.0685540	0.5166078
C	4.1730293	-11.7214909	-0.9706485
C	2.8001150	-10.6347664	-2.8225521
C	4.6900218	-11.3533292	0.2390838
C	4.6441831	-9.2676702	1.7079449
C	6.1845624	-9.1746969	1.6648172
C	4.1550389	-9.9524863	2.9962898
C	4.1097188	-7.8408303	1.6453994
C	3.9128928	-10.9475160	-3.8468238
C	2.2892273	-9.2357661	-3.1559680
C	1.6386650	-11.6405634	-2.9144189
H	1.1422246	-11.5405817	-3.8900548
H	0.9071385	-11.4542379	-2.1164720
H	1.9688978	-12.6868054	-2.8318755
H	3.4837469	-10.8716682	-4.8554512
H	4.3498479	-11.9436402	-3.7274387
H	4.7186665	-10.2039821	-3.7659253
H	1.9320741	-9.2409710	-4.1953792
H	3.0737595	-8.4761962	-3.0553477
H	1.4652925	-8.9297269	-2.5010545
H	4.4180888	-7.3223157	0.7291942
H	4.4994215	-7.2913931	2.5141871
H	3.0130346	-7.8106972	1.6819581
H	4.6343429	-10.9285007	3.1373046
H	3.0665049	-10.0947609	2.9634003

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 H     4.4012918   -9.3225327    3.8627240
 H     6.5123189   -8.7318158    0.7136792
 H     6.6619538  -10.1504912    1.7952897
 H     6.5189055   -8.5140178    2.4768589
 N     4.4360400  -12.9144752   -1.6528801
 N     5.5282432  -12.0928504    1.0933536
 H     3.5929983  -13.3905822   -1.9758190
 H     4.9635581  -13.5458028   -1.0480889
 H     5.0639032  -12.8640360    1.5738998
 H     6.3995311  -12.4084388    0.6698300
```

HEP complex R_1=C(CH$_3$)$_3$ R_2=Cl

```
69
 Energy =   -7353.2937109670
 H    -2.6579989   -5.4104657    3.0312874
 C    -2.9474063   -5.7900625    2.0521258
 C    -4.2227802   -5.5384966    1.5459849
 H    -4.9284748   -4.9602320    2.1429652
 C    -4.6106297   -6.0119653    0.2813906
 H    -5.6126786   -5.7941741   -0.0889051
 C    -3.7377110   -6.7538784   -0.5143639
 H    -4.0513739   -7.1083404   -1.4935993
 C    -2.4590770   -7.0136072   -0.0081412
 C    -2.0710544   -6.5341336    1.2564331
 N    -1.3576498   -7.7029203   -0.5116814
 N    -0.7527694   -6.9518023    1.4553479
 C    -1.3058749   -8.3980794   -1.8151987
 C    -1.3476453   -7.3986605   -2.9732570
 H    -2.3023797   -6.8563959   -3.0184328
 H    -0.5336618   -6.6674730   -2.8761059
 H    -1.2210307   -7.9341885   -3.9244766
 C    -2.3509539   -9.5132665   -1.9044856
 H    -3.3808897   -9.1330096   -1.9111738
 H    -2.1974101  -10.0723301   -2.8378919
 H    -2.2384529  -10.2108980   -1.0639376
 C    -0.0227581   -6.6109148    2.7034651
 C     1.0651283   -5.5658124    2.4490670
 H     1.8165240   -5.9263276    1.7366414
 H     0.6306441   -4.6477093    2.0306879
 H     1.5585884   -5.3127138    3.3983306
 C     0.4512159   -7.8584966    3.4465747
 H    -0.7923103   -6.1404686    3.3309026
 H     1.1723472   -8.4355691    2.8567075
```

H	0.9243269	-7.5568481	4.3918523
H	-0.3915324	-8.5246883	3.6737218
C	-0.3080748	-7.6596148	0.3691283
H	-0.3173692	-8.8761431	-1.7987053
Pd	1.4765342	-8.5591152	-0.0146461
Br	2.2589825	-6.3937316	-1.0166851
Br	0.4869407	-10.6572741	0.9094637
C	3.2077284	-9.7664468	-0.3709812
N	3.2725347	-10.7511850	-1.3392667
N	4.0804084	-10.1664602	0.6220451
C	4.0532504	-11.8070138	-0.8767417
C	2.6892494	-10.6966128	-2.7417108
C	4.5629532	-11.4403881	0.3336407
C	4.5595110	-9.3482661	1.8059748
C	6.0989659	-9.2623354	1.7467148
C	4.0580095	-10.0024336	3.1044925
C	4.0349919	-7.9193750	1.7196581
C	3.7862468	-11.0690498	-3.7628618
C	2.2609236	-9.2718453	-3.0803722
C	1.4884467	-11.6521833	-2.8149791
H	1.0381258	-11.5940399	-3.8161425
H	0.7355053	-11.3763727	-2.0644592
H	1.7834380	-12.6938422	-2.6354061
H	3.3877147	-10.8795588	-4.7687382
H	4.0926551	-12.1173112	-3.7194968
H	4.6720115	-10.4329686	-3.6272455
H	1.8861430	-9.2690360	-4.1132167
H	3.0921116	-8.5598131	-3.0049853
H	1.4667837	-8.9067871	-2.4203412
H	4.3376469	-7.4168598	0.7929559
H	4.4403933	-7.3609877	2.5751924
H	2.9391499	-7.8792916	1.7721803
H	4.4867689	-10.9985604	3.2630256
H	2.9643327	-10.0962084	3.0841077
H	4.3420838	-9.3712342	3.9577583
H	6.4181150	-8.8186117	0.7934149
H	6.5954718	-10.2294523	1.8710172
H	6.4402822	-8.6035657	2.5566931
Cl	4.2599893	-13.3562296	-1.5762628
Cl	5.5364331	-12.4513063	1.3146256

HEP complex R_1=C(CH$_3$)$_3$ R_2=Br

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```
 Energy =  -11581.6487818700
 H   -2.5416255   -5.2953998    2.9688321
 C   -2.8682485   -5.7227780    2.0216153
 C   -4.1500983   -5.4671604    1.5343880
 H   -4.8249149   -4.8379054    2.1152805
 C   -4.5830698   -6.0007418    0.3090995
 H   -5.5893141   -5.7787600   -0.0470311
 C   -3.7499973   -6.8077445   -0.4657941
 H   -4.0980322   -7.2069383   -1.4157616
 C   -2.4654511   -7.0726911    0.0222718
 C   -2.0329718   -6.5333974    1.2480152
 N   -1.3932381   -7.8149295   -0.4693633
 N   -0.7208962   -6.9723654    1.4382482
 C   -1.3911920   -8.5882039   -1.7295860
 C   -1.4451732   -7.6597448   -2.9445532
 H   -2.3903221   -7.1014997   -2.9978880
 H   -0.6149201   -6.9410506   -2.9122920
 H   -1.3548340   -8.2543541   -3.8644971
 C   -2.4619228   -9.6824252   -1.7225530
 H   -3.4828480   -9.2783269   -1.7259990
 H   -2.3464712  -10.3002461   -2.6234449
 H   -2.3414684  -10.3303487   -0.8445955
 C    0.0442306   -6.5897618    2.6529915
 C    1.1111223   -5.5395281    2.3358095
 H    1.8446404   -5.9122885    1.6107790
 H    0.6524581   -4.6388365    1.9055653
 H    1.6308438   -5.2536080    3.2615624
 C    0.5561956   -7.8119426    3.4123841
 H   -0.7111073   -6.1125361    3.2926482
 H    1.2571310   -8.4003235    2.8095505
 H    1.0646498   -7.4809525    4.3288432
 H   -0.2719251   -8.4774149    3.6902909
 C   -0.3200198   -7.7450331    0.3797709
 H   -0.4118740   -9.0848171   -1.7097173
Pd    1.4463468   -8.6690624   -0.0072913
Br    2.1791367   -6.5420459   -1.1306830
Br    0.4588670  -10.7289346    1.0004077
 C    3.1781024   -9.8992186   -0.3328214
 N    3.2192635  -10.9330855   -1.2483940
 N    4.0558653  -10.2580724    0.6723873
 C    3.9903485  -11.9744346   -0.7392063
 C    2.6496936  -10.9148179   -2.6581740
 C    4.5159386  -11.5534476    0.4484162
Br    4.1792084  -13.7262918   -1.3961044
Br    5.5583124  -12.6438976    1.5704187
 C    4.5708223   -9.3606695    1.7823701
```

C	6.1092545	-9.2992681	1.6876839
C	4.0864272	-9.8999552	3.1386321
C	4.0675663	-7.9338634	1.5922763
C	3.7714437	-11.2842827	-3.6515270
C	2.1950557	-9.5065628	-3.0294504
C	1.4623184	-11.8868652	-2.7343292
H	1.0309645	-11.8501456	-3.7446619
H	0.6917349	-11.6029789	-2.0049705
H	1.7614529	-12.9223736	-2.5314451
H	3.3787322	-11.1600714	-4.6699941
H	4.1240381	-12.3147168	-3.5546907
H	4.6262948	-10.6036007	-3.5345230
H	1.8420814	-9.5300834	-4.0696174
H	3.0040870	-8.7703241	-2.9483197
H	1.3761688	-9.1552910	-2.3914104
H	4.3603743	-7.5122727	0.6231376
H	4.4996146	-7.3159357	2.3920070
H	2.9744800	-7.8670755	1.6604832
H	4.5051028	-10.8862639	3.3703354
H	2.9916019	-9.9796948	3.1466471
H	4.3947866	-9.2059185	3.9321233
H	6.4140130	-8.9213141	0.7019539
H	6.5980207	-10.2624933	1.8633167
H	6.4745344	-8.5957460	2.4478574

HEP complex R_1=C(CH$_3$)$_3$ R_2=I

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Energy = -7028.4698120620

H	-2.6274965	-5.3879538	3.0287287
C	-2.9272444	-5.7759196	2.0560623
C	-4.2039520	-5.5193531	1.5558575
H	-4.9009479	-4.9296596	2.1517662
C	-4.6041090	-6.0024780	0.2987652
H	-5.6075021	-5.7819810	-0.0664265
C	-3.7418333	-6.7579800	-0.4959087
H	-4.0649676	-7.1193167	-1.4695578
C	-2.4618521	-7.0229521	0.0045275
C	-2.0626059	-6.5355772	1.2626185
N	-1.3675410	-7.7238481	-0.4997004
N	-0.7472657	-6.9626972	1.4591860
C	-1.3299951	-8.4364853	-1.7945989
C	-1.3938833	-7.4539643	-2.9663755
H	-2.3536546	-6.9208762	-3.0104742

H	-0.5857306	-6.7139005	-2.8884580
H	-1.2723197	-8.0021559	-3.9110106
C	-2.3732321	-9.5555725	-1.8492789
H	-3.4034948	-9.1761473	-1.8322794
H	-2.2430652	-10.1230981	-2.7809273
H	-2.2375077	-10.2447750	-1.0052624
C	-0.0119803	-6.6217513	2.7043427
C	1.0482056	-5.5471849	2.4552789
H	1.8091721	-5.8842922	1.7414661
H	0.5903309	-4.6379332	2.0423608
H	1.5344981	-5.2869036	3.4064256
C	0.5007393	-7.8678599	3.4228260
H	-0.7865390	-6.1805133	3.3467477
H	1.2252191	-8.4182276	2.8119571
H	0.9829730	-7.5690781	4.3643738
H	-0.3226991	-8.5565661	3.6528284
C	-0.3132310	-7.6799493	0.3750730
H	-0.3380922	-8.9087118	-1.7870124
Pd	1.4695036	-8.5718397	-0.0157789
Br	2.2129007	-6.3828689	-1.0055219
Br	0.4842151	-10.6779685	0.8902646
C	3.2101617	-9.7889352	-0.3731197
N	3.2666376	-10.7734683	-1.3396417
N	4.0645651	-10.2025490	0.6291489
C	4.0183798	-11.8513198	-0.8691422
C	2.7286887	-10.6598658	-2.7576857
C	4.5212137	-11.4930687	0.3557376
C	4.5556506	-9.3462314	1.7827140
C	6.0953833	-9.2857768	1.7289471
C	4.0297980	-9.9215056	3.1079037
C	4.0664013	-7.9091374	1.6307346
C	3.8646300	-10.9871798	-3.7487256
C	2.3096006	-9.2236166	-3.0583036
C	1.5213254	-11.5962774	-2.9183043
H	1.1110476	-11.4862778	-3.9322765
H	0.7430996	-11.3412530	-2.1863338
H	1.7906087	-12.6504050	-2.7769608
H	3.5003852	-10.7841029	-4.7651353
H	4.1926261	-12.0304867	-3.7184193
H	4.7316643	-10.3377221	-3.5640094
H	1.9673690	-9.1867944	-4.1017761
H	3.1351842	-8.5124531	-2.9341086
H	1.4938881	-8.8816278	-2.4123732
H	4.3685596	-7.4612998	0.6766442
H	4.5010456	-7.3197726	2.4503609
H	2.9740987	-7.8320699	1.6986172

H	4.4431653	-10.9120675	3.3309456
H	2.9357652	-10.0046682	3.0763141
H	4.3088364	-9.2467423	3.9287137
H	6.4257794	-8.8613542	0.7707434
H	6.5797681	-10.2576132	1.8692430
H	6.4434243	-8.6226497	2.5323994
I	4.2054292	-13.7787650	-1.6595792
I	5.6195744	-12.7967728	1.5667326

HEP complex R_1=C(CH$_3$)$_3$ R_2=OCH$_3$

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Energy = -6663.1172748200

H	-2.5974689	-5.2985115	2.9972520
C	-2.9162024	-5.7406582	2.0540498
C	-4.2173595	-5.5496179	1.5885795
H	-4.9137909	-4.9564636	2.1818372
C	-4.6423841	-6.1026774	0.3691560
H	-5.6644211	-5.9319203	0.0299530
C	-3.7816014	-6.8655381	-0.4204744
H	-4.1244368	-7.2822514	-1.3647782
C	-2.4770285	-7.0648600	0.0456764
C	-2.0522112	-6.5058545	1.2650611
N	-1.3765985	-7.7507538	-0.4646606
N	-0.7162442	-6.8766231	1.4303796
C	-1.3680120	-8.5430730	-1.7118392
C	-1.4958949	-7.6410636	-2.9414617
H	-2.4688939	-7.1322749	-2.9843475
H	-0.7033055	-6.8800028	-2.9397179
H	-1.3935309	-8.2464720	-3.8528395
C	-2.3825500	-9.6889387	-1.6569539
H	-3.4225022	-9.3369501	-1.6355029
H	-2.2617617	-10.3176369	-2.5498172
H	-2.2019857	-10.3137288	-0.7722694
C	0.0399821	-6.4842242	2.6467967
C	1.1068334	-5.4329750	2.3350328
H	1.8368012	-5.7974320	1.6033094
H	0.6463816	-4.5282728	1.9147206
H	1.6299948	-5.1557596	3.2614447
C	0.5438883	-7.7076395	3.4122337
H	-0.7195758	-6.0045442	3.2794860
H	1.2383976	-8.3058431	2.8116203
H	1.0553024	-7.3787444	4.3279427
H	-0.2915709	-8.3625002	3.6941273
C	-0.2905493	-7.6286146	0.3644567

H	-0.3660659	-8.9931148	-1.7085474
Pd	1.5280303	-8.4672747	-0.0586448
Br	2.2201245	-6.3012725	-1.1248081
Br	0.6599301	-10.6130013	0.8878732
C	3.3147053	-9.5519654	-0.4393546
N	3.5038686	-10.4827193	-1.4430530
N	4.2116261	-9.9028546	0.5477533
C	4.4173478	-11.4550871	-1.0265993
C	2.8605117	-10.5414236	-2.8099941
C	4.8388522	-11.1076464	0.2214081
O	4.7194556	-12.5703790	-1.7402055
O	5.6797882	-11.7903472	1.0460840
C	4.6275529	-9.1114472	1.7663085
C	6.1651073	-8.9764425	1.7548597
C	4.1357761	-9.8406534	3.0279504
C	4.0511021	-7.7012193	1.7184282
C	3.9561886	-10.7400690	-3.8802699
C	2.1664944	-9.2246946	-3.1361940
C	1.8526954	-11.7022455	-2.8206797
H	1.3457738	-11.7404729	-3.7954462
H	1.1008634	-11.5619255	-2.0323433
H	2.3521200	-12.6657665	-2.6555800
H	3.4967096	-10.6138608	-4.8700003
H	4.4096924	-11.7344687	-3.8447347
H	4.7400292	-9.9759581	-3.7779172
H	1.7388778	-9.3062470	-4.1454649
H	2.8568153	-8.3726315	-3.1107923
H	1.3578563	-9.0005465	-2.4317586
H	4.3690200	-7.1563708	0.8206411
H	4.4006298	-7.1581264	2.6080172
H	2.9535135	-7.7063739	1.7229275
H	4.6405114	-10.8057743	3.1587209
H	3.0525927	-10.0139223	2.9734898
H	4.3514743	-9.2264145	3.9133962
H	6.4968189	-8.4798438	0.8320587
H	6.6757922	-9.9398898	1.8461453
H	6.4658849	-8.3449825	2.6023872
C	5.1302093	-13.0458594	1.5240370
C	6.1294071	-12.7577502	-2.0067584
H	6.5175401	-11.9283819	-2.6169064
H	6.2066173	-13.6986102	-2.5629742
H	6.7013865	-12.8251059	-1.0710167
H	5.8859043	-13.4658596	2.1976706
H	4.9470613	-13.7348738	0.6870293
H	4.1900059	-12.8714357	2.0669047

HEP complex R_1=C(CH_3)$_3$ R_2=COH

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73
 Energy =   -6660.7212163300
 H   -2.7031716   -5.2740497    2.8763364
 C   -2.9414417   -5.6478838    1.8813054
 C   -4.1643391   -5.3383412    1.2871096
 H   -4.8775171   -4.7163922    1.8285619
 C   -4.4929823   -5.8163985    0.0077026
 H   -5.4580122   -5.5594600   -0.4297301
 C   -3.6099326   -6.6171417   -0.7158342
 H   -3.8813517   -6.9808519   -1.7042889
 C   -2.3815057   -6.9308515   -0.1224908
 C   -2.0543101   -6.4520788    1.1585801
 N   -1.2890041   -7.6906771   -0.5362940
 N   -0.7808119   -6.9443300    1.4577230
 C   -1.1665463   -8.3575783   -1.8497795
 C   -1.1646334   -7.3373716   -2.9911000
 H   -2.1156808   -6.7942940   -3.0724293
 H   -0.3543739   -6.6098579   -2.8495506
 H   -0.9950903   -7.8593051   -3.9429591
 C   -2.2027158   -9.4736369   -2.0027939
 H   -3.2312868   -9.0891149   -2.0250498
 H   -2.0279118  -10.0085154   -2.9463709
 H   -2.1205435  -10.1927353   -1.1765586
 C   -0.1071535   -6.5683231    2.7276270
 C    1.1847711   -5.7946114    2.4683393
 H    1.9184629   -6.3984793    1.9248082
 H    0.9875964   -4.8959423    1.8684371
 H    1.6210357   -5.4825212    3.4279955
 C    0.0283033   -7.7545124    3.6820517
 H   -0.8114529   -5.8631023    3.1895530
 H    0.6609518   -8.5478028    3.2684368
 H    0.4614741   -7.4082628    4.6311680
 H   -0.9540362   -8.1992053    3.8921730
 C   -0.3111621   -7.7165071    0.4253835
 H   -0.1676504   -8.8130113   -1.8071599
Pd    1.4047364   -8.8247435    0.1579826
Br    2.4301236   -6.8581127   -0.9952205
Br    0.3542436  -10.7062155    1.4463922
 C    3.0929344  -10.0184699   -0.2150404
 N    3.3584831  -10.7936988   -1.3541380
 N    4.1460874  -10.2537645    0.6258283
 C    4.5513916  -11.4649588   -1.2060341
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C	2.4167841	-10.9779401	-2.5456457
C	5.0340142	-11.1737783	0.0518197
C	5.3775220	-12.2535953	-2.1925766
C	6.1953603	-11.8693788	0.5917516
C	4.4519607	-9.6231444	1.9727470
C	5.9087307	-9.1101620	1.9578437
C	4.1918637	-10.6767959	3.0651696
C	3.5783212	-8.4062975	2.2422507
C	2.8763349	-12.1328432	-3.4501921
C	2.4026858	-9.6836146	-3.3670839
C	1.0298688	-11.3629613	-2.0214950
H	0.3488972	-11.4642895	-2.8776890
H	0.6242253	-10.6195811	-1.3277101
H	1.0623388	-12.3214757	-1.4859914
H	2.0525086	-12.3396427	-4.1456504
H	3.0549425	-13.0615802	-2.8866164
H	3.7597271	-11.8895890	-4.0463716
H	1.7162846	-9.8064786	-4.2169447
H	3.4046637	-9.4703842	-3.7637696
H	2.0852785	-8.8206998	-2.7697481
H	3.7296837	-7.6246453	1.4869037
H	3.8577403	-8.0047272	3.2268186
H	2.5131808	-8.6668525	2.2707326
H	4.8073719	-11.5781133	2.9490501
H	3.1344515	-10.9757577	3.0470099
H	4.4166557	-10.2425722	4.0491603
H	6.0616775	-8.4240936	1.1138760
H	6.6685464	-9.8974687	1.9063932
H	6.0872760	-8.5503504	2.8853208
O	5.9134469	-11.7256266	-3.1467864
O	6.9331477	-12.5398106	-0.1279592
H	6.3727020	-11.8306545	1.6850663
H	5.4812990	-13.3377922	-1.9733660

HEP complex R_1=C(CH_3)$_3$ R_2=$COCH_3$

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Energy = -6739.3811413590

H	-2.7224547	-5.4429429	3.0200686
C	-2.9916033	-5.8288056	2.0375687
C	-4.2667392	-5.6074306	1.5174129
H	-4.9924504	-5.0459443	2.1061362
C	-4.6300123	-6.0918303	0.2497130
H	-5.6337372	-5.9002153	-0.1305028
C	-3.7312503	-6.8134666	-0.5359316

H	-4.0274041	-7.1784412	-1.5167275
C	-2.4522502	-7.0424074	-0.0158158
C	-2.0898537	-6.5542977	1.2531981
N	-1.3287484	-7.7067537	-0.5053719
N	-0.7654595	-6.9436837	1.4694517
C	-1.2385671	-8.3954825	-1.8113637
C	-1.3223530	-7.3956675	-2.9670549
H	-2.2986055	-6.8938236	-3.0125017
H	-0.5393209	-6.6316937	-2.8677249
H	-1.1727707	-7.9236759	-3.9190863
C	-2.2345549	-9.5541307	-1.9038709
H	-3.2794679	-9.2162282	-1.8990728
H	-2.0655348	-10.0997956	-2.8424403
H	-2.0879462	-10.2529672	-1.0693767
C	-0.0569925	-6.5755811	2.7223454
C	1.0245022	-5.5236150	2.4674642
H	1.7903476	-5.8867495	1.7721752
H	0.5874336	-4.6165736	2.0280998
H	1.5009419	-5.2506107	3.4200707
C	0.4170111	-7.8057670	3.4939843
H	-0.8394524	-6.1016323	3.3306370
H	1.1521454	-8.3863346	2.9250373
H	0.8730407	-7.4838196	4.4409153
H	-0.4226093	-8.4760386	3.7201246
C	-0.2940166	-7.6454014	0.3906391
H	-0.2264035	-8.8249115	-1.7941744
Pd	1.5036757	-8.5340692	0.0089799
Br	2.2481113	-6.3385041	-0.9874184
Br	0.5596501	-10.6140936	1.0068131
C	3.2353265	-9.7095133	-0.3794835
N	3.3631161	-10.6448715	-1.4073451
N	4.1725349	-10.0689175	0.5479016
C	4.2590237	-11.6269209	-1.0508775
C	2.6366802	-10.5990777	-2.7491325
C	4.7795815	-11.2998615	0.1910486
C	4.5269246	-12.9412960	-1.7756576
C	5.6269326	-12.3164669	0.8624723
C	4.5706042	-9.2558397	1.7570270
C	6.1033566	-9.0563756	1.7071993
C	4.0250189	-9.9514059	3.0190065
C	3.9942602	-7.8421739	1.7180109
C	3.5332013	-11.1755095	-3.8609554
C	2.3592529	-9.1473721	-3.1386930
C	1.3405392	-11.4155147	-2.6353335
H	0.8061979	-11.3775358	-3.5953839
H	0.6942895	-11.0157942	-1.8431409

H	1.5627601	-12.4633592	-2.3951438
H	3.0908239	-10.8877013	-4.8237781
H	3.5866956	-12.2675170	-3.8505643
H	4.5451180	-10.7478157	-3.8262061
H	1.8405947	-9.1460780	-4.1068697
H	3.2898611	-8.5725937	-3.2412664
H	1.7398787	-8.6182237	-2.4093222
H	4.2576680	-7.3071826	0.7978093
H	4.4073728	-7.2934439	2.5775485
H	2.8993402	-7.8373450	1.8048627
H	4.2974498	-11.0083288	3.0946173
H	2.9278846	-9.9100404	3.0041999
H	4.3868468	-9.4336014	3.9183724
H	6.3452926	-8.3346825	0.9150268
H	6.6787312	-9.9620719	1.5109003
H	6.4463401	-8.6352626	2.6619143
O	3.6152089	-13.7474240	-1.8810279
O	5.7273659	-13.3985871	0.2677427
C	6.4145449	-12.2085967	2.1551002
C	5.8715028	-13.1412594	-2.4458206
H	6.6555950	-12.5082282	-2.0142385
H	5.7704403	-12.8914766	-3.5128888
H	6.1549761	-14.1966337	-2.3666046
H	6.1131916	-11.4269757	2.8514073
H	7.4712433	-12.0440777	1.8900312
H	6.3574609	-13.1888002	2.6443843

HEP complex R_1=C(CH_3)$_3$ R_2=$COOCH_3$

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Energy = -6889.9358671010

H	-2.5950394	-5.2883355	2.9519653
C	-2.9028515	-5.7400930	2.0097477
C	-4.1890659	-5.5309176	1.5121796
H	-4.8858474	-4.9121866	2.0781676
C	-4.5988500	-6.0981273	0.2940975
H	-5.6093598	-5.9129309	-0.0710448
C	-3.7377900	-6.8931632	-0.4623551
H	-4.0709293	-7.3219368	-1.4046673
C	-2.4475234	-7.1090118	0.0347498
C	-2.0388472	-6.5375173	1.2536847
N	-1.3505486	-7.8266674	-0.4384266
N	-0.7157680	-6.9356545	1.4588317
C	-1.3208613	-8.6168204	-1.6875596
C	-1.4271582	-7.7075697	-2.9148155
H	-2.3998051	-7.1996863	-2.9715542
H	-0.6351691	-6.9461680	-2.8953495

H	-1.3090936	-8.3073940	-3.8279678
C	-2.3426288	-9.7567878	-1.6573221
H	-3.3798767	-9.3960774	-1.6568556
H	-2.2087306	-10.3828674	-2.5502548
H	-2.1878042	-10.3857979	-0.7707805
C	0.0343940	-6.4885650	2.6602686
C	1.0423836	-5.3899595	2.3151976
H	1.8057967	-5.7469388	1.6129513
H	0.5393707	-4.5325078	1.8471733
H	1.5321900	-5.0408223	3.2353007
C	0.6205409	-7.6619040	3.4394818
H	-0.7423663	-6.0407610	3.2951375
H	1.3605215	-8.2098082	2.8460689
H	1.1055047	-7.2854061	4.3510324
H	-0.1629828	-8.3750717	3.7269995
C	-0.2856660	-7.7165665	0.4178317
H	-0.3191962	-9.0682668	-1.6744397
Pd	1.5032523	-8.6294962	0.0512618
Br	2.2323162	-6.4833007	-1.0566897
Br	0.5372972	-10.6708710	1.1118095
C	3.2498197	-9.7775444	-0.3148112
N	3.4778959	-10.6427877	-1.3766833
N	4.2006668	-10.1016924	0.6234120
C	4.5113843	-11.5132615	-1.0656580
C	2.6701550	-10.7340445	-2.6674753
C	4.9496985	-11.2054416	0.1955215
C	4.9926005	-12.7095162	-1.8384952
C	5.8627619	-12.1288905	0.9143189
C	4.5721574	-9.2740186	1.8480004
C	6.1044937	-9.2909416	2.0182356
C	3.8531713	-9.8330971	3.0853608
C	4.1858118	-7.8107632	1.6294961
C	3.5415212	-11.2649399	-3.8195610
C	2.2033168	-9.3424897	-3.0902251
C	1.4915832	-11.6871328	-2.4224091
H	0.8838018	-11.7553276	-3.3361044
H	0.8619761	-11.3336244	-1.5953783
H	1.8500232	-12.6946582	-2.1698477
H	2.9816753	-11.1029679	-4.7502007
H	3.7350238	-12.3414927	-3.7560104
H	4.4913557	-10.7214746	-3.9017502
H	1.6303518	-9.4396342	-4.0227278
H	3.0510872	-8.6680966	-3.2677109
H	1.5689516	-8.8633058	-2.3387028
H	4.6277157	-7.3991042	0.7131248
H	4.5479838	-7.2305149	2.4898435

H	3.1002260	-7.6712814	1.5558001
H	4.1901688	-10.8470830	3.3218878
H	2.7694518	-9.8654192	2.9150440
H	4.0578710	-9.1835003	3.9479162
H	6.6072221	-8.9655993	1.0967310
H	6.5035200	-10.2624415	2.3231061
H	6.3640867	-8.5769919	2.8108247
O	4.4572707	-13.7999420	-1.7913535
O	6.7916881	-12.7033952	0.3733789
O	5.4872351	-12.3693433	2.1963790
O	6.1074646	-12.4240334	-2.5366573
C	6.3022661	-13.3406346	2.8952412
H	6.2573010	-14.3107584	2.3856152
H	5.8694410	-13.4090735	3.8977943
H	7.3465037	-13.0049979	2.9420685
C	6.7003314	-13.5496268	-3.2266012
H	6.9841743	-14.3231007	-2.5025419
H	7.5821153	-13.1459903	-3.7324680
H	5.9910096	-13.9702785	-3.9518031