Supporting Information

Nickel-catalyzed aryl trifluoromethyl sulfides synthesis: A DFT study

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Table S1. Computed relative Gibbs energies (in kcal mol^{-1}) for different halobenzenes.

Species	PhI	PhBr	PhCl
A1	0.0	0.0	0.0
ADTS	13.0	13.7	15.4
A2	2.9	3.4	3.8
OA1	26.2	29.7	35.8
A3	-31.0	-30.1	-27.4
A4	-33.3	-23.3	-18.6
RE1	-1.5	8.5	13.2
A5	-9.2	0.8	5.5
SET	26.3	38.4	57.6
B1	1.3	11.1	46.4
MECP	3.0	3.0	3.0
$A1^T$	1.4	1.4	1.4
$B1^T$	0.3	4.7	-0.6
HAT	3.6	11.3	16.3
B2	-6.2	6.1	7.4
LDTS	8.3	10.3	11.2
B3	6.7	8.6	9.0
B4	3.5	13.5	18.2
B5	8.1	18.3	23.3
OA2	10.1	24.6	33.3
B6	-2.0	11.4	20.6
RE2	7.9	21.8	29.2
B7	-1.9	13.9	20.7
Overall	-10.7	-0.8	4.0

Table S2. Computed relative Gibbs energies (in kcal mol^{-1}) for substituted iodobenzenes.

Species	PhI	4-iodotoluene	methyl 4-iodobenzoate
A1	0.0	0.0	0.0
ADTS	13.0	14.8	-
A2	2.9	3.9	-
OA1	26.2	27.1	26.2
A3	-31.0	-27.8	-
A4	-33.3	-30.3	-29.8
RE1	-1.5	0.8	-1.9
A5	-9.1	-6.1	-
SET	26.3	29.0	-
B1	1.3	3.8	5.6
MECP	3.0	3.0	3.0
$A1^T$	1.4	1.4	1.4
$B1^T$	0.3	1.7	4.3
HAT	3.6	5.4	9.8
B2	-6.2	-3.9	-1.3
LDTS	8.3	10.7	13.2
B3	6.7	9.0	11.6
B4	3.5	5.8	8.4
B5	8.1	10.6	14.0
OA2	10.1	14.4	17.7
B6	-2.0	2.8	7.2
RE2	7.9	13.0	17.5
B7	-1.9	2.4	6.0
Overall	-10.7	-9.7	-9.0

Table S3. Computed free energy values (Hartree) for the species involved in the iodobenzene catalytic cycles.

Species	Free energy
PhI	-527.6867
PhI^{-}	-527.7870
$Ph^{\cdot}$	-231.3806
I^{-}	-296.4085
SCF_3^{-}	-735.9440
$PhSCF_3$	-967.2393
4,4'-Dimethoxy-2,2'-bipyridine (dmbpy)	-723.9392
A1	-2956.9852
ADTS1	-3484.6512
A2	-2760.7282
OA1	-2760.6910
A3	-2760.7822
A4	-3200.3213
RE1	-3200.2706
A5	-3200.2829
B1	-2956.8829
MECP	-2957.3579
A1T	-2956.9830
B1T	-3484.6714
HAT	-3484.6662
B2	-3253.3012
LDTS	-3253.2780
B3	-2529.3416
B4	-2968.8822
B5	-3496.5615
OA2	-3496.5584
B6	-3496.5776
RE2	-3496.5618
B7	-3496.5775
Ni_L [Ni(dmbpy)]	-2232.9856

Table S4. Computed free energy values (Hartree) for the species involved in the bromobenzene catalytic cycles.

Species	**Free energy**
PhBr	-649.2327
$PhBr^{\bullet-}$	-649.3174
Br^-	-231.3806
ADTS1	-3606.1961
A2	-2882.2735
OA1	-2882.2315
A3	-2882.3268
B1T	-3606.2104
HAT	-3606.2000
B2	-3374.8277
LDTS	-3374.8210
B3	-2650.8845
B5	-3618.1072
OA2	-3618.0971
B6	-3618.1182
RE2	-3618.1016
B7	-3618.1143

Table S5. Computed free energy values (Hartree) for the species involved in the chlorobenzene catalytic cycles.

Species	**Free energy**
PhCl	-691.7183
$PhCl^{-}$	-691.7467
Cl^{-}	-231.3806
ADTS1	-3648.6789
A2	-2924.7583
OA1	-2924.7073
A3	-2924.8081
B1T	-3648.7045
HA5	-3648.6775
B2	-3417.3111
LDTS	-3417.3051
B3	-2693.3695
B5	-3660.5923
OA2	-3660.5764
B6	-3660.5967
RE2	-3660.5829
B7	-3660.5964

Table S6. Computed free energy values (Hartree) for the species involved in the 4-iodotoluene catalytic cycles.

Species	**Free energy**
*p*MePhI	-566.9625
*p*MePhI$^{\cdot-}$	-567.0588
*p*MePh$^{\cdot}$	-270.6527
*p*MePhSCF$_3$	-1006.5135
ADTS1	-3523.9242
A2	-2800.0023
OA1	-2799.9653
A3	-2800.0529
A4	-3239.5925
RE1	-3239.5429
A5	-3239.5538
B1T	-3523.9450
HAT	-3523.9391
B5	-3535.8370
OA2	-3535.8311
B6	-3535.8495
RE2	-3535.8333
B7	-3535.8501

Table S7. Computed free energy values (Hartree) for the species involved in the methyl 4-iodotoluene catalytic cycles.

Species	**Free energy**
pCO_2MePhI	-755.4656
pCO_2MePhI$^{\cdot-}$	-755.5591
pCO_2MePh$^{\cdot}$	-459.1517
pCO_2MePhSCF_3	-1195.0155
OA1	-2988.4699
A4	-3428.0947
RE1	-3428.0503
B1T	-3712.4440
HAT	-3712.4352
B5	-3724.3388
OA2	-3724.3329
B6	-3724.3497
RE2	-3724.3333
B7	-3724.3515

Table S10. Computed energies of the SET calculations.

Species	Free energy
A1	-2956.9852
$A1^+$ with A1 geometry	-2956.8766
$A1^+$ with the solvent cavity of A1	-2956.8563
PhI	-527.6867
$PhI^{\cdot-}$ with PhBr geometry	-527.7390
$PhI^{\cdot-}$ with the solvent cavity of PhI	-527.7082
PhBr	-649.2327
$PhBr^{\cdot-}$ with PhI geometry	-649.2753
$PhBr^{\cdot-}$ with the solvent cavity of PhBr	-649.2201
PhCl	-691.7183
$PhCl^{\cdot-}$ with PhCl geometry	-691.7576
$PhCl^{\cdot-}$ with the solvent cavity of PhCl	-691.7263
*p*MePhI	-566.9625
*p*MePhI$^{\cdot-}$ with *p*MePhI geometry	-567.0104
*p*MePhI$^{\cdot-}$ with the solvent cavity of *p*MePhI	-566.9799

Table S11. Computed components of the SET calculations.

Substrate	λ_S	λ_N	λ	ΔG	$\Delta G^{\ddagger}$
PhI	67.4	35.3	102.7	1.3	26.3
PhBr	41.5	88.8	130.3	11.1	38.4
PhCl	43.5	75.9	119.4	46.4	57.6
*p*MePhI	38.1	70.0	108.1	3.8	29.0

Optimized geometries

Substrate: Iodobenzene

57
A1
N 1.462605 -1.187941 0.510691
N 1.490571 1.158703 -0.553295
C 1.365458 -2.467625 0.961319
C 2.452790 -3.311737 1.175226
C 3.755058 -2.822409 0.880697
C 3.813889 2.762638 -0.864009
C 2.525792 3.270812 -1.187559
C 1.422208 2.441045 -1.002552
C 2.740061 -0.711252 0.230338
C 3.884761 -1.514967 0.395095
C 3.914027 1.451663 -0.380946
C 2.754947 0.663480 -0.245686
H 0.351463 -2.812696 1.171038
H 2.284111 -4.313683 1.566778
H 2.380400 4.276177 -1.579906
H 0.418486 2.800840 -1.235361
Ni -0.000013 -0.000081 -0.028770
N -1.462533 1.187823 0.510859
N -1.490662 -1.158796 -0.553175
C -1.365300 2.467551 0.961353
C -2.740027 0.711171 0.230621
C -1.422367 -2.441117 -1.002517
C -2.754992 -0.663579 -0.245377
C -2.452578 3.311748 1.175201
H -0.351278 2.812584 1.170997
C -3.884676 1.514949 0.395364
C -2.525994 -3.270843 -1.187467
H -0.418678 -2.800904 -1.235476
C -3.914096 -1.451732 -0.380527
C -3.754882 2.822458 0.880771
H -2.283812 4.313738 1.566606
C -3.814040 -2.762679 -0.863696
H -2.380664 -4.276185 -1.579894
H -4.890415 -1.056663 -0.098566
H -4.872907 1.134239 0.135926
H 4.872959 -1.134231 0.135573
H 4.890386 1.056593 -0.099129
O -4.979282 -3.470021 -0.976029
O -4.907095 3.545234 1.024066
O 4.979113 3.469996 -0.976466
O 4.907325 -3.545087 1.024093
C -4.897942 -4.805644 -1.511399
H -5.929789 -5.179668 -1.523992
H -4.490531 -4.792167 -2.536548
H -4.273204 -5.448911 -0.868762
C -4.795790 4.872706 1.574090
H -5.822150 5.259378 1.617596
H -4.363163 4.840897 2.588472
H -4.179349 5.516821 0.924343
C 4.796120 -4.872509 1.574257
H 4.179559 -5.516694 0.924696
H 5.822488 -5.259183 1.617624
H 4.363680 -4.840585 2.588714
C 4.897586 4.806015 -1.510807
H 4.272833 5.448741 -0.867645
H 5.929392 5.180163 -1.523191
H 4.490115 4.793306 -2.535945

57
A1T
N 1.533394 1.235691 -0.425848
N 1.533216 -1.235833 0.425634
C 1.454116 2.473023 -0.960311
C 2.555132 3.240624 -1.350854
C 3.848236 2.670353 -1.190514
C 3.847842 -2.670707 1.190597
C 2.554669 -3.240891 1.350707
C 1.453770 -2.473191 0.960036
C 2.795412 0.673291 -0.275893
C 3.959429 1.381131 -0.654630
C 3.959210 -1.381479 0.654765
C 2.795311 -0.673534 0.275876
H 0.442621 2.866851 -1.078726
H 2.400536 4.235199 -1.764199
H 2.399941 -4.235483 1.763963
H 0.442231 -2.866954 1.078279
Ni 0.000000 -0.000001 0.000020
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N -1.533217 1.235815 0.425673
C -1.454112 -2.472990 -0.960406
C -2.795411 -0.673282 -0.275931
C -1.453773 2.473155 0.960117
C -2.795313 0.673524 0.275885
C -2.555126 -3.240580 -1.350975
H -0.442616 -2.866810 -1.078833
C -3.959427 -1.381111 -0.654692
C -2.554673 3.240845 1.350801
H -0.442233 2.866909 1.078384
C -3.959213 1.381461 0.654785
C -3.848231 -2.670317 -1.190616
H -2.400528 -4.235141 -1.764352
C -3.847847 2.670671 1.190658
H -2.399946 4.235423 1.764091
H -4.946414 0.930366 0.557056
H -4.946579 -0.929941 -0.556820
H 4.946581 0.929956 -0.556772
H 4.946410 -0.930378 0.557061
O -5.013888 3.290290 1.539292
O -5.014364 -3.289826 -1.539143
O 5.013882 -3.290332 1.539225
O 5.014370 3.289872 -1.539020
C -4.928607 4.610725 2.112640
H -5.965100 4.905901 2.320419
H -4.347972 4.594871 3.050228
H -4.471523 5.318206 1.400516
C -4.929238 -4.610293 -2.112445
H -5.965767 -4.905379 -2.320180
H -4.348619 -4.594523 -3.050042
H -4.472203 -5.317794 -1.400310
C 4.929246 4.610346 -2.112307
H 4.472210 5.317839 -1.400164
H 5.965775 4.905434 -2.320036
H 4.348628 4.594586 -3.049905
C 4.928596 -4.610773 2.112561
H 4.471517 -5.318247 1.400428
H 5.965089 -4.905950 2.320344
H 4.347956 -4.594926 3.050145

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A2
Ni -0.044011 -0.949897 -0.561633
N -1.995665 -1.047071 -0.257881
N -0.356784 0.986552 -0.300571
C -2.780096 -2.148520 -0.245590
C -4.163783 -2.123923 -0.041998
C -4.783254 -0.872586 0.166162
C -1.117462 3.683243 0.073921
C 0.231444 3.341450 -0.161882
C 0.549424 1.990996 -0.339710
C -2.602869 0.169407 -0.050305
C -3.979345 0.286955 0.161057
C -2.076697 2.649343 0.118316
C -1.671076 1.325569 -0.072691
H -2.262428 -3.094898 -0.406686
H -4.723901 -3.057195 -0.048588
H 1.023098 4.087342 -0.205712
H 1.580925 1.687410 -0.517280
H 3.325564 -2.192172 2.082851
C 2.634892 -2.303508 1.246165
C 1.677095 -3.379634 1.245946
C 2.676053 -1.453572 0.159400
C 0.825859 -3.569366 0.169941
C 1.777596 -1.531849 -0.967741
C 0.817319 -2.658015 -0.955099
H 0.149984 -4.429721 0.155624
H 2.114368 -1.107781 -1.921946
H 0.436209 -3.043553 -1.912345
I 4.220843 0.113005 0.109931
H 1.654960 -4.060662 2.100994
H -4.448075 1.256361 0.324357
H -3.120206 2.902640 0.300788
O -6.110991 -0.683308 0.375276
O -1.582936 4.943662 0.264925
C -0.624823 6.026277 0.232681
H -0.132181 6.077536 -0.751886
H -1.209937 6.936994 0.409898
H 0.129424 5.898764 1.026215
C -6.960156 -1.853276 0.399132

H	-6.667658	-2.526458	1.221673
H	-7.974903	-1.471675	0.565998
H	-6.909747	-2.388191	-0.563266

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A3

Ni	0.690694	-0.366425	0.001521
N	-0.165347	1.393838	0.010346
N	-1.245157	-0.987908	-0.002960
C	0.448642	2.602147	0.006744
C	-0.225697	3.823282	-0.030163
C	-1.635105	3.812074	-0.071456
C	-4.023894	-1.500110	0.065890
C	-3.094291	-2.560282	0.056277
C	-1.732944	-2.246760	0.022874
C	-1.542258	1.385522	-0.017434
C	-2.290329	2.564006	-0.061719
C	-3.531946	-0.178595	0.039370
C	-2.152409	0.040336	0.003761
H	1.534638	2.587425	0.033322
H	0.353539	4.744237	-0.029879
H	-3.399356	-3.604431	0.075929
H	-0.991633	-3.044015	0.016728
C	2.432756	0.365646	0.075291
C	3.011386	0.672383	1.326599
C	3.124499	0.730795	-1.100465
C	4.243205	1.354092	1.400526
H	2.501382	0.386654	2.250950
C	4.355919	1.412822	-1.027065
H	2.703251	0.488729	-2.080089
C	4.919480	1.729128	0.224001
H	4.674720	1.586768	2.378822
H	4.876307	1.690366	-1.948709
H	5.876117	2.254849	0.281571
I	1.845257	-2.680025	-0.124693
H	-3.377669	2.539619	-0.093794
H	-4.239976	0.647721	0.055707
O	-2.426715	4.906760	-0.120065
O	-5.368359	-1.640163	0.102184
C	-1.784788	6.205466	-0.140656
H	-2.604927	6.932672	-0.173278
H	-1.183907	6.350836	0.771036
H	-1.150379	6.304978	-1.035900
C	-5.906912	-2.983833	0.163824
H	-6.995300	-2.856138	0.201738
H	-5.622252	-3.554389	-0.734688
H	-5.550352	-3.497658	1.070795

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A4

Ni	0.689599	-0.239960	-0.386006
N	-0.446818	1.351168	-0.112555
N	-1.120198	-1.163662	-0.305959
C	-0.038430	2.641174	-0.062717
C	-0.902207	3.730392	0.067092
C	-2.288065	3.481887	0.146653
C	-3.739140	-2.166351	0.013153
C	-2.652009	-3.041069	-0.193742
C	-1.377654	-2.487646	-0.344287
C	-1.799623	1.111713	-0.035110
C	-2.730568	2.144092	0.091555
C	-3.484857	-0.779239	0.063576
C	-2.176276	-0.316726	-0.095812
H	1.033989	2.804868	-0.129748
H	-0.485971	4.735037	0.098764
H	-2.772796	-4.121462	-0.237758
H	-0.512972	-3.130847	-0.506822
C	2.297130	0.737074	-0.245242
C	2.761150	1.071655	1.046594
C	2.979725	1.259980	-1.364904
C	3.869755	1.925438	1.215288
H	2.255899	0.673788	1.931024
C	4.081087	2.123764	-1.197840
H	2.653937	0.999863	-2.375726
C	4.530603	2.460433	0.093253
H	4.213123	2.172540	2.224431
H	4.591897	2.525680	-2.078159
H	5.389482	3.124118	0.222913
S	1.869343	-2.019583	-1.020065
C	2.725205	-2.541815	0.462133
F	3.942292	-1.930052	0.695460
F	2.010379	-2.364128	1.634298
F	3.018367	-3.895735	0.410234
H	-3.797679	1.937004	0.143213
H	-4.314238	-0.095477	0.235076
O	-3.246293	4.426553	0.268979
O	-5.026455	-2.546205	0.176047
C	-2.826467	5.810759	0.355985
H	-2.290171	6.107844	-0.559288
H	-3.753971	6.386945	0.456110
H	-2.185679	5.961060	1.239248
C	-5.325879	-3.963018	0.123405
H	-6.410364	-4.034692	0.269099
H	-5.043944	-4.378112	-0.857428
H	-4.797930	-4.497001	0.929518

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A5

Ni	-0.164677	-0.445870	1.056465
N	-1.121726	1.225834	0.605426
N	-1.819530	-1.284195	0.386932
C	-0.680126	2.498871	0.722013
C	-1.424371	3.623755	0.351822
C	-2.716200	3.421909	-0.180365
C	-4.314786	-2.189671	-0.580954
C	-3.330061	-3.108512	-0.158166
C	-2.113088	-2.602470	0.309774
C	-2.380703	1.033606	0.085209
C	-3.192367	2.099931	-0.311405
C	-4.025077	-0.810584	-0.509363
C	-2.782897	-0.392100	-0.025148
H	0.324156	2.612782	1.131949
H	-0.994788	4.615846	0.477372
H	-3.487844	-4.185025	-0.187342
H	-1.325132	-3.280492	0.639808
H	3.064832	-2.283495	-1.226959
C	2.653220	-1.750654	-0.367659
C	3.025167	-0.376602	-0.136020
C	1.803392	-2.390396	0.519027
C	2.538695	0.316591	0.970996
C	1.218009	-1.698679	1.651418
H	1.565409	-3.447067	0.364363
C	1.616028	-0.303387	1.885205
H	2.869607	1.340445	1.161790
H	0.854211	-2.313037	2.486297
H	1.521139	0.146167	2.882621
S	4.089705	0.473226	-1.297869
C	5.745148	-0.059374	-0.707787
F	6.701670	0.574829	-1.451583
F	5.983355	0.243096	0.604133
F	5.968716	-1.404300	-0.828342
H	-4.185585	1.933869	-0.726284
H	-4.777502	-0.094093	-0.835921
O	-5.540086	-2.522340	-1.059521
O	-3.555694	4.406578	-0.588305
C	-3.095553	5.773001	-0.473035
H	-2.187321	5.926183	-1.078429
H	-3.916370	6.389172	-0.859818
H	-2.894733	6.024614	0.581075
C	-5.862352	-3.928215	-1.164726
H	-5.829666	-4.407414	-0.172931
H	-6.881986	-3.963114	-1.567388
H	-5.163868	-4.432727	-1.852102

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ADTS

N	2.320090	1.059987	-0.269234
N	1.962269	-1.517596	0.379274
C	2.511592	2.384759	-0.464682
C	3.756977	3.010571	-0.536818
C	4.915976	2.212743	-0.376540
C	3.889030	-3.482461	-0.331008
C	2.609794	-3.857575	0.148601
C	1.706064	-2.841762	0.466060
C	3.456083	0.279720	-0.174855
C	4.748934	0.831246	-0.195651
C	4.176346	-2.113725	-0.453133
C	3.214452	-1.162426	-0.072679
H	1.606671	2.979177	-0.580616
H	3.809884	4.082937	-0.714811
H	2.321622	-4.898568	0.282420
H	0.708919	-3.114277	0.818743
Ni	0.532225	0.132898	0.243595
N	-0.804765	1.799577	-0.029742
N	-0.814008	-0.649954	-1.099338
C	-0.637837	3.077865	0.363711
C	-1.737094	1.568576	-1.010862
C	-0.874267	-1.929103	-1.529528
C	-1.877802	0.165385	-1.422034
C	-1.349390	4.168971	-0.142551
H	0.102013	3.229632	1.149528

C	-2.475649	2.605355	-1.607713
C	-1.939117	-2.479696	-2.246188
H	-0.013197	-2.550661	-1.286844
C	-3.007429	-0.314785	-2.102514
C	-2.297965	3.926055	-1.164762
H	-1.174423	5.164423	0.261565
C	-3.052596	-1.653349	-2.523218
H	-1.892909	-3.519634	-2.563587
H	-3.862784	0.333574	-2.288331
H	-3.167200	2.402912	-2.424897
H	5.625196	0.198558	-0.057231
H	5.138231	-1.803006	-0.859840
O	-4.183313	-2.051905	-3.164725
O	-3.049667	4.880470	-1.776903
O	4.869109	-4.347998	-0.705794
O	6.193370	2.679484	-0.377438
C	-4.263793	-3.432550	-3.563528
H	-5.247833	-3.546933	-4.035765
H	-3.470174	-3.680738	-4.288164
H	-4.187027	-4.100582	-2.689206
C	-2.858728	6.243026	-1.355477
H	-3.541957	6.841767	-1.971194
H	-3.110231	6.366737	-0.288789
H	-1.818354	6.567637	-1.527699
C	6.378445	4.099596	-0.521357
H	5.888396	4.645867	0.302151
H	7.463409	4.260448	-0.482758
H	5.983002	4.454871	-1.487609
C	4.583545	-5.755006	-0.602029
H	3.728891	-6.032223	-1.242140
H	5.490439	-6.266302	-0.949154
H	4.370393	-6.039193	0.442020
H	-0.163583	-1.677242	1.955092
C	-0.381731	-0.624186	2.114431
C	-1.719099	-0.228487	2.359406
C	0.659592	0.283552	2.516539
C	-2.066776	1.016641	2.881032
C	0.317641	1.520178	3.120532
H	1.684833	-0.082282	2.585838
C	-1.024822	1.890103	3.275717
H	-1.284234	2.856487	3.715035
I	-3.308229	-1.601355	1.720311
H	-3.109756	1.305850	3.012455
H	1.112292	2.191558	3.455415

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B1

N	-1.534042	1.221840	0.464725
N	-1.536753	-1.219210	-0.468240
C	-1.444806	2.454647	1.009733
C	-2.548594	3.223242	1.389546
C	-3.836624	2.678250	1.191450
C	-3.842941	-2.672525	-1.189643
C	-2.556100	-3.219174	-1.390933
C	-1.450418	-2.452090	-1.013579
C	-2.785698	0.687013	0.287102
C	-3.944938	1.386409	0.632262
C	-3.948240	-1.380524	-0.630277
C	-2.787271	-0.682662	-0.287812
H	-0.433280	2.839459	1.145742
H	-2.392220	4.208542	1.823822
H	-2.402014	-4.204635	-1.825658
H	-0.439706	-2.838258	-1.151780
Ni	0.000001	-0.000146	-0.002579
N	1.534191	-1.222150	0.464235
N	1.536631	1.219161	-0.468062
C	1.445113	-2.455038	1.009094
C	2.785774	-0.687030	0.286978
C	1.450147	2.452053	-1.013349
C	2.787197	0.682679	-0.287834
C	2.548998	-3.223392	1.389101
H	0.433652	-2.840115	1.144834
C	3.945104	-1.386171	0.632347
C	2.555751	3.219174	-1.390856
H	0.439402	2.838198	-1.151372
C	3.948097	1.380592	-0.630420
C	3.836951	-2.678073	1.191427
H	2.392763	-4.208786	1.823216
C	3.842654	2.672600	-1.189749
H	2.401565	4.204627	-1.825564
H	4.936891	0.948125	-0.486093
H	4.934676	-0.954699	0.490429
H	-4.934610	0.955223	0.490164
H	-4.937029	-0.948064	-0.485890
O	5.008215	3.287134	-1.498355
O	5.001080	-3.293793	1.503071
O	-5.008601	-3.286972	-1.498061
O	-5.000715	3.294153	1.502882
C	4.944610	4.615770	-2.071295
H	5.987918	4.905284	-2.245233
H	4.390716	4.598944	-3.023582
H	4.467233	5.314958	-1.365783
C	4.934681	-4.622325	2.075898
H	5.977269	-4.912931	2.252317
H	4.378587	-4.604941	3.026895
H	4.458255	-5.321045	1.369277
C	-4.934212	4.622605	2.075895
H	-4.457405	5.321301	1.369509
H	-5.976785	4.913432	2.252037
H	-4.378391	4.604962	3.027046
C	-4.945202	-4.615712	-2.070780
H	-4.468043	-5.314861	-1.365079
H	-5.988545	-4.905038	-2.244812
H	-4.391168	-4.599173	-3.022991

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B1T

N	1.488831	1.182589	-0.196161
N	1.493322	-1.284450	0.670329
C	1.400760	2.410391	-0.750854
C	2.490849	3.148974	-1.215821
C	3.780249	2.557420	-1.119935
C	3.821045	-2.739913	1.347286
C	2.529487	-3.288759	1.577445
C	1.422077	-2.512274	1.227169
C	2.744841	0.600938	-0.108509
C	3.897616	1.274932	-0.569659
C	3.923235	-1.458039	0.791455
C	2.752445	-0.741106	0.458440
H	0.391144	2.814904	-0.835143
H	2.330858	4.136809	-1.643025
H	2.380880	-4.274366	2.013797
H	0.412369	-2.889302	1.399792
Ni	-0.045628	-0.046413	0.261016
N	-1.593198	-1.296376	-0.081250
N	-1.570486	1.212900	0.658814
C	-1.523406	-2.548734	-0.581741
C	-2.845297	-0.706614	0.012516
C	-1.482039	2.464029	1.158917
C	-2.835143	0.658915	0.519365
C	-2.626517	-3.300372	-0.991348
H	-0.518760	-2.966482	-0.662914
C	-4.010920	-1.394706	-0.391957
C	-2.577907	3.251297	1.521548
H	-0.468108	2.852147	1.272978
C	-3.994634	1.386728	0.867452
C	-3.910835	-2.698036	-0.894419
H	-2.480152	-4.307115	-1.377281
C	-3.875238	2.690055	1.367159
H	-2.416379	4.254936	1.909608
H	-4.984573	0.940379	0.776774
H	-4.988442	-0.915258	-0.346698
H	4.878486	0.802198	-0.524871
H	4.909818	-1.020029	0.642306
O	-5.037238	3.329356	1.688773
O	-5.076070	-3.297795	-1.276363
O	4.993400	-3.371268	1.646449
O	4.934634	3.148461	-1.545858
C	-4.943367	4.656273	2.246812
H	-5.978419	4.964242	2.442522
H	-4.369824	4.645220	3.188739
H	-4.473641	5.350172	1.529760
C	-4.995503	-4.619721	-1.847640
H	-6.030374	-4.897682	-2.085093
H	-4.388095	-4.612175	-2.768213
H	-4.571003	-5.335033	-1.123449
C	4.839698	4.463442	-2.130474
H	4.423752	5.184513	-1.406966
H	5.869542	4.742890	-2.387208
H	4.217947	4.443879	-3.041216
C	4.917601	-4.691637	2.222670
H	4.423555	-5.392302	1.528849
H	5.958296	-4.998719	2.387375
H	4.375315	-4.669806	3.182639
C	-1.429202	-0.199904	-7.457449
C	-0.260118	0.124644	-8.169244
C	0.930543	0.394125	-7.470364
C	0.958151	0.341407	-6.062992
C	-0.217548	0.015544	-5.368009
C	-1.414047	-0.257448	-6.049934
H	-2.358965	-0.409962	-7.992402

H	-0.276782	0.167306	-9.260663
H	1.843977	0.646152	-8.015242
H	1.883219	0.551829	-5.522840
H	-2.323009	-0.508813	-5.500069
I	-0.181762	-0.058053	-3.157702

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B2

N	1.501588	1.187818	-0.302391
N	1.483372	-1.258603	0.616444
C	1.417621	2.407288	-0.872555
C	2.525458	3.153315	-1.284534
C	3.807616	2.589973	-1.105824
C	3.777520	-2.684773	1.431091
C	2.489035	-3.240037	1.594471
C	1.390257	-2.485120	1.174460
C	2.745421	0.639559	-0.134123
C	3.909306	1.309460	-0.522207
C	3.891021	-1.400151	0.859506
C	2.736159	-0.718350	0.465129
H	0.407888	2.791587	-1.017504
H	2.374529	4.127408	-1.744923
H	2.328626	-4.222711	2.033574
H	0.378063	-2.875694	1.287847
Ni	-0.048115	-0.050163	0.093257
N	-1.610179	-1.292529	-0.228126
N	-1.559261	1.170000	0.643638
C	-1.546429	-2.527465	-0.767435
C	-2.847706	-0.743198	-0.020088
C	-1.447554	2.413070	1.160491
C	-2.818200	0.633791	0.533190
C	-2.668355	-3.289081	-1.106478
H	-0.542544	-2.912554	-0.946732
C	-4.024902	-1.431352	-0.328885
C	-2.533190	3.188519	1.577513
H	-0.431045	2.800181	1.242546
C	-3.961135	1.338939	0.920989
C	-3.943848	-2.727755	-0.879292
H	-2.533700	-4.274975	-1.546497
C	-3.828399	2.639434	1.450810
H	-2.358468	4.182889	1.983873
H	-4.955025	0.903417	0.830645
H	-5.004991	-0.982714	-0.174299
H	4.892464	0.855540	-0.407413
H	4.878926	-0.956135	0.745783
O	-4.978946	3.262698	1.808212
O	-5.123784	-3.334190	-1.159126
O	4.938364	-3.287127	1.791214
O	4.974770	3.180161	-1.463064
C	-4.880828	4.591774	2.369686
H	-5.914000	4.893895	2.580484
H	-4.293357	4.575672	3.302284
H	-4.423092	5.284834	1.645096
C	-5.080489	-4.656041	-1.745696
H	-6.128885	-4.936382	-1.905104
H	-4.542438	-4.634554	-2.706993
H	-4.596869	-5.367332	-1.056233
C	4.909494	4.490097	-2.073493
H	4.456720	5.216604	-1.378970
H	5.950931	4.763906	-2.282253
H	4.332523	4.451310	-3.011410
C	4.861318	-4.609521	2.371630
H	4.405014	-5.317059	1.660197
H	5.899947	-4.896384	2.576844
H	4.282334	-4.588316	3.309369
I	-0.078774	-0.103623	-3.610848

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B3

N	-0.254847	-1.246542	-0.040021
N	-0.290509	1.350507	-0.100629
C	-0.141725	-2.594037	-0.026902
C	-1.235697	-3.463651	-0.009302
C	-2.533222	-2.905084	-0.011213
C	-2.604254	2.953386	-0.002828
C	-1.322170	3.542631	-0.071443
C	-0.208406	2.699069	-0.115590
C	-1.517632	-0.704379	-0.033822
C	-2.664940	-1.499802	-0.025836
C	-2.702678	1.545077	0.011679
C	-1.537141	0.777786	-0.041743
H	0.877334	-2.983124	-0.031327
H	-1.065283	-4.538377	0.001910
H	-1.177311	4.620886	-0.086666
H	0.800790	3.110573	-0.163905
Ni	1.207067	0.064574	-0.116075
I	3.735454	0.415844	-0.219304
H	-3.685150	1.078984	0.072863
H	-3.659635	-1.056666	-0.035796
O	-3.772107	3.636700	0.054261
O	-3.686018	-3.615629	-0.000785
C	-3.709157	5.083309	0.057335
H	-3.238067	5.450178	-0.868719
H	-4.752159	5.417826	0.109411
H	-3.149322	5.441074	0.936510
C	-3.588959	-5.059748	0.028746
H	-4.625113	-5.418488	0.035562
H	-3.063907	-5.428351	-0.867192
H	-3.064644	-5.390756	0.939761

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B4

Ni	-1.219014	-0.121784	-0.619866
N	0.347314	-1.308088	-0.317583
N	0.169086	1.279829	-0.366885
C	0.342267	-2.658436	-0.311963
C	1.482529	-3.437411	-0.092195
C	2.708902	-2.774975	0.135943
C	2.290221	3.071942	0.102702
C	0.989916	3.551750	-0.167514
C	-0.024501	2.616054	-0.393018
C	1.538101	-0.665524	-0.090166
C	2.725992	-1.362407	0.136603
C	2.505346	1.676346	0.130153
C	1.433027	0.814982	-0.106310
H	-0.625246	-3.129284	-0.492943
H	1.399052	-4.521997	-0.103100
H	0.757063	4.613988	-0.203283
H	-1.044357	2.941972	-0.602577
S	-3.367721	-0.261689	-1.086389
C	-4.086497	-0.181065	0.553863
F	-3.705891	-1.207228	1.406632
F	-3.797478	0.981217	1.253802
F	-5.469382	-0.241328	0.522101
H	3.502460	1.293641	0.342458
H	3.666141	-0.840315	0.310226
O	3.370590	3.848810	0.348371
O	3.895783	-3.387022	0.356361
C	3.180357	5.284119	0.372889
H	2.449182	5.560145	1.149564
H	4.165299	5.702214	0.613378
H	2.844269	5.645131	-0.612533
C	3.924163	-4.835057	0.356818
H	3.607280	-5.224772	-0.623812
H	4.969762	-5.102034	0.552093
H	3.275042	-5.234063	1.152783

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B5

Ni	-0.168265	-0.254694	-0.068984
N	1.707971	-0.978106	-0.335099
N	0.862329	1.473362	-0.047565
C	2.051994	-2.271446	-0.496384
C	3.363612	-2.705484	-0.708416
C	4.386617	-1.732036	-0.756028
C	2.511481	3.753813	0.037570
C	1.112624	3.870977	0.198465
C	0.345587	2.704174	0.148518
C	2.698618	-0.034001	-0.381396
C	4.038964	-0.375698	-0.588760
C	3.064352	2.471249	-0.158468
C	2.221017	1.356646	-0.194744
H	1.231445	-2.988483	-0.448828
H	3.565936	-3.768519	-0.824094
H	0.621245	4.827823	0.362936
H	-0.737009	2.749213	0.274733
S	-1.308358	-1.103089	1.698317
C	0.010106	-1.523425	2.820535
F	0.784015	-2.612700	2.433959
F	0.932656	-0.509968	3.049573
F	-0.454284	-1.864247	4.086647
H	4.820702	0.381533	-0.622829
H	4.142351	2.368135	-0.272730
O	5.700998	-1.994412	-0.955864
O	3.386403	4.787278	0.059377
C	6.096308	-3.377105	-1.115618
H	5.594765	-3.824243	-1.989230
H	7.181131	-3.351302	-1.275560
H	5.858667	-3.952907	-0.206505
C	2.853378	6.121406	0.238610
H	3.724896	6.786782	0.218235

H	2.163467	6.372427	-0.583090
H	2.335288	6.202705	1.207548
H	-0.003486	-1.894283	-3.263981
C	-0.836234	-1.487485	-2.687165
C	-1.967084	-2.267311	-2.434326
C	-0.760692	-0.152949	-2.194759
C	-3.077089	-1.737436	-1.724597
H	-2.017592	-3.296198	-2.798487
C	-1.856744	0.383566	-1.446192
H	0.024889	0.515313	-2.553110
C	-3.007080	-0.426299	-1.258272
H	-3.961083	-2.351011	-1.551161
H	-1.890338	1.445602	-1.204594
I	-4.689836	0.418941	-0.184591

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B6

Ni	-0.632627	-0.342390	0.049592
N	0.261129	1.406813	-0.324663
N	1.326946	-0.980944	-0.073320
C	-0.345867	2.612086	-0.325528
C	0.324602	3.810999	-0.567353
C	1.711495	3.759958	-0.823380
C	4.049397	-1.578602	-0.434915
C	3.133393	-2.588174	-0.069670
C	1.792853	-2.231920	0.095663
C	1.615045	1.352907	-0.533641
C	2.357757	2.505072	-0.796575
C	3.570440	-0.261126	-0.607889
C	2.212903	0.002165	-0.417084
H	-1.413992	2.609322	-0.122062
H	-0.232595	4.744837	-0.549014
H	3.434620	-3.622058	0.084684
H	1.050637	-2.979696	0.375464
C	-2.379807	0.319923	-0.390637
C	-2.507483	0.618030	-1.759461
C	-3.427312	0.591343	0.501581
C	-3.690912	1.217802	-2.235300
H	-1.695134	0.403361	-2.458463
C	-4.604688	1.199441	0.018957
H	-3.338277	0.338018	1.558246
C	-4.739554	1.513125	-1.345902
H	-3.782951	1.453034	-3.299124
H	-5.418696	1.415360	0.716219
H	-5.656700	1.978683	-1.714695
S	-1.606646	-2.358163	0.312459
C	-1.787880	-2.897815	-1.394632
F	-2.990388	-2.570311	-1.981326
F	-0.823559	-2.402084	-2.250253
F	-1.704835	-4.271431	-1.480481
H	3.431503	2.460170	-0.967854
H	4.270486	0.524641	-0.883847
O	2.491786	4.828015	-1.085238
O	5.371408	-1.763369	-0.635253
C	1.864367	6.135656	-1.117763
H	1.419214	6.369387	-0.138110
H	2.675170	6.837575	-1.345317
H	1.095651	6.169348	-1.905668
C	5.904911	-3.101235	-0.465575
H	6.977281	-3.011527	-0.675372
H	5.745577	-3.448171	0.567571
H	5.432683	-3.794798	-1.179097
I	-0.476408	0.126197	2.821160

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B7

Ni	-0.265752	-0.204014	0.183523
N	-1.667051	1.194028	-0.180342
N	-1.864414	-1.407654	0.004534
C	-1.471088	2.526447	-0.238105
C	-2.486532	3.445957	-0.514830
C	-3.789892	2.949098	-0.740381
C	-4.259546	-2.864116	-0.261394
C	-3.049534	-3.521118	0.054035
C	-1.892326	-2.746687	0.170681
C	-2.929512	0.709807	-0.393551
C	-4.006581	1.556417	-0.673539
C	-4.245079	-1.463010	-0.426300
C	-3.043265	-0.765102	-0.280403
H	-0.450688	2.860794	-0.045635
H	-2.256158	4.509091	-0.540758
H	-2.992382	-4.596428	0.209686
H	-0.937914	-3.214759	0.414924
H	-5.010370	1.166562	-0.835129
H	-5.175204	-0.946852	-0.657576
O	-4.874362	3.710629	-1.018517
O	-5.457977	-3.472242	-0.419140
C	-4.690573	5.143874	-1.107597
H	-3.974783	5.390540	-1.908201
H	-5.681472	5.547551	-1.348292
H	-4.338918	5.548037	-0.144800
C	-5.516925	-4.909893	-0.254128
H	-6.562585	-5.179130	-0.445776
H	-4.856236	-5.407410	-0.981958
H	-5.233398	-5.190784	0.772927
H	-0.205123	-0.683576	-2.363432
C	0.670236	-0.493902	-1.738023
C	1.419674	0.708781	-1.917610
C	1.240580	-1.548375	-0.958959
C	2.665157	0.866857	-1.306975
H	1.007399	1.514558	-2.527713
C	2.518843	-1.394787	-0.375593
H	0.746967	-2.519473	-0.911975
C	3.222513	-0.192241	-0.543141
H	3.216240	1.801510	-1.422162
H	2.945194	-2.205821	0.216169
S	4.783917	0.038497	0.310058
C	5.947236	-0.364424	-1.049244
F	5.842113	0.473098	-2.125513
F	7.221306	-0.256751	-0.572569
F	5.801176	-1.630445	-1.543974
I	0.951606	0.625579	2.427564

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dmbpy

N	0.882909	-1.600425	-0.007652
N	-0.882909	1.600425	-0.007652
C	2.145611	-2.056326	0.000989
C	3.292445	-1.245233	0.003205
C	3.099598	0.151244	-0.008297
C	-3.099598	-0.151244	-0.008296
C	-3.292445	1.245233	0.003205
C	-2.145611	2.056326	0.000989
C	0.706432	-0.250760	-0.015623
C	1.782056	0.651615	-0.018919
C	-1.782056	-0.651614	-0.018918
C	-0.706432	0.250761	-0.015622
H	2.263360	-3.144292	0.007568
H	4.281762	-1.699077	0.012694
H	-4.281762	1.699077	0.012695
H	-2.263360	3.144292	0.007568
H	1.605045	1.726029	-0.025773
H	-1.605045	-1.726029	-0.025772
O	4.095262	1.075836	-0.009623
O	-4.095261	-1.075836	-0.009621
C	-5.458239	-0.596704	0.037017
H	-6.083107	-1.498318	0.037739
H	-5.631484	-0.013848	0.956407
H	-5.683880	0.020014	-0.848351
C	5.458239	0.596704	0.037020
H	5.683883	-0.020014	-0.848348
H	6.083107	1.498318	0.037742
H	5.631482	0.013849	0.956410

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HAT

N	1.456966	1.255378	-0.169036
N	1.450661	-1.251609	0.580264
C	1.377139	2.494247	-0.701605
C	2.479804	3.249002	-1.105257
C	3.765913	2.667616	-0.975449
C	3.757296	-2.675839	1.383441
C	2.470731	-3.259274	1.495551
C	1.370798	-2.502524	1.086016
C	2.706313	0.689625	-0.047129
C	3.869258	1.370269	-0.446772
C	3.862647	-1.370138	0.874858
C	2.702788	-0.680590	0.484382
H	0.368791	2.891959	-0.819871
H	2.327594	4.243973	-1.518461
H	2.317005	-4.262505	1.888081
H	0.364080	-2.914408	1.165726
Ni	-0.097547	-0.017337	0.143922
N	-1.683292	-1.270534	-0.080357
N	-1.593328	1.214099	0.736618
C	-1.660134	-2.501587	-0.636713
C	-2.913959	-0.694566	0.145914
C	-1.459588	2.444306	1.280812
C	-2.856716	0.660324	0.711432
C	-2.798978	-3.237912	-0.967432
H	-0.669488	-2.909910	-0.836519

C	-4.111877	-1.354988	-0.178880
C	-2.517898	3.199554	1.790735
H	-0.443197	2.839104	1.308189
C	-3.977047	1.349913	1.205067
C	-4.064861	-2.644078	-0.734056
H	-2.688735	-4.227855	-1.405575
C	-3.818151	2.637353	1.744803
H	-2.323784	4.186018	2.207423
H	-4.967562	0.896216	1.191871
H	-5.077523	-0.873797	-0.029754
H	4.848820	0.898248	-0.380577
H	4.843899	-0.901325	0.810166
O	-4.944858	3.248405	2.201253
O	-5.260596	-3.224397	-1.025325
O	4.919815	-3.281751	1.747028
O	4.929723	3.267819	-1.344862
C	-4.809225	4.565428	2.778102
H	-5.824469	4.860792	3.071003
H	-4.153957	4.536308	3.664377
H	-4.408689	5.275768	2.036042
C	-5.243169	-4.546533	-1.606803
H	-6.296396	-4.803278	-1.776148
H	-4.696228	-4.544292	-2.563935
H	-4.784063	-5.269614	-0.912240
C	4.851785	4.588728	-1.924046
H	4.413187	5.302714	-1.207346
H	5.888818	4.869109	-2.147293
H	4.257442	4.572515	-2.852403
C	4.840588	-4.610618	2.307363
H	4.400776	-5.314132	1.581304
H	5.877328	-4.895376	2.526240
H	4.246750	-4.606520	3.236439
C	-1.028029	-0.719571	-7.755701
C	0.066426	-0.140407	-8.426190
C	1.101245	0.466031	-7.688485
C	1.042983	0.494580	-6.277508
C	-0.052002	-0.086604	-5.628951
C	-1.089396	-0.693831	-6.344614
H	-1.833917	-1.191293	-8.326674
H	0.112678	-0.161595	-9.517973
H	1.953391	0.916707	-8.206801
H	1.849072	0.966193	-5.706757
H	-1.941088	-1.145870	-5.826761
I	-0.134324	-0.054895	-3.113926

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LDTS

N	1.479883	1.133397	-1.064374
N	1.287730	-1.145848	0.183797
C	1.495052	2.292797	-1.757532
C	2.586482	3.165080	-1.787372
C	3.743782	2.808746	-1.058417
C	3.328594	-2.305997	1.756840
C	2.083377	-2.956123	1.594069
C	1.110785	-2.334491	0.808930
C	2.606081	0.783535	-0.359267
C	3.745578	1.596298	-0.339879
C	3.524460	-1.061513	1.126527
C	2.498605	-0.510465	0.350411
H	0.587524	2.512840	-2.320603
H	2.524996	4.082033	-2.370306
H	1.861881	-3.915211	2.058574
H	0.135464	-2.799241	0.664961
Ni	-0.019627	-0.169673	-0.932148
N	-2.020297	-1.610305	-0.532760
N	-1.927755	1.111037	0.005907
C	-2.115740	-2.848603	-1.042909
C	-3.161271	-0.980178	-0.151102
C	-1.781601	2.361913	0.472681
C	-3.023294	0.405126	0.392376
C	-3.320953	-3.546060	-1.195679
H	-1.176376	-3.309437	-1.356002
C	-4.420229	-1.587273	-0.276838
C	-2.688318	2.992591	1.335635
H	-0.886966	2.893312	0.138404
C	-3.981165	0.940003	1.267390
C	-4.508838	-2.891625	-0.805714
H	-3.318386	-4.547666	-1.621294
C	-3.818110	2.254860	1.749942
H	-2.505177	4.012900	1.668463
H	-4.837135	0.353578	1.599466
H	-5.333875	-1.058538	-0.007625
H	4.638177	1.309309	0.214483
H	4.476761	-0.547970	1.250400
O	-4.776381	2.707096	2.598540
O	-5.756213	-3.415296	-0.909241
O	4.370617	-2.786915	2.484666
O	4.880407	3.548231	-0.993177
C	-4.628106	4.042089	3.133340
H	-5.497962	4.192419	3.784464
H	-3.697165	4.123134	3.718087
H	-4.629335	4.787255	2.321259
C	-5.887480	-4.728050	-1.502092
H	-6.963622	-4.940443	-1.501172
H	-5.502219	-4.724279	-2.534605
H	-5.351886	-5.480161	-0.900049
C	4.924687	4.780988	-1.748097
H	4.155085	5.483062	-1.387423
H	5.925489	5.193519	-1.570508
H	4.780637	4.581108	-2.822299
C	4.208239	-4.075292	3.118999
H	4.020802	-4.857385	2.364807
H	5.157645	-4.267332	3.633984
H	3.381304	-4.047152	3.847710
I	-0.842130	-0.150784	-3.804027

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MECP

N	1.497895	1.193683	-0.503382
N	1.497679	-1.193331	0.503262
C	1.412230	2.434835	-1.029109
C	2.512591	3.221823	-1.378191
C	3.809776	2.682066	-1.162463
C	3.809467	-2.681790	1.162318
C	2.512062	-3.221578	1.378021
C	1.412007	-2.434240	1.028829
C	2.766751	0.670075	-0.280601
C	3.927399	1.405916	-0.602657
C	3.927229	-1.405815	0.602656
C	2.766647	-0.669701	0.280484
H	0.396061	2.803652	-1.185628
H	2.353755	4.208375	-1.809787
H	2.353179	-4.208038	1.809502
H	0.395617	-2.803101	1.185348
Ni	0.000000	0.000342	-0.000091
N	-1.497889	-1.193001	-0.503373
N	-1.497677	1.193977	0.503359
C	-1.412303	-2.434136	-1.029124
C	-2.766813	-0.669413	-0.280503
C	-1.411951	2.434873	1.028987
C	-2.766593	0.670348	0.280627
C	-2.512596	-3.221106	-1.378145
H	-0.396074	-2.802933	-1.185711
C	-3.927335	-1.405301	-0.602543
C	-2.512037	3.222199	1.378271
H	-0.395599	2.803734	1.185470
C	-3.927285	1.406388	0.602845
C	-3.809818	-2.681349	-1.162325
H	-2.353793	-4.207689	-1.809776
C	-3.809434	2.682448	1.162619
H	-2.353141	4.208609	1.809786
H	-4.921027	0.993507	0.432835
H	-4.921261	-0.992280	-0.432350
H	4.921211	0.992946	-0.432556
H	4.921075	-0.992858	0.432589
O	-4.980730	3.326835	1.470588
O	-4.981286	-3.325652	-1.470137
O	4.980770	-3.326268	1.470251
O	4.981249	3.326302	-1.470293
C	-4.887487	4.615474	2.088286
H	-5.921469	4.917708	2.297831
H	-4.312991	4.561807	3.029951
H	-4.413580	5.346609	1.409452
C	-4.888238	-4.614279	-2.087831
H	-5.922272	-4.916399	-2.297251
H	-4.313845	-4.560678	-3.029566
H	-4.414321	-5.345463	-1.409051
C	4.888183	4.614967	-2.087927
H	4.414284	5.346120	-1.409108
H	5.922226	4.917107	-2.297346
H	4.313791	4.561417	-3.029660
C	4.887538	-4.614886	2.087965
H	4.413624	-5.346031	1.409143
H	5.921512	-4.917105	2.297512
H	4.313033	-4.561199	3.029627

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Ni_L

N	1.299502	1.181839	-0.383651
N	-1.299469	1.180957	0.389648
C	2.662396	1.237043	-0.420145

C 3.504710 0.139788 -0.223802
C 2.917635 -1.119649 0.053046
C -2.916923 -1.120210 -0.052708
C -3.504416 0.138287 0.227381
C -2.662444 1.235289 0.426643
C 0.732383 -0.054228 -0.064773
C 1.516267 -1.196607 0.150938
C -1.515451 -1.196493 -0.150333
C -0.732001 -0.054445 0.068405
H 3.085650 2.213911 -0.660062
H 4.581520 0.272537 -0.315320
H -4.581283 0.270395 0.319252
H -3.086148 2.211357 0.669152
Ni -0.001171 2.542699 -0.003172
H 1.046912 -2.140632 0.429627
H -1.045769 -2.139677 -0.431343
O -3.608298 -2.279352 -0.263379
O 3.609409 -2.279119 0.260394
C 5.047807 -2.220584 0.185261
H 5.451675 -1.524510 0.939974
H 5.393844 -3.241038 0.393644
H 5.375034 -1.911098 -0.821738
C -5.046712 -2.221389 -0.188394
H -5.450558 -1.522876 -0.940871
H -5.392467 -3.241219 -0.400284
H -5.374241 -1.915331 0.819560

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OA1
Ni -0.215035 -1.291336 -0.929817
N 1.705571 -1.141744 -0.625491
N -0.050039 0.602225 -1.655687
C 2.680626 -2.054752 -0.396603
C 3.981813 -1.727066 0.000917
C 4.308899 -0.358704 0.153189
C -0.177237 3.277149 -0.700346
C -1.182893 2.764341 -1.551229
C -1.068822 1.438721 -1.984380
C 2.042250 0.193351 -0.519823
C 3.323494 0.607363 -0.126421
C 0.899060 2.439152 -0.349474
C 0.948026 1.130558 -0.850601
H 2.386114 -3.099244 -0.510912
H 4.698852 -2.523351 0.192582
H -2.034571 3.362104 -1.872409
H -1.836212 1.010402 -2.633915
C -1.978540 -0.501122 1.296212
C -2.421305 0.815987 1.135589
C -1.201012 -0.909423 2.388485
C -2.063283 1.765257 2.114307
H -3.006876 1.109822 0.265147
C -0.847253 0.055108 3.352142
H -0.864191 -1.942160 2.483315
C -1.274806 1.389668 3.215854
H -2.398251 2.799283 2.004723
H -0.228179 -0.241766 4.202400
H -0.991596 2.133321 3.964021
I -2.510236 -2.025881 -0.280441
H 3.572563 1.666310 -0.061955
H 1.664893 2.804216 0.335277
O 5.527033 0.113971 0.536120
O -0.169162 4.533955 -0.165707
C 6.574558 -0.847231 0.784791
H 6.785272 -1.436121 -0.123374
H 7.455213 -0.253218 1.060210
H 6.299068 -1.519261 1.614390
C -1.262138 5.409622 -0.507654
H -2.225456 4.977836 -0.187541
H -1.071262 6.344298 0.035168
H -1.282207 5.601983 -1.593646

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OA2
Ni -0.716482 -0.485582 0.350984
N 1.279104 -0.615439 0.028778
N -0.250198 1.496781 0.313294
C 1.975002 -1.751608 -0.156384
C 3.337602 -1.782934 -0.467277
C 4.016102 -0.552717 -0.598194
C 0.679177 4.153857 0.344585
C -0.686202 3.866902 0.562465
C -1.089383 2.528808 0.535192
C 1.932845 0.578954 -0.094912
C 3.293664 0.644357 -0.407106
C 1.568473 3.081158 0.124258
C 1.077603 1.772472 0.118285
H 1.408979 -2.674889 -0.045488
H 3.835129 -2.741263 -0.600416
H -1.423337 4.645348 0.748552
H -2.135003 2.262530 0.691026
C -1.312486 -0.876242 -1.644824
C -1.080660 -2.269567 -1.731427
C -0.673987 0.026907 -2.529470
C -0.077931 -2.733542 -2.602392
H -1.640825 -2.962782 -1.105771
C 0.324501 -0.460017 -3.383846
H -0.912860 1.089072 -2.498113
C 0.633470 -1.836294 -3.417588
H 0.140042 -3.803742 -2.637803
H 0.863563 0.240876 -4.026251
H 1.409962 -2.205373 -4.090963
S -1.324912 -1.992762 2.012561
C 0.016762 -1.782546 3.157468
F 1.209048 -2.401988 2.792849
F 0.381090 -0.462446 3.402567
F -0.269457 -2.305629 4.413096
H 3.809096 1.597788 -0.510259
H 2.625210 3.292109 -0.030689
O 5.328785 -0.416804 -0.902890
O 1.221907 5.393828 0.330805
C 6.104992 -1.623480 -1.095142
H 5.700176 -2.211396 -1.934690
H 7.120353 -1.280752 -1.328180
H 6.110350 -2.228470 -0.174041
C 0.343899 6.519523 0.573653
H 0.986144 7.406248 0.511551
H -0.443155 6.565076 -0.196150
H -0.106802 6.445305 1.576347
I -3.393992 -0.234607 -0.818786

12
PhI
C -0.592520 0.000000 0.000039
C -1.275503 -1.226462 0.000121
C -2.683569 -1.216240 0.000305
C -3.389029 0.000001 0.000407
C -2.683569 1.216240 0.000304
C -1.275501 1.226462 0.000121
H -0.731785 -2.171768 0.000040
H -3.221927 -2.166789 0.000370
H -4.481100 0.000000 0.000562
H -3.221924 2.166791 0.000369
H -0.731785 2.171768 0.000038
I 1.580880 0.000000 -0.000173

12
PhI$^{\cdot-}$
C 1.384064 0.000251 0.216528
C 2.024717 -1.230416 0.130259
C 3.428810 -1.222874 -0.052359
C 4.122743 -0.000250 -0.143015
C 3.429254 1.222628 -0.052407
C 2.025163 1.230683 0.130212
H 1.478241 -2.175211 0.196707
H 3.971395 -2.170105 -0.126413
H 5.205919 -0.000450 -0.288247
H 3.972177 2.169661 -0.126525
H 1.479031 2.175680 0.196634
I -2.162175 0.000006 -0.023160

11
Ph$^{\cdot}$
C 1.223213 0.637579 0.000005
C -0.000005 1.334146 -0.000002
C -1.223202 0.637604 -0.000002
C -1.235625 -0.779041 0.000003
C -0.000009 -1.407303 0.000001
C 1.235632 -0.779027 -0.000006
H 2.170396 1.183876 0.000012
H 0.000026 2.426463 -0.000003
H -2.170413 1.183851 0.000000
H -2.180265 -1.328946 0.000002
H 2.180238 -1.328991 -0.000004

16
PhSCF3
C 0.735576 -0.036151 0.546681
C 1.399626 -1.241229 0.241626
C 2.703809 -1.196521 -0.278777
C 3.339095 0.040359 -0.489393
C 2.672381 1.238862 -0.177763

C	1.369029	1.206710	0.345794
H	0.902718	-2.198749	0.404648
H	3.220925	-2.128057	-0.517969
H	4.353525	0.070061	-0.892563
H	3.165388	2.199892	-0.338133
H	0.849341	2.134050	0.591241
S	-0.923486	-0.091484	1.255297
C	-1.913625	0.016643	-0.283884
F	-1.734453	1.185075	-0.966820
F	-1.650932	-0.986689	-1.170336
F	-3.231445	-0.063440	0.052971

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RE1

Ni	-0.713556	-0.063909	-0.207256
N	0.962536	-1.126860	-0.409521
N	0.598691	1.421176	0.116951
C	1.073849	-2.462981	-0.582471
C	2.286551	-3.157047	-0.573198
C	3.473270	-2.421977	-0.353791
C	2.675494	3.327489	0.295042
C	1.323156	3.721291	0.413045
C	0.339392	2.734381	0.311405
C	2.119532	-0.413898	-0.192103
C	3.375728	-1.030245	-0.156803
C	2.965078	1.963639	0.092302
C	1.915964	1.039431	0.014131
H	0.132352	-2.994195	-0.730652
H	2.289332	-4.234381	-0.729574
H	1.030195	4.756915	0.574388
H	-0.715752	3.000985	0.387495
C	-2.274928	-1.190776	0.069960
C	-2.273014	-0.759718	1.446648
C	-2.372353	-2.593902	-0.225128
C	-2.156296	-1.734135	2.463452
H	-2.448603	0.280375	1.720145
C	-2.273785	-3.522761	0.809072
H	-2.468426	-2.922692	-1.262334
C	-2.133907	-3.103685	2.159249
H	-2.113429	-1.404746	3.505560
H	-2.303715	-4.589933	0.571673
H	-2.059948	-3.845484	2.957614
S	-2.599653	0.041900	-1.300041
C	-3.939942	1.164209	-0.593408
F	-4.970821	0.478235	-0.018288
F	-3.489427	2.053004	0.344131
F	-4.469984	1.907090	-1.615757
H	4.282145	-0.457877	0.035495
H	4.003618	1.653140	-0.014718
O	3.739050	4.168560	0.354553
O	4.723263	-2.951938	-0.305779
C	3.471677	5.579175	0.528711
H	2.954542	5.759198	1.485186
H	4.455895	6.063220	0.535329
H	2.865432	5.963076	-0.307987
C	4.854110	-4.380931	-0.477039
H	4.475603	-4.690212	-1.465039
H	5.929724	-4.584558	-0.405741
H	4.312610	-4.917281	0.319538

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RE2

Ni	-0.716217	0.075262	-0.428408
N	0.820346	-1.239790	-0.292811
N	0.866286	1.381309	-0.386416
C	0.685876	-2.574520	-0.187499
C	1.739965	-3.429616	0.144590
C	3.009409	-2.859675	0.384658
C	3.219957	2.917370	-0.505710
C	1.956813	3.520595	-0.691913
C	0.822582	2.707671	-0.621681
C	2.049411	-0.684292	-0.076126
C	3.158975	-1.460975	0.265718
C	3.278260	1.524972	-0.278433
C	2.091934	0.789695	-0.236878
H	-0.314181	-2.963361	-0.375999
H	1.559869	-4.500350	0.211566
H	1.841570	4.584285	-0.889487
H	-0.169720	3.135535	-0.758222
C	-1.515997	-0.411192	1.352579
C	-0.636401	-0.109368	2.413143
C	-2.289490	-1.592452	1.368710
C	-0.459966	-1.051579	3.441690
H	-0.051569	0.807897	2.411790
C	-2.098546	-2.521381	2.404966
H	-2.997738	-1.796406	0.566019
C	-1.183001	-2.258573	3.441651
H	0.254579	-0.836158	4.240179
H	-2.677096	-3.448401	2.400634
H	-1.044373	-2.981247	4.248624
S	-2.554612	1.185942	0.219387
C	-2.334424	2.480361	1.501948
F	-2.820106	2.118416	2.727681
F	-1.050039	2.895614	1.703308
F	-3.048088	3.584589	1.112897
H	4.131523	-1.007505	0.450637
H	4.247128	1.040632	-0.167131
O	4.118077	-3.552719	0.729898
O	4.403760	3.567138	-0.542406
C	4.001336	-4.989987	0.870310
H	3.692447	-5.445292	-0.084071
H	5.004086	-5.335274	1.149377
H	3.278067	-5.239552	1.663097
C	4.389504	4.990214	-0.817540
H	5.442646	5.295028	-0.810831
H	3.942028	5.184042	-1.805352
H	3.831812	5.526865	-0.033719
I	-2.001461	-1.160760	-2.558817

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$SCF3^-$

S	1.508163	0.000126	-0.000028
C	-0.225828	0.000197	-0.000127
F	-0.843871	1.257419	-0.204111
F	-0.843409	-0.805760	-0.986511
F	-0.843347	-0.452014	1.190756

Substrate: Bromobenzene

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A2_Br

Ni	-0.054831	-0.958569	-0.562188
N	-2.004792	-1.052861	-0.254409
N	-0.363415	0.976726	-0.305512
C	-2.791644	-2.152642	-0.240406
C	-4.175812	-2.124321	-0.040311
C	-4.793189	-0.871096	0.162517
C	-1.113071	3.674885	0.075316
C	0.234768	3.328548	-0.161658
C	0.546646	1.977168	-0.342514
C	-2.610236	0.165628	-0.052133
C	-3.986809	0.286764	0.155686
C	-2.076493	2.644702	0.118128
C	-1.676055	1.319777	-0.075585
H	-2.275593	-3.100641	-0.397096
H	-4.737895	-3.056411	-0.045462
H	1.029149	4.071698	-0.204179
H	1.576171	1.668215	-0.522750
H	3.332239	-2.160701	2.077636
C	2.640696	-2.287737	1.244032
C	1.695419	-3.375255	1.247539
C	2.662467	-1.444408	0.154956
C	0.840864	-3.573866	0.175845
C	1.768074	-1.529167	-0.971398
C	0.817314	-2.663510	-0.950675
H	0.173134	-4.440534	0.165769
H	2.106802	-1.109104	-1.926845
H	0.437668	-3.055452	-1.905705
H	1.683548	-4.054966	2.103630
H	-4.453533	1.257872	0.314584
H	-3.118841	2.901640	0.302386
O	-6.120915	-0.678465	0.368100
O	-1.573577	4.936592	0.268977
C	-0.611240	6.015560	0.241824
H	-0.116183	6.067771	-0.741490
H	-1.193122	6.928085	0.420433
H	0.140677	5.882674	1.036756
C	-6.972669	-1.846562	0.392656
H	-6.683531	-2.518550	1.217354
H	-7.986930	-1.462318	0.556428
H	-6.921269	-2.383583	-0.568510
Br	4.048034	0.006167	0.103252

41
A3_Br

Ni	0.680592	-0.344917	0.100219
N	-0.174191	1.406806	0.043301
N	-1.251852	-0.966979	0.072514
C	0.439790	2.615798	0.026779
C	-0.234825	3.836659	-0.012651
C	-1.644779	3.826564	-0.039285
C	-4.024231	-1.495980	0.044778
C	-3.088180	-2.551194	0.072657
C	-1.728109	-2.229380	0.086448
C	-1.552381	1.400312	0.021117
C	-2.300268	2.578911	-0.019636
C	-3.541476	-0.170771	0.029326
C	-2.162595	0.055765	0.041315
H	1.525942	2.600366	0.045639
H	0.345026	4.757182	-0.023142
H	-3.389086	-3.596794	0.084470
H	-0.974874	-3.016188	0.110199
C	2.426124	0.375591	0.116441
C	3.046466	0.731290	1.333791
C	3.089989	0.670285	-1.094329
C	4.293984	1.388181	1.340424
H	2.557536	0.501849	2.284858
C	4.337886	1.326549	-1.089260
H	2.635358	0.392461	-2.049555
C	4.944017	1.690585	0.128455
H	4.758285	1.658846	2.293748
H	4.836774	1.548620	-2.037658
H	5.912479	2.197637	0.133065
H	-3.388017	2.553134	-0.039637
H	-4.254500	0.651219	0.009155
O	-2.436260	4.922016	-0.082651
O	-5.368724	-1.645414	0.031227
C	-1.793746	6.219949	-0.117309
H	-2.613594	6.947822	-0.142450
H	-1.180628	6.369198	0.785614
H	-1.171078	6.315001	-1.021289
C	-5.899084	-2.993273	0.046829
H	-6.989072	-2.874040	0.037259
H	-5.568242	-3.546205	-0.846926
H	-5.581297	-3.520652	0.960478
Br	1.697485	-2.507384	0.193032

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ADTS_Br

N	2.404336	1.055388	-0.469889
N	1.943529	-1.494921	0.121314
C	2.618559	2.371439	-0.704249
C	3.863635	3.000851	-0.646180
C	4.992350	2.217066	-0.293661
C	3.947561	-3.487213	-0.148858
C	2.597165	-3.843203	0.098626
C	1.659708	-2.812194	0.203908
C	3.522613	0.282046	-0.204695
C	4.808306	0.844065	-0.077679
C	4.269724	-2.126675	-0.261925
C	3.263216	-1.153960	-0.101035
H	1.736295	2.953929	-0.968654
H	3.940695	4.062539	-0.874623
H	2.276870	-4.876890	0.217245
H	0.612761	-3.066022	0.381877
Ni	0.608226	0.165237	-0.074430
N	-0.708148	1.779962	-0.205626
N	-0.828040	-0.625120	-1.301203
C	-0.489977	3.056329	0.172418
C	-1.797940	1.547060	-1.014735
C	-0.887859	-1.883773	-1.790609
C	-1.955098	0.157958	-1.454458
C	-1.299576	4.142283	-0.171138
H	0.375242	3.212883	0.816710
C	-2.662271	2.579357	-1.423305
C	-2.011431	-2.450027	-2.398305
H	0.026400	-2.469910	-1.702452
C	-3.140365	-0.341514	-2.020555
C	-2.428152	3.893498	-0.989990
H	-1.062128	5.133857	0.211510
C	-3.182154	-1.659400	-2.498683
H	-1.960852	-3.469153	-2.777930
H	-4.035579	0.277180	-2.076870
H	-3.497421	2.377358	-2.094043
H	5.661101	0.224997	0.201809
H	5.293930	-1.837131	-0.497441
O	-4.365625	-2.080045	-3.030734
O	-3.307903	4.844664	-1.417359
O	4.970432	-4.375719	-0.306078
O	6.259608	2.701239	-0.142324
C	-4.436910	-3.436198	-3.516861
H	-5.463478	-3.561722	-3.884140
H	-3.721103	-3.594761	-4.340959
H	-4.237002	-4.152522	-2.702438
C	-3.067958	6.207969	-1.012616
H	-3.871140	6.795721	-1.474905
H	-3.114704	6.304624	0.084931
H	-2.087451	6.557372	-1.377860
C	6.459769	4.118173	-0.323086
H	5.846328	4.693186	0.390905
H	7.525690	4.290228	-0.126066
H	6.214371	4.420184	-1.355083
C	4.658113	-5.780820	-0.204280
H	3.933854	-6.076085	-0.981777
H	5.610446	-6.303806	-0.359008
H	4.255447	-6.020475	0.793967
H	-0.215270	-1.671071	1.687202
C	-0.390148	-0.628068	1.933323
C	-1.689703	-0.180164	2.218519
C	0.702666	0.257700	2.203228
C	-1.967891	1.090425	2.735745
C	0.443718	1.510138	2.822142
H	1.718156	-0.139075	2.226180
C	-0.875429	1.929485	3.051920
H	-1.073534	2.914870	3.481981
H	-2.993004	1.416495	2.914984
H	1.280572	2.161093	3.086967
Br	-3.201757	-1.409257	1.834932

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B1T_Br

N	1.492900	1.227216	-0.204098
N	1.494560	-1.255558	0.616831
C	1.406710	2.467735	-0.727987
C	2.498336	3.218127	-1.172968
C	3.787430	2.623989	-1.086408
C	3.820605	-2.724463	1.272828
C	2.528204	-3.279734	1.483712

C	1.421646	-2.495607	1.144753
C	2.749785	0.643153	-0.123465
C	3.904407	1.330541	-0.562751
C	3.925449	-1.432508	0.742278
C	2.755464	-0.708203	0.417508
H	0.397393	2.877359	-0.796927
H	2.340191	4.217058	-1.574562
H	2.378191	-4.275354	1.896238
H	0.410995	-2.877942	1.302293
Ni	-0.038500	-0.003446	0.232168
N	-1.583871	-1.226098	-0.179228
N	-1.559029	1.244115	0.676558
C	-1.512670	-2.455818	-0.729537
C	-2.836132	-0.638413	-0.065974
C	-1.469758	2.474879	1.223219
C	-2.825638	0.703538	0.498676
C	-2.615274	-3.192324	-1.170564
H	-0.506363	-2.867312	-0.825033
C	-4.001495	-1.311262	-0.498473
C	-2.565801	3.256452	1.600275
H	-0.454527	2.851706	1.363067
C	-3.985443	1.425343	0.861638
C	-3.899861	-2.594490	-1.050099
H	-2.468260	-4.183451	-1.594888
C	-3.864392	2.708392	1.410508
H	-2.403343	4.244800	2.025463
H	-4.976881	0.989013	0.741357
H	-4.979913	-0.835727	-0.432036
H	4.886352	0.859489	-0.522307
H	4.912998	-0.992043	0.606803
O	-5.027135	3.343077	1.742610
O	-5.065918	-3.181649	-1.452430
O	4.992539	-3.361115	1.567197
O	4.943771	3.225234	-1.495807
C	-4.932340	4.661618	2.318864
H	-5.967495	4.971062	2.512014
H	-4.365141	4.636994	3.264401
H	-4.455222	5.363159	1.614034
C	-4.988271	-4.497258	-2.036948
H	-6.023845	-4.771478	-2.276046
H	-4.382140	-4.482768	-2.958455
H	-4.563867	-5.220349	-1.320301
C	4.847561	4.543735	-2.070949
H	4.428834	5.259740	-1.343937
H	5.877328	4.827254	-2.323832
H	4.227630	4.529789	-2.983263
C	4.913999	-4.684550	2.134730
H	4.425038	-5.382126	1.434074
H	5.953838	-4.992143	2.304349
H	4.365474	-4.669162	3.091399
C	-1.420805	-0.702773	-7.179218
C	-0.349244	-0.252803	-7.971394
C	0.798767	0.278076	-7.356275
C	0.883264	0.362179	-5.953276
C	-0.197077	-0.093577	-5.183915
C	-1.351897	-0.626625	-5.775010
H	-2.317097	-1.116665	-7.647334
H	-0.408349	-0.315187	-9.060093
H	1.636576	0.629876	-7.963008
H	1.774797	0.773529	-5.477451
H	-2.183269	-0.976730	-5.161100
Br	-0.089458	0.009819	-3.204722

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B2_Br

N	-1.961897	-0.596063	-0.600551
N	-0.884703	1.581951	0.369588
C	-2.454390	-1.687891	-1.219366
C	-3.805662	-2.047729	-1.210716
C	-4.711834	-1.201226	-0.531074
C	-2.236509	3.415841	2.048757
C	-0.866201	3.589986	1.741400
C	-0.253291	2.649172	0.910823
C	-2.839711	0.227693	0.052243
C	-4.214530	-0.045551	0.100259
C	-2.910276	2.307883	1.503157
C	-2.217224	1.418669	0.669485
H	-1.720022	-2.290682	-1.754677
H	-4.127585	-2.948768	-1.729820
H	-0.284685	4.423604	2.131604
H	0.804005	2.747331	0.660408
Ni	-0.002773	0.005242	-0.626094
H	1.727130	2.285215	-1.766848
C	2.456176	1.685938	-1.220539
C	3.809919	2.036462	-1.218000
C	4.709626	1.196226	-0.522702
H	4.138290	2.925355	-1.753712
C	4.203389	0.056642	0.130756
C	2.826893	-0.207500	0.086579
N	1.955414	0.609340	-0.582375
C	2.196310	-1.383449	0.725924
N	0.864648	-1.545948	0.426110
C	2.882660	-2.259671	1.578307
C	0.225990	-2.599219	0.984364
C	2.201389	-3.353480	2.143598
H	-0.830784	-2.696811	0.730995
C	0.831500	-3.527147	1.835188
H	0.244752	-4.350723	2.238610
H	-3.961423	2.153809	1.744715
H	-4.908869	0.626760	0.602018
H	3.934005	-2.106615	1.819421
H	4.892466	-0.610823	0.646083
O	-2.968190	4.239425	2.847525
O	-6.052129	-1.407794	-0.440934
O	6.051345	1.393762	-0.436981
O	2.927116	-4.164294	2.960291
C	-2.301264	5.385774	3.418697
H	-1.929801	6.055533	2.625516
H	-3.065222	5.898901	4.016045
H	-1.466100	5.068719	4.065232
C	-6.598019	-2.578303	-1.089084
H	-7.677870	-2.538691	-0.898997
H	-6.402660	-2.548412	-2.173568
H	-6.171279	-3.496729	-0.653344
C	2.253704	-5.295867	3.553099
H	3.013339	-5.798774	4.164463
H	1.417195	-4.961919	4.189177
H	1.882885	-5.980911	2.772864
C	6.605395	2.550511	-1.102754
H	6.183878	3.478122	-0.681620
H	7.684807	2.506935	-0.911165
H	6.410588	2.505305	-2.186779
Br	0.058485	-0.095110	-3.351571

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B3_Br

N	-0.488036	-1.305400	0.007864
N	-0.038975	1.249773	0.005224
C	-0.627893	-2.650618	0.008912
C	-1.863892	-3.303111	0.006897
C	-3.035547	-2.513879	0.003528
C	-2.020136	3.255323	0.000201
C	-0.649377	3.597256	0.001678
C	0.289306	2.561640	0.004206
C	-1.629023	-0.539589	0.004822
C	-2.904184	-1.109038	0.002648
C	-2.376806	1.890163	0.001185
C	-1.372677	0.919495	0.003700
H	0.300896	-3.222939	0.011455
H	-1.895936	-4.390972	0.007999
H	-0.308288	4.630741	0.001000
H	1.357804	2.782415	0.005467
Ni	1.203323	-0.288244	0.008769
H	-3.430459	1.614841	0.000043
H	-3.799833	-0.489934	0.000106
O	-3.043635	4.142710	-0.002086
O	-4.300524	-2.998797	0.000994
C	-2.713982	5.551671	-0.004049
H	-2.138302	5.811722	-0.907107
H	-3.677759	6.075161	-0.006491
H	-2.141143	5.814898	0.899897
C	-4.472135	-4.435692	0.000470
H	-5.557045	-4.596899	-0.001950
H	-4.020515	-4.877480	-0.902376
H	-4.024610	-4.877702	0.905239
Br	3.530313	-0.635832	0.011308

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B5_Br

Ni	-0.509004	-0.205457	-0.070655
N	1.335468	-0.997836	-0.354976
N	0.586785	1.484918	-0.052960
C	1.629331	-2.302205	-0.527391
C	2.923242	-2.785328	-0.741819
C	3.983574	-1.852380	-0.781032
C	2.328724	3.694985	0.061601
C	0.935063	3.868353	0.215657
C	0.121024	2.734709	0.151278
C	2.362454	-0.092793	-0.392825
C	3.688555	-0.485114	-0.602193
C	2.828852	2.392551	-0.144332

C	1.940324	1.314198	-0.195584
H	0.782143	-2.987715	-0.486688
H	3.083752	-3.854521	-0.865674
H	0.482769	4.843294	0.384911
H	-0.959125	2.824763	0.273664
S	-1.660685	-1.054070	1.687876
C	-0.349572	-1.540589	2.791291
F	0.373886	-2.657000	2.384627
F	0.617376	-0.569664	3.021986
F	-0.815381	-1.875827	4.058135
H	4.499353	0.241380	-0.628148
H	3.901999	2.246530	-0.256195
O	5.286929	-2.163380	-0.983382
O	3.245254	4.691024	0.098720
C	5.629119	-3.558666	-1.157999
H	5.110374	-3.976266	-2.036165
H	6.714019	-3.572199	-1.318534
H	5.369936	-4.134531	-0.254813
C	2.766743	6.043588	0.293534
H	3.665405	6.672099	0.284486
H	2.090448	6.333629	-0.526763
H	2.249101	6.132952	1.262029
H	-0.493735	-1.881767	-3.231367
C	-1.294796	-1.417287	-2.653517
C	-2.469394	-2.123124	-2.382701
C	-1.132277	-0.083645	-2.179039
C	-3.540363	-1.517822	-1.673647
H	-2.585614	-3.151470	-2.732516
C	-2.186532	0.528345	-1.428084
H	-0.313714	0.532093	-2.556891
C	-3.378865	-0.209956	-1.228097
H	-4.461250	-2.070324	-1.487433
H	-2.156622	1.593592	-1.202317
Br	-4.861817	0.670604	-0.269993

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B6_Br

Ni	-0.660571	-0.328820	0.287060
N	0.225510	1.421976	-0.133422
N	1.301753	-0.964577	0.112232
C	-0.384560	2.624970	-0.135798
C	0.284027	3.827496	-0.367563
C	1.673103	3.781738	-0.611483
C	4.019129	-1.556420	-0.293614
C	3.110246	-2.569180	0.080207
C	1.771554	-2.215091	0.267826
C	1.579332	1.372315	-0.340687
C	2.321397	2.527936	-0.591878
C	3.535893	-0.238682	-0.451407
C	2.180753	0.021419	-0.237849
H	-1.454812	2.619440	0.057481
H	-0.276010	4.759720	-0.350730
H	3.414946	-3.603724	0.222827
H	1.034176	-2.965134	0.554739
C	-2.418618	0.326277	-0.127116
C	-2.598426	0.581430	-1.498434
C	-3.421707	0.644131	0.799479
C	-3.790933	1.187805	-1.942921
H	-1.821783	0.326851	-2.223831
C	-4.609162	1.255862	0.346998
H	-3.283105	0.427696	1.858724
C	-4.796385	1.528913	-1.020613
H	-3.924610	1.390326	-3.009103
H	-5.389448	1.508706	1.070136
H	-5.720905	1.998022	-1.365855
S	-1.630304	-2.354778	0.544319
C	-1.800684	-2.898263	-1.161033
F	-3.014196	-2.603148	-1.745374
F	-0.852891	-2.376930	-2.020877
F	-1.681146	-4.269842	-1.251270
H	3.396335	2.486861	-0.756705
H	4.230395	0.549037	-0.735786
O	2.453394	4.854456	-0.856362
O	5.338487	-1.738370	-0.516336
C	1.824190	6.161235	-0.868226
H	1.374894	6.376505	0.113836
H	2.634704	6.868525	-1.079902
H	1.058393	6.208503	-1.658385
C	5.875737	-3.076486	-0.363765
H	6.945362	-2.983870	-0.586118
H	5.730189	-3.432133	0.668516
H	5.395506	-3.765226	-1.076675
Br	-0.513842	0.100219	2.826998

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HAT_B

N	1.484383	1.164097	-0.209577
N	1.473483	-1.305340	0.649567
C	1.403934	2.382432	-0.784554
C	2.503239	3.116423	-1.235176
C	3.789675	2.529673	-1.106555
C	3.785965	-2.729835	1.437833
C	2.493630	-3.290837	1.613893
C	1.392721	-2.531560	1.210001
C	2.735199	0.589893	-0.089683
C	3.896137	1.253023	-0.535999
C	3.895070	-1.448464	0.877244
C	2.732165	-0.752378	0.492065
H	0.395746	2.782900	-0.895531
H	2.350600	4.098475	-1.678282
H	2.337836	-4.275414	2.050232
H	0.381908	-2.921673	1.339497
Ni	-0.064747	-0.074155	0.180937
N	-1.638598	-1.318070	-0.067641
N	-1.568319	1.190009	0.669535
C	-1.598409	-2.571877	-0.566503
C	-2.878233	-0.724968	0.082242
C	-1.449995	2.439329	1.169193
C	-2.837590	0.645016	0.592391
C	-2.724609	-3.318495	-0.918724
H	-0.601577	-2.995368	-0.694903
C	-4.064986	-1.400066	-0.269304
C	-2.524698	3.229151	1.585624
H	-0.430417	2.822572	1.237328
C	-3.975807	1.372709	0.993095
C	-3.997854	-2.708136	-0.769739
H	-2.601745	-4.328968	-1.303099
C	-3.828985	2.676780	1.488797
H	-2.341251	4.230355	1.970882
H	-4.970469	0.930389	0.945560
H	-5.035275	-0.911925	-0.183727
H	4.874998	0.779246	-0.466844
H	4.880903	-0.997932	0.765158
O	-4.972331	3.319453	1.860162
O	-5.182905	-3.298652	-1.096196
O	4.951583	-3.341964	1.791223
O	4.951533	3.113628	-1.517163
C	-4.849228	4.646064	2.414435
H	-5.874628	4.961217	2.645686
H	-4.243939	4.629757	3.336172
H	-4.399589	5.336282	1.681311
C	-5.139952	-4.626280	-1.660399
H	-6.185622	-4.889838	-1.863979
H	-4.560403	-4.633719	-2.598558
H	-4.703666	-5.341999	-0.943656
C	4.870243	4.425191	-2.112964
H	4.444421	5.151763	-1.400917
H	5.904996	4.699337	-2.354860
H	4.263368	4.400464	-3.033404
C	4.870162	-4.660754	2.371635
H	4.410619	-5.370507	1.663653
H	5.907843	-4.953206	2.576347
H	4.293159	-4.640106	3.311149
C	-1.150758	-0.453701	-7.421123
C	-0.113868	0.247099	-8.065710
C	0.907331	0.849849	-7.306988
C	0.896541	0.755762	-5.898071
C	-0.145403	0.053589	-5.292491
C	-1.172436	-0.556244	-6.012627
H	-1.945712	-0.922748	-8.008127
H	-0.101639	0.323005	-9.155542
H	1.714927	1.393906	-7.805191
H	1.685944	1.222636	-5.303873
H	-1.975828	-1.098488	-5.508200
Br	-0.165501	-0.080263	-3.014969

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LDTS_Br

N	-2.307984	-0.700853	-1.342231
N	-1.064525	1.471963	-0.201297
C	-3.026609	-1.552022	-2.088917
C	-4.369842	-1.868180	-1.837451
C	-4.999267	-1.241192	-0.739040
C	-1.376521	1.851606	2.587353
C	-0.358918	2.526633	1.876945
C	-0.259830	2.296216	0.499174
C	-2.915412	-0.085562	-0.293009
C	-4.256407	-0.328338	0.038377
C	-2.251506	1.012693	1.869903
C	-2.066472	0.853158	0.489444
H	-2.496666	-1.998743	-2.933136

H -4.892269 -2.571281 -2.483801
H 0.345555 3.197579 2.365869
H 0.532034 2.784484 -0.073786
Ni 0.020594 -0.178634 -1.586245
H 2.058923 1.512581 -3.150498
C 2.558578 1.333786 -2.197377
C 3.807031 1.898547 -1.919312
C 4.406605 1.608562 -0.672605
H 4.284876 2.535331 -2.661502
C 3.719289 0.771634 0.228642
C 2.464652 0.259997 -0.126873
N 1.884722 0.538417 -1.339388
C 1.655729 -0.616043 0.749532
N 0.499078 -1.081434 0.172487
C 2.013390 -0.939185 2.064596
C -0.280182 -1.904059 0.908993
C 1.180714 -1.785403 2.821204
H -1.187577 -2.254400 0.417351
C 0.007318 -2.293087 2.219612
H -0.674013 -2.960338 2.744438
H -3.031247 0.464381 2.399055
H -4.734580 0.193970 0.866922
H 2.916235 -0.537245 2.522373
H 4.181049 0.528753 1.184551
O -1.578191 1.931326 3.930940
O -6.290689 -1.436890 -0.366802
O 5.613970 2.075448 -0.259993
O 1.580215 -2.045797 4.094542
C -0.639972 2.711500 4.703928
H -0.658093 3.768138 4.390196
H -0.976415 2.624054 5.744714
H 0.379542 2.304164 4.598935
C -7.086947 -2.351504 -1.154117
H -8.079157 -2.349910 -0.686320
H -7.158887 -2.001879 -2.196843
H -6.655244 -3.365325 -1.124217
C 0.744631 -2.909860 4.896102
H 1.248748 -2.981897 5.867882
H -0.259414 -2.471986 5.020941
H 0.666258 -3.909004 4.436968
C 6.358244 2.913669 -1.172612
H 5.788430 3.825686 -1.414814
H 7.280495 3.176510 -0.639923
H 6.597042 2.361922 -2.096599
Br -0.150603 -0.203559 -4.115167

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OA1_Br
Ni -0.113593 -1.313561 -0.668338
N 1.792614 -1.132486 -0.489155
N 0.014337 0.590884 -1.507143
C 2.768704 -2.053796 -0.286901
C 4.103568 -1.731775 -0.020367
C 4.468629 -0.365721 0.023950
C -0.025778 3.304034 -0.659983
C -1.087245 2.769086 -1.424199
C -1.012301 1.425023 -1.808246
C 2.163966 0.198448 -0.490281
C 3.480321 0.604680 -0.230321
C 1.064321 2.468078 -0.344665
C 1.064302 1.139477 -0.790923
H 2.446811 -3.095553 -0.313268
H 4.820132 -2.531308 0.157669
H -1.951770 3.363816 -1.715320
H -1.821258 0.981233 -2.394080
C -2.095664 -0.534428 1.274380
C -2.643704 0.724732 1.028426
C -1.440469 -0.879549 2.460327
C -2.511708 1.702427 2.035936
H -3.138221 0.957276 0.086364
C -1.313026 0.117423 3.447802
H -1.030017 -1.877536 2.612530
C -1.844677 1.404106 3.236848
H -2.929966 2.697754 1.869253
H -0.788743 -0.118786 4.376746
H -1.740298 2.170719 4.007493
H 3.750200 1.660351 -0.249349
H 1.879602 2.852550 0.269106
O 5.724019 0.096851 0.276824
O 0.027979 4.580589 -0.179161
C 6.764628 -0.877987 0.502357
H 6.884641 -1.528896 -0.379613
H 7.679512 -0.295009 0.667173
H 6.540078 -1.488821 1.392409
C -1.083162 5.450773 -0.474480
H -2.020084 5.041790 -0.059818
H -0.844573 6.406462 0.009643
H -1.187334 5.595681 -1.562912
Br -2.322033 -2.005409 -0.179302

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OA2_Br
Ni 0.165396 -1.093158 0.199770
N 0.906635 0.786751 0.101388
N -1.583940 -0.044950 0.183812
C 2.207082 1.113561 -0.007233
C 2.661579 2.423666 -0.185095
C 1.700900 3.455229 -0.253700
C -3.828959 1.647499 0.323992
C -3.981717 0.244835 0.376768
C -2.830473 -0.544307 0.303016
C -0.027815 1.782378 0.036199
C 0.334674 3.120513 -0.137118
C -2.527834 2.181758 0.209773
C -1.432799 1.316389 0.146596
H 2.909582 0.283793 0.053459
H 3.729708 2.615386 -0.264206
H -4.953591 -0.234081 0.475426
H -2.904768 -1.631188 0.336145
C 0.448947 -1.558484 -1.813483
C 1.832265 -1.821863 -1.912466
C -0.193475 -0.626324 -2.658880
C 2.607766 -0.995258 -2.746285
H 2.291985 -2.611506 -1.320152
C 0.603869 0.183556 -3.480464
H -1.273761 -0.495425 -2.618669
C 2.003645 0.012140 -3.519468
H 3.688192 -1.152922 -2.789636
H 0.125128 0.951144 -4.093685
H 2.613514 0.644712 -4.167764
S 1.411644 -2.277493 1.769234
C 1.541611 -1.056622 3.053618
F 2.534920 -0.098913 2.860937
F 0.390147 -0.308116 3.274282
F 1.840395 -1.614631 4.290095
H -0.412150 3.910795 -0.192388
H -2.397966 3.262314 0.183590
O 1.980755 4.767315 -0.433537
O -4.840923 2.543581 0.378172
C 3.370912 5.150696 -0.560925
H 3.831840 4.649127 -1.427107
H 3.357909 6.236433 -0.715503
H 3.924096 4.902698 0.359289
C -6.190751 2.034700 0.510497
H -6.833451 2.922980 0.531018
H -6.447505 1.397732 -0.351165
H -6.295414 1.466583 1.448500
Br -0.778114 -3.255413 -1.166909

12
PhBr
C 0.132997 0.000000 0.000008
C 0.806913 1.228386 0.000093
C 2.214858 1.216655 0.000273
C 2.919701 0.000000 0.000362
C 2.214858 -1.216655 0.000272
C 0.806913 -1.228386 0.000092
H 0.261014 2.172228 0.000025
H 2.753022 2.167019 0.000343
H 4.011577 0.000000 0.000502
H 2.753023 -2.167019 0.000342
H 0.261014 -2.172228 0.000024
Br -1.846203 0.000000 -0.000224

12
PhBr_rad
C 0.741793 0.001152 0.003369
C 1.402958 1.226760 0.002088
C 2.818644 1.221276 -0.000788
C 3.519514 -0.001141 -0.002225
C 2.816614 -1.222394 -0.000786
C 1.400929 -1.225544 0.002090
H 0.856853 2.174941 0.003122
H 3.367533 2.168355 -0.001936
H 4.612684 -0.002057 -0.004512
H 3.363929 -2.170384 -0.001931
H 0.853263 -2.172808 0.003134
Br -2.550199 0.000037 -0.000582

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RE2_Br

Ni	-0.518270	-0.590722	-0.766845
N	1.483816	-0.397554	-0.468460
N	-0.375949	1.446521	-0.512578
C	2.356047	-1.420754	-0.435190
C	3.694703	-1.278772	-0.058161
C	4.149877	0.008054	0.303101
C	0.095038	4.199778	-0.179957
C	-1.184461	3.728760	-0.546114
C	-1.358904	2.350278	-0.693852
C	1.917326	0.849059	-0.119178
C	3.238828	1.085857	0.268533
C	1.140008	3.264271	-0.017624
C	0.877291	1.905070	-0.203759
H	1.953042	-2.389744	-0.728966
H	4.345560	-2.150473	-0.052994
H	-2.027575	4.396038	-0.711283
H	-2.333175	1.945837	-0.965141
C	-0.872633	-1.542380	0.979483
C	-0.609785	-0.717606	2.094163
C	-0.510064	-2.908307	0.995907
C	0.105939	-1.244857	3.183469
H	-0.901459	0.330353	2.093961
C	0.205194	-3.416547	2.092050
H	-0.752364	-3.546661	0.146618
C	0.519122	-2.589657	3.188251
H	0.344053	-0.591590	4.026949
H	0.508567	-4.466543	2.088262
H	1.069181	-2.992670	4.041436
S	-2.637898	-1.208350	-0.287516
C	-3.589453	-0.279791	0.974234
F	-3.734618	-0.951118	2.157598
F	-3.104162	0.956760	1.292926
F	-4.856258	-0.086883	0.482179
H	3.581133	2.080343	0.548897
H	2.136746	3.622460	0.234255
O	5.411970	0.305790	0.689257
O	0.417620	5.496629	0.022604
C	6.374178	-0.775096	0.751665
H	6.512321	-1.224261	-0.244916
H	7.307813	-0.310408	1.090573
H	6.045237	-1.540569	1.472649
C	-0.620206	6.491236	-0.160896
H	-0.138991	7.452981	0.053308
H	-0.989120	6.472496	-1.198769
H	-1.450158	6.315385	0.541919
Br	-0.377074	-2.194619	-2.716672

Substrate: Chlorobenzene

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A2_Cl

N	-0.363289	0.973281	-0.295551
C	-2.794852	-2.154243	-0.230887
C	-4.179873	-2.124038	-0.037221
C	-4.797209	-0.869535	0.157751
C	-1.113271	3.672963	0.077268
C	0.236296	3.324738	-0.146666
C	0.548453	1.972928	-0.324213
C	-2.612430	0.164778	-0.051567
C	-3.989947	0.287626	0.149463
C	-2.077816	2.643744	0.114709
C	-1.677194	1.318053	-0.073951
H	-2.278902	-3.103312	-0.381403
H	-4.742604	-3.055746	-0.041167
H	1.031729	4.067074	-0.182459
H	1.579354	1.663493	-0.495661
H	3.355132	-2.136508	2.055229
C	2.656072	-2.274382	1.228737
C	1.714812	-3.362485	1.248640
C	2.675295	-1.430503	0.135585
C	0.849618	-3.570669	0.186659
C	1.763746	-1.536910	-0.981071
C	0.816780	-2.668975	-0.946862
H	0.182065	-4.437540	0.189982
H	2.092722	-1.117397	-1.940844
H	0.424953	-3.066768	-1.894277
H	1.711052	-4.037175	2.108703
H	-4.456731	1.259707	0.302141
H	-3.121267	2.901900	0.290936
O	-6.125844	-0.675135	0.356969
O	-1.574055	4.935860	0.263659
C	-0.609391	6.012922	0.245503
H	-0.101002	6.060874	-0.731216
H	-1.191584	6.927291	0.413331
H	0.131573	5.880875	1.050839
C	-6.978451	-1.842506	0.381804
H	-6.692863	-2.512510	1.209360
H	-7.993029	-1.457102	0.540947
H	-6.924186	-2.382145	-0.577748
Cl	3.908147	-0.131976	0.066207

39
A3_Cl

N	-1.251384	-0.953708	0.027127
C	0.429862	2.628903	0.014842
C	-0.247582	3.848278	-0.021139
C	-1.657413	3.835421	-0.050649
C	-4.016539	-1.501857	0.053266
C	-3.073054	-2.551196	0.049644
C	-1.715119	-2.220173	0.038207
C	-1.560501	1.409359	0.005064
C	-2.310430	2.586287	-0.034733
C	-3.544635	-0.172280	0.039016
C	-2.167527	0.063478	0.023239
H	1.515965	2.616033	0.034486
H	0.330385	4.769992	-0.027964
H	-3.367065	-3.598743	0.057769
H	-0.953700	-2.999519	0.039153
C	2.421001	0.392819	0.099974
C	3.024108	0.721555	1.333418
C	3.111462	0.689043	-1.095205
C	4.283661	1.354707	1.370613
H	2.512275	0.492784	2.272732
C	4.370682	1.322691	-1.058871
H	2.668745	0.432578	-2.061993
C	4.960317	1.660239	0.174366
H	4.735364	1.605425	2.335299
H	4.890846	1.547776	-1.994938
H	5.937456	2.149484	0.203056
H	-3.398070	2.557829	-0.058688
H	-4.263898	0.644599	0.045660
O	-2.450940	4.929091	-0.093876
O	-5.359752	-1.661167	0.070883
C	-1.811177	6.228601	-0.125069
H	-2.632604	6.954613	-0.151708
H	-1.201150	6.377911	0.779909
H	-1.186113	6.326075	-1.027102
C	-5.880299	-3.012542	0.108152
H	-6.970878	-2.900403	0.128951
H	-5.571976	-3.568453	-0.791799
H	-5.532300	-3.532216	1.015146
Cl	1.588357	-2.351320	0.059383

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ADTS_Cl

N	2.374891	1.063159	-0.374753
N	1.957155	-1.505812	0.219688
C	2.579725	2.385164	-0.581457
C	3.825565	3.012594	-0.566406
C	4.969803	2.221589	-0.294933
C	3.947189	-3.478396	-0.245363
C	2.622801	-3.847628	0.099394
C	1.690341	-2.827869	0.297233
C	3.503065	0.285743	-0.181445
C	4.792190	0.843351	-0.104970
C	4.249885	-2.112382	-0.351204
C	3.253782	-1.153590	-0.092546
H	1.685459	2.973996	-0.781457
H	3.891514	4.080858	-0.763628
H	2.321454	-4.886513	0.219006
H	0.660603	-3.092685	0.545076
Ni	0.579294	0.154617	0.045722
N	-0.751510	1.791108	-0.136383
N	-0.827702	-0.635982	-1.221648
C	-0.555891	3.069211	0.247794
C	-1.773962	1.560661	-1.027770
C	-0.899265	-1.909746	-1.669312
C	-1.931961	0.163438	-1.441564
C	-1.320602	4.157429	-0.177483
H	0.249429	3.221172	0.966064
C	-2.579167	2.596623	-1.533360
C	-2.010895	-2.471733	-2.299479
H	-0.004420	-2.513050	-1.520856
C	-3.106120	-0.330895	-2.032518
C	-2.367722	3.914628	-1.099598
H	-1.111518	5.150882	0.214868
C	-3.159801	-1.662814	-2.471496
H	-1.970582	-3.504269	-2.640727
H	-3.985134	0.303827	-2.138722
H	-3.347823	2.394679	-2.278796
H	5.656491	0.217185	0.114923
H	5.250665	-1.809058	-0.657136
O	-4.329498	-2.072856	-3.032075
O	-3.185134	4.868500	-1.623790
O	4.958603	-4.350040	-0.506549
O	6.242472	2.694156	-0.197995
C	-4.414122	-3.445136	-3.457033
H	-5.431144	-3.570170	-3.850213
H	-3.678343	-3.658689	-4.250740
H	-4.252636	-4.131331	-2.608758
C	-2.956487	6.230138	-1.219121
H	-3.700393	6.827879	-1.761223
H	-3.102260	6.350553	-0.132451
H	-1.939611	6.559028	-1.493616
C	6.435288	4.112225	-0.346873
H	5.866536	4.669877	0.416497
H	7.510778	4.279655	-0.205660
H	6.133377	4.451093	-1.352223
C	4.660312	-5.755507	-0.420689
H	3.862368	-6.033525	-1.129900
H	5.591589	-6.271397	-0.687481
H	4.358517	-6.033967	0.602949
H	-0.209989	-1.685182	1.775605
C	-0.397727	-0.637221	1.992498
C	-1.718621	-0.211531	2.246102
C	0.675053	0.250875	2.323168
C	-2.015686	1.050378	2.771809
C	0.383260	1.497334	2.935922
H	1.693565	-0.135548	2.366782
C	-0.945471	1.898865	3.128741
H	-1.167192	2.875462	3.565844
H	-3.050078	1.359040	2.927771
H	1.203791	2.153199	3.236292
Cl	-3.055360	-1.319886	1.838867

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B1T_Cl

N	1.588762	1.251502	-0.207892
N	1.664290	-1.307450	0.328426
C	1.483636	2.543938	-0.586329
C	2.565796	3.389582	-0.841457
C	3.874165	2.846208	-0.711919
C	4.005577	-2.722623	1.050660
C	2.732993	-3.354421	1.095749
C	1.617216	-2.594742	0.732714
C	2.866804	0.720528	-0.080336
C	4.015001	1.504958	-0.336124
C	4.081678	-1.379875	0.659766

C	2.904023	-0.682237	0.306004
H	0.465029	2.916429	-0.704554
H	2.386788	4.422068	-1.135301
H	2.603755	-4.390895	1.400647
H	0.621573	-3.041000	0.763149
Ni	0.103011	-0.121602	-0.133312
N	-1.242172	-1.405093	-0.920636
N	-1.571219	0.977994	0.107186
C	-0.985353	-2.593216	-1.505116
C	-2.528465	-0.897058	-1.032949
C	-1.688446	2.171627	0.725709
C	-2.723244	0.405542	-0.415722
C	-1.926194	-3.356071	-2.201915
H	0.042367	-2.946719	-1.418845
C	-3.535882	-1.600573	-1.729304
C	-2.880028	2.894953	0.838356
H	-0.766543	2.572659	1.151256
C	-3.970105	1.066376	-0.334112
C	-3.241908	-2.834905	-2.319193
H	-1.629908	-4.305038	-2.644929
C	-4.055590	2.321337	0.280801
H	-2.881242	3.857601	1.345710
H	-4.872192	0.611125	-0.742068
H	-4.536042	-1.182842	-1.839437
H	5.013825	1.075346	-0.263210
H	5.051092	-0.882108	0.654303
O	-5.289452	2.907135	0.307551
O	-4.258769	-3.447911	-2.996194
O	5.182217	-3.331345	1.382065
O	5.025681	3.542354	-0.945262
C	-5.403583	4.204387	0.926433
H	-6.459448	4.485830	0.824362
H	-5.129739	4.155161	1.993638
H	-4.765768	4.941851	0.410821
C	-3.974096	-4.711632	-3.627920
H	-4.911047	-5.015609	-4.112290
H	-3.178413	-4.602733	-4.384120
H	-3.676385	-5.465389	-2.879771
C	4.904480	4.926174	-1.332470
H	4.400810	5.509828	-0.543769
H	5.933374	5.285134	-1.463755
H	4.349129	5.019882	-2.280834
C	5.128503	-4.709087	1.805645
H	4.719792	-5.349521	1.006259
H	6.168192	-4.989969	2.017152
H	4.518130	-4.812779	2.718432
C	-1.195797	1.543697	-3.257684
C	-2.332683	1.111579	-3.959298
C	-2.297754	-0.100368	-4.672396
C	-1.127821	-0.882625	-4.690028
C	-0.005879	-0.427682	-3.983148
C	-0.018780	0.773907	-3.259481
H	-1.221706	2.472988	-2.685694
H	-3.247585	1.707305	-3.937227
H	-3.181578	-0.450734	-5.209922
H	-1.096818	-1.827956	-5.232887
H	0.860818	1.093545	-2.706151
Cl	1.474439	-1.405390	-3.980059

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B2_Cl

N	1.492655	1.176976	-0.256823
N	1.485033	-1.261151	0.683034
C	1.402173	2.390397	-0.840161
C	2.504229	3.124688	-1.287624
C	3.787705	2.559005	-1.128106
C	3.787926	-2.699229	1.445605
C	2.500583	-3.246152	1.641576
C	1.396505	-2.485604	1.245497
C	2.738896	0.623919	-0.112420
C	3.896357	1.284796	-0.531028
C	3.896063	-1.417247	0.865967
C	2.736634	-0.729738	0.497530
H	0.392117	2.783397	-0.959228
H	2.347716	4.093346	-1.757605
H	2.344590	-4.226892	2.086411
H	0.384961	-2.870756	1.381524
Ni	-0.046920	-0.037920	0.203556
N	-1.592348	-1.260337	-0.208228
N	-1.570221	1.186178	0.703290
C	-1.511698	-2.488683	-0.761166
C	-2.837975	-0.721543	-0.013638
C	-1.471752	2.427340	1.226322
C	-2.825243	0.651201	0.552298
C	-2.623136	-3.253102	-1.127523
H	-0.502401	-2.868402	-0.922484
C	-4.004614	-1.416688	-0.342761
C	-2.568540	3.201476	1.616005
H	-0.457833	2.814552	1.335857
C	-3.978154	1.355096	0.910518
C	-3.906038	-2.706018	-0.908152
H	-2.474708	-4.232270	-1.577995
C	-3.859506	2.652843	1.451666
H	-2.404692	4.194563	2.029568
H	-4.969883	0.922752	0.787095
H	-4.990620	-0.979952	-0.191913
H	4.880056	0.828709	-0.430330
H	4.883914	-0.980958	0.725440
O	-5.018913	3.273356	1.780849
O	-5.077114	-3.319465	-1.206695
O	4.952960	-3.306494	1.779529
O	4.949325	3.140918	-1.513504
C	-4.938127	4.603506	2.344026
H	-5.976570	4.900184	2.535438
H	-4.367446	4.590385	3.286874
H	-4.470372	5.297851	1.627185
C	-5.016416	-4.637144	-1.801634
H	-6.060765	-4.926603	-1.970795
H	-4.471578	-4.603853	-2.758703
H	-4.530974	-5.347941	-1.112987
C	4.876787	4.445504	-2.135003
H	4.434099	5.178468	-1.440844
H	5.915555	4.716245	-2.360242
H	4.287289	4.398216	-3.064637
C	4.883842	-4.630008	2.359694
H	4.414171	-5.335018	1.654584
H	5.925351	-4.918658	2.546650
H	4.320483	-4.608885	3.306741
Cl	-0.067556	-0.061267	-4.010004

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B3_Cl

C	-0.631805	-2.652854	0.008287
C	-1.867801	-3.305401	0.006385
C	-3.039725	-2.516491	0.003288
C	-2.017341	3.253235	-0.000154
C	-0.645644	3.591612	0.001397
C	0.290575	2.553463	0.003995
C	-1.633664	-0.542264	0.004452
C	-2.908710	-1.111587	0.002427
C	-2.378029	1.889030	0.000765
C	-1.376032	0.916341	0.003372
H	0.297467	-3.224279	0.010683
H	-1.899709	-4.393259	0.007382
H	-0.302141	4.624321	0.000734
H	1.359993	2.769885	0.005340
Ni	1.201643	-0.298826	0.009397
H	-3.432326	1.616010	-0.000455
H	-3.804125	-0.492104	0.000091
O	-3.038405	4.143302	-0.002454
O	-4.304506	-3.001830	0.001029
C	-2.705133	5.551430	-0.003658
H	-2.128905	5.810442	-0.906649
H	-3.667601	6.077331	-0.005695
H	-2.131537	5.812613	0.900383
C	-4.475630	-4.438804	0.000848
H	-5.560482	-4.600376	-0.001257
H	-4.024101	-4.880604	-0.902030
H	-4.027712	-4.880457	0.905589
Cl	3.386998	-0.536208	0.014711

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B5_Cl

Ni	-0.504010	-0.208779	-0.074185
N	1.339809	-0.999470	-0.356296
N	0.589513	1.482445	-0.055176
C	1.634735	-2.303925	-0.527313
C	2.928981	-2.786236	-0.741449
C	3.988656	-1.852539	-0.781688
C	2.329993	3.693695	0.061770
C	0.936142	3.865918	0.215416
C	0.122781	2.731832	0.149836
C	2.366404	-0.093772	-0.394293
C	3.692732	-0.485409	-0.603495
C	2.831130	2.391780	-0.144844
C	1.943329	1.312859	-0.197171
H	0.788053	-2.990030	-0.485644
H	3.090272	-3.855423	-0.864390
H	0.483086	4.840428	0.385155
H	-0.957502	2.821045	0.271474
S	-1.666418	-1.063181	1.675576

C -0.361384 -1.535001 2.792744
F 0.373570 -2.647261 2.396362
F 0.596066 -0.555767 3.026795
F -0.835366 -1.868278 4.056876
H 4.503037 0.241630 -0.629895
H 3.904440 2.246521 -0.256210
O 5.292219 -2.162767 -0.984269
O 3.245827 4.690446 0.099987
C 5.635136 -3.557811 -1.159075
H 5.116176 -3.975701 -2.036983
H 6.719964 -3.570715 -1.320181
H 5.376783 -4.133899 -0.255788
C 2.766168 6.042411 0.295839
H 3.664318 6.671678 0.287827
H 2.090026 6.332710 -0.524497
H 2.247974 6.130524 1.264162
H -0.502310 -1.882486 -3.243812
C -1.300591 -1.417629 -2.662381
C -2.475665 -2.122006 -2.386972
C -1.135717 -0.084698 -2.186984
C -3.539756 -1.517364 -1.670561
H -2.594053 -3.149425 -2.738593
C -2.184969 0.526152 -1.432092
H -0.315130 0.528949 -2.563507
C -3.381415 -0.207629 -1.219431
H -4.460971 -2.067174 -1.475230
H -2.155821 1.590802 -1.201386
Cl -4.702930 0.580180 -0.343372

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B6_Cl
Ni -0.677763 -0.329195 0.337050
N 0.218251 1.425033 -0.081770
N 1.292799 -0.965216 0.156242
C -0.389599 2.628847 -0.083822
C 0.276315 3.827407 -0.342891
C 1.659809 3.775549 -0.615874
C 3.999456 -1.567229 -0.298798
C 3.095160 -2.575712 0.097087
C 1.761354 -2.216523 0.308182
C 1.567733 1.369536 -0.313983
C 2.306842 2.520905 -0.592010
C 3.517690 -0.248206 -0.451838
C 2.167826 0.017167 -0.213100
H -1.456054 2.626802 0.130692
H -0.281785 4.760742 -0.325679
H 3.399364 -3.610522 0.238068
H 1.026185 -2.963797 0.607982
C -2.431039 0.326971 -0.111048
C -2.586149 0.594253 -1.481891
C -3.443642 0.640316 0.805334
C -3.767353 1.215213 -1.936795
H -1.800581 0.339761 -2.197426
C -4.619772 1.265475 0.341450
H -3.322138 0.410143 1.863693
C -4.783596 1.554521 -1.025751
H -3.883322 1.429990 -3.002583
H -5.408662 1.516589 1.055675
H -5.699074 2.034572 -1.379761
S -1.652264 -2.368571 0.504466
C -1.694469 -2.887313 -1.217057
F -2.873937 -2.609149 -1.874280
F -0.705049 -2.327338 -2.002606
F -1.534836 -4.252942 -1.322694
H 3.378121 2.476015 -0.778547
H 4.209076 0.535874 -0.753356
O 2.436337 4.842702 -0.894007
O 5.313150 -1.754558 -0.548067
C 1.807181 6.149300 -0.930694
H 1.370424 6.390515 0.051061
H 2.614974 6.850446 -1.171060
H 1.031187 6.175843 -1.711794
C 5.848356 -3.094721 -0.406071
H 6.913865 -3.005972 -0.648699
H 5.721401 -3.450468 0.628589
H 5.351941 -3.781103 -1.110129
Cl -0.633434 0.032562 2.697526

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HAT_B
N 1.520346 1.216798 -0.112078
N 1.497866 -1.274229 0.685982
C 1.450124 2.455697 -0.642921
C 2.556018 3.206490 -1.048669
C 3.841900 2.615824 -0.914924
C 3.800000 -2.727849 1.450648
C 2.503785 -3.292364 1.597159
C 1.408934 -2.516838 1.206641
C 2.772645 0.636953 0.013784
C 3.941051 1.322971 -0.384475
C 3.919488 -1.432723 0.928909
C 2.761491 -0.718413 0.551950
H 0.443450 2.862341 -0.751879
H 2.409617 4.203850 -1.458287
H 2.341943 -4.290009 2.000364
H 0.395545 -2.908231 1.313904
Ni -0.029049 -0.017490 0.258491
N -1.590602 -1.246078 -0.083928
N -1.542715 1.236334 0.737084
C -1.534763 -2.478713 -0.630310
C -2.837383 -0.659912 0.061997
C -1.438117 2.471313 1.272789
C -2.811201 0.689900 0.614492
C -2.649979 -3.217092 -1.033232
H -0.532262 -2.890675 -0.755551
C -4.014783 -1.333141 -0.330679
C -2.522789 3.249224 1.686530
H -0.420507 2.853681 1.372644
C -3.959415 1.407093 1.014055
C -3.930363 -2.619988 -0.878206
H -2.514357 -4.210382 -1.456145
C -3.824582 2.695744 1.548318
H -2.349504 4.240512 2.100672
H -4.952267 0.965106 0.933327
H -4.989937 -0.855155 -0.240788
H 4.920569 0.851064 -0.311481
H 4.908391 -0.983321 0.841579
O -4.976753 3.327344 1.916321
O -5.106953 -3.207163 -1.244826
O 4.960736 -3.355028 1.799158
O 5.010581 3.215755 -1.286059
C -4.867521 4.647183 2.487997
H -5.897564 4.955645 2.707785
H -4.276120 4.623548 3.418593
H -4.409930 5.347984 1.769817
C -5.047189 -4.524874 -1.828340
H -6.088582 -4.794472 -2.046065
H -4.459348 -4.514604 -2.761471
H -4.611568 -5.247908 -1.118450
C 4.934894 4.535304 -1.863415
H 4.498071 5.251717 -1.147606
H 5.972297 4.815082 -2.087277
H 4.340674 4.523473 -2.792490
C 4.866688 -4.678035 2.366247
H 4.407984 -5.379437 1.649349
H 5.900977 -4.979515 2.575591
H 4.283263 -4.662657 3.302049
C -1.343204 -0.813200 -6.952630
C -0.369376 -0.165577 -7.735682
C 0.684055 0.535488 -7.119451
C 0.774490 0.596458 -5.712129
C -0.212328 -0.060795 -4.982995
C -1.272675 -0.767006 -5.543797
H -2.162482 -1.356796 -7.430016
H -0.431338 -0.207035 -8.825257
H 1.441388 1.038172 -7.726486
H 1.585573 1.135719 -5.220027
H -2.019834 -1.264228 -4.922928
Cl -0.096366 0.007493 -2.908155

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LDTS_Cl
N 1.812846 1.414059 -1.821679
N 1.510895 -1.046229 -0.625856
C 2.136007 2.464891 -2.590280
C 3.264296 3.271587 -2.380383
C 4.112259 2.946402 -1.298899
C 2.127908 -1.299832 2.123291
C 1.400903 -2.308232 1.452027
C 1.126403 -2.119755 0.091482
C 2.634745 1.092693 -0.786628
C 3.790353 1.832745 -0.495973
C 2.554537 -0.176582 1.387550
C 2.236951 -0.091254 0.024124
H 1.455307 2.675019 -3.418027
H 3.463241 4.111048 -3.044456
H 1.049291 -3.206500 1.957284
H 0.548263 -2.870962 -0.452232
Ni -0.138290 0.014833 -2.008584
N -1.643553 -1.301269 -1.715100
N -0.921958 0.770461 -0.294948

C	-1.984317	-2.327775	-2.523554
C	-2.291586	-1.187640	-0.510324
C	-0.496857	1.855139	0.390837
C	-1.855106	-0.036801	0.310220
C	-2.954558	-3.282853	-2.204718
H	-1.444135	-2.370068	-3.470246
C	-3.281528	-2.095643	-0.113088
C	-0.930825	2.193219	1.674891
H	0.239166	2.474491	-0.120628
C	-2.333822	0.217429	1.602016
C	-3.623216	-3.164050	-0.965102
H	-3.172304	-4.083757	-2.909031
C	-1.867269	1.343508	2.305918
H	-0.537570	3.085874	2.157841
H	-3.055611	-0.444478	2.078258
H	-3.798006	-1.992657	0.840213
H	4.455340	1.544966	0.318114
H	3.096221	0.624845	1.890278
O	-2.363183	1.523239	3.558753
O	-4.588189	-4.008492	-0.515458
O	2.446527	-1.315072	3.445869
O	5.242169	3.621593	-0.964824
C	-1.901423	2.671877	4.304217
H	-2.415648	2.616093	5.271599
H	-0.809800	2.625669	4.451830
H	-2.173561	3.605512	3.784739
C	-4.959945	-5.115522	-1.367056
H	-5.736485	-5.659731	-0.815391
H	-5.363544	-4.748704	-2.325049
H	-4.093235	-5.771714	-1.549922
C	5.629907	4.737240	-1.798234
H	4.854555	5.520466	-1.783072
H	6.560409	5.118008	-1.359437
H	5.807251	4.402142	-2.833238
C	2.009308	-2.448975	4.226453
H	2.457412	-3.380167	3.842306
H	2.362473	-2.253679	5.246752
H	0.909542	-2.526828	4.215040
Cl	0.172724	-0.221070	-4.343587

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OA1_Cl

Ni	-1.084488	0.715433	0.745284
N	0.804698	0.489389	0.705050
N	-0.731837	2.102950	-0.627118
C	1.523714	-0.395531	1.434202
C	2.911938	-0.522893	1.341551
C	3.604688	0.315385	0.440383
C	0.133776	4.013522	-2.505664
C	-1.238658	3.870583	-2.205404
C	-1.610494	2.905848	-1.263125
C	1.478741	1.308163	-0.173311
C	2.864510	1.242351	-0.324918
C	1.063227	3.178206	-1.847959
C	0.602111	2.239407	-0.923226
H	0.945409	-1.021142	2.114690
H	3.420701	-1.260231	1.959611
H	-2.003510	4.483658	-2.678240
H	-2.659992	2.762488	-0.998145
C	-1.754015	-0.773938	2.279744
C	-1.549169	-0.434447	3.640080
C	-1.738263	-2.139128	1.901417
C	-1.380957	-1.444559	4.604492
H	-1.536066	0.615310	3.945294
C	-1.569469	-3.141299	2.874357
H	-1.870439	-2.417261	0.852383
C	-1.395161	-2.805090	4.232891
H	-1.226246	-1.164092	5.651215
H	-1.561966	-4.191216	2.564874
H	-1.267060	-3.586798	4.985538
H	3.385801	1.892666	-1.025960
H	2.124082	3.281249	-2.071681
O	4.945127	0.309150	0.241537
O	0.648771	4.902620	-3.388437
C	5.736973	-0.627552	1.009682
H	5.445799	-1.663524	0.772010
H	6.774956	-0.446422	0.705265
H	5.619235	-0.437472	2.088764
C	-0.273320	5.768599	-4.091559
H	-0.836052	6.392745	-3.378839
H	0.354795	6.399152	-4.732554
H	-0.967686	5.172791	-4.705836
Cl	-3.346164	0.333194	1.378314

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OA2_Cl

Ni	0.145186	-1.091118	0.186512
N	0.881527	0.793620	0.148454
N	-1.612451	-0.031255	0.157920
C	2.183244	1.116262	0.043008
C	2.642263	2.426296	-0.120283
C	1.685187	3.462319	-0.177049
C	-3.853813	1.656742	0.343762
C	-4.009302	0.253305	0.342165
C	-2.858890	-0.535078	0.246851
C	-0.050037	1.791832	0.085904
C	0.317318	3.130541	-0.070079
C	-2.551206	2.194042	0.257380
C	-1.458031	1.328587	0.170981
H	2.882418	0.282692	0.092484
H	3.711081	2.615218	-0.196438
H	-4.983094	-0.226068	0.415660
H	-2.933244	-1.622690	0.236793
C	0.528942	-1.467870	-1.783448
C	1.890245	-1.798476	-1.937492
C	-0.135804	-0.606436	-2.680783
C	2.634601	-1.112455	-2.914929
H	2.360860	-2.532184	-1.284077
C	0.630447	0.064808	-3.646434
H	-1.204599	-0.421758	-2.582736
C	2.014954	-0.176363	-3.762999
H	3.702119	-1.325229	-3.011995
H	0.137090	0.777527	-4.312169
H	2.598501	0.344010	-4.525263
S	1.441993	-2.219098	1.790974
C	1.557795	-0.984089	3.061455
F	2.567030	-0.040344	2.884314
F	0.410211	-0.220261	3.245471
F	1.818827	-1.531900	4.311293
H	-0.427718	3.922690	-0.124446
H	-2.419055	3.274538	0.273018
O	1.969822	4.774922	-0.339834
O	-4.865140	2.550524	0.426289
C	3.361729	5.155591	-0.459809
H	3.823107	4.662155	-1.330301
H	3.352041	6.242959	-0.602348
H	3.911470	4.895635	0.459087
C	-6.215321	2.038522	0.547152
H	-6.857011	2.926426	0.594891
H	-6.474774	1.426963	-0.331838
H	-6.317635	1.444190	1.469037
Cl	-0.653191	-3.022634	-1.006367

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PhCl

C	-0.505159	0.000000	-0.000068
C	0.178148	1.226525	0.000019
C	1.584197	1.216155	0.000199
C	2.289805	0.000000	0.000288
C	1.584197	-1.216155	0.000198
C	0.178148	-1.226525	0.000018
H	-0.371774	2.168717	-0.000048
H	2.122834	2.166132	0.000269
H	3.381663	0.000000	0.000427
H	2.122834	-2.166132	0.000268
H	-0.371774	-2.168717	-0.000049
Cl	-2.278812	0.000000	-0.000282

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PhCl_rad

C	-0.487852	0.000000	-0.000080
C	0.153054	1.245925	-0.000013
C	1.626011	1.234869	0.000198
C	2.303619	0.000000	0.000286
C	1.626011	-1.234870	0.000198
C	0.153054	-1.245924	-0.000014
H	-0.413271	2.178342	-0.000059
H	2.174939	2.180498	0.000276
H	3.401166	0.000000	0.000444
H	2.174938	-2.180499	0.000276
H	-0.413271	-2.178341	-0.000061
Cl	-2.303993	0.000000	-0.000254

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RE2_Cl

Ni	-0.515634	-0.604871	-0.804392
N	1.491384	-0.413079	-0.498910
N	-0.368334	1.431959	-0.538564
C	2.362754	-1.436838	-0.471687
C	3.700271	-1.298676	-0.088812
C	4.153536	-0.015767	0.288370

C	0.096162	4.177621	-0.138102
C	-1.177237	3.714707	-0.534279
C	-1.348694	2.339453	-0.714559
C	1.921944	0.828709	-0.130982
C	3.241406	1.061639	0.265467
C	1.140006	3.239185	0.014223
C	0.880979	1.884661	-0.205916
H	1.960371	-2.403731	-0.773089
H	4.351261	-2.170252	-0.091050
H	-2.018569	4.385106	-0.696400
H	-2.319034	1.941235	-1.007629
C	-0.866323	-1.504676	0.970497
C	-0.627892	-0.642688	2.061420
C	-0.486307	-2.863962	1.031577
C	0.084422	-1.125709	3.173270
H	-0.936799	0.399686	2.026041
C	0.226009	-3.327734	2.149363
H	-0.711917	-3.532630	0.201228
C	0.517775	-2.463222	3.222305
H	0.303837	-0.443731	3.998883
H	0.544650	-4.372724	2.180392
H	1.066061	-2.831811	4.092035
S	-2.642799	-1.229148	-0.314543
C	-3.616613	-0.307902	0.930573
F	-3.728814	-0.954192	2.131172
F	-3.172589	0.952757	1.215858
F	-4.893343	-0.171078	0.445543
H	3.581577	2.053018	0.559331
H	2.133169	3.591437	0.287500
O	5.414594	0.278662	0.679880
O	0.414624	5.468608	0.103572
C	6.379544	-0.800766	0.725357
H	6.515648	-1.236602	-0.277398
H	7.313069	-0.338314	1.067546
H	6.054515	-1.576397	1.437162
C	-0.621979	6.467218	-0.064532
H	-0.147245	7.421405	0.193424
H	-0.971002	6.484223	-1.109148
H	-1.464837	6.264673	0.615455
Cl	-0.387278	-2.184900	-2.562368

Substrate: 4-iodotoluene

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A2_pMe

Ni	-0.086027	-0.843607	-0.514308
N	-2.056051	-0.866553	-0.323619
N	-0.345856	1.106510	-0.296781
C	-2.888149	-1.929574	-0.412921
C	-4.278214	-1.851905	-0.281188
C	-4.854983	-0.585145	-0.045675
C	-1.000970	3.803164	0.246648
C	0.334430	3.423240	-0.007096
C	0.599321	2.074991	-0.269027
C	-2.624189	0.367597	-0.106968
C	-4.004582	0.537425	0.035483
C	-2.000295	2.807556	0.222499
C	-1.646965	1.483493	-0.051703
H	-2.405010	-2.888864	-0.595945
H	-4.875386	-2.758278	-0.361302
H	1.155866	4.137659	-0.003404
H	1.619166	1.743564	-0.462099
H	3.395326	-1.763064	2.176267
C	2.663885	-1.962530	1.391963
C	1.667387	-2.983570	1.588011
C	2.685943	-1.283623	0.192783
C	0.763597	-3.325773	0.592193
C	1.728719	-1.498279	-0.865491
C	0.758701	-2.594959	-0.665133
H	2.024026	-1.219083	-1.884720
H	0.367606	-3.130784	-1.543973
I	4.289839	0.179259	-0.169643
H	1.657548	-3.524680	2.538844
H	-4.440862	1.520608	0.206862
H	-3.032841	3.088905	0.424826
O	-6.183143	-0.348485	0.106630
O	-1.417432	5.066267	0.517994
C	-0.416689	6.109367	0.559049
H	0.087303	6.199849	-0.416955
H	-0.966415	7.030849	0.787170
H	0.322814	5.903109	1.350023
C	-7.074538	-1.486560	0.069077
H	-6.836247	-2.188021	0.885466
H	-8.080433	-1.071618	0.208036
H	-7.007510	-2.000751	-0.903561
C	-0.222031	-4.458231	0.782676
H	0.040299	-5.079950	1.654424
H	-1.245978	-4.075159	0.938458
H	-0.256326	-5.106108	-0.111955

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A3_pMe

Ni	-0.365023	-0.557315	0.005877
N	0.073016	1.351948	0.007765
N	1.662461	-0.725900	0.009577
C	-0.797771	2.390478	0.009039
C	-0.415941	3.732253	0.001145
C	0.959739	4.040552	-0.008409
C	4.487046	-0.594470	0.009318
C	3.821923	-1.837983	0.017598
C	2.424516	-1.841221	0.016849
C	1.416492	1.655274	0.000844
C	1.880200	2.972869	-0.007055
C	3.707483	0.580546	0.002218
C	2.313718	0.481394	0.003557
H	-1.852523	2.131216	0.016268
H	-1.186725	4.500123	0.002164
H	4.355268	-2.786662	0.024162
H	1.886951	-2.788132	0.021901
C	-2.229539	-0.230738	0.009177
C	-2.926576	-0.021200	-1.200824
C	-2.924602	-0.044441	1.222006
C	-4.272063	0.394395	-1.193758
H	-2.418936	-0.168047	-2.158432
C	-4.272068	0.370946	1.223191
H	-2.417196	-0.209564	2.176768
C	-4.967537	0.600274	0.017848
H	-4.789938	0.559122	-2.144720
H	-4.790395	0.516936	2.176650
I	-0.972523	-3.070151	-0.020753
H	2.945493	3.193658	-0.013128
H	4.210272	1.545595	-0.003636
O	1.480339	5.288191	-0.019007
O	5.828971	-0.425073	0.008052
C	0.556754	6.405023	-0.022508
H	1.187920	7.301636	-0.034670
H	-0.078682	6.374498	-0.922279
H	-0.066380	6.390378	0.886243
C	6.657821	-1.613314	0.013663
H	7.690969	-1.245999	0.010136
H	6.468350	-2.209028	0.920749
H	6.465710	-2.219209	-0.886102
C	-6.425263	1.020714	0.017148
H	-6.615314	1.814543	-0.725488
H	-7.086367	0.172690	-0.239221
H	-6.732909	1.393657	1.007954

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A4_pMe

Ni	0.333659	-0.481160	-0.290145
N	-0.482382	1.305397	-0.073567
N	-1.621056	-1.041470	-0.216754
C	0.161960	2.496392	-0.049275
C	-0.482226	3.733985	0.002251
C	-1.892170	3.756951	0.021062
C	-4.386073	-1.511832	0.112611
C	-3.485584	-2.585702	-0.047860
C	-2.128017	-2.292742	-0.202121
C	-1.857757	1.331156	-0.046332
C	-2.579015	2.525994	-0.008548
C	-3.871146	-0.198260	0.109618
C	-2.498366	-0.000190	-0.057582
H	1.247682	2.451750	-0.071175
H	0.118171	4.641163	0.021889
H	-3.810025	-3.624231	-0.050241
H	-1.403338	-3.098360	-0.316710
C	2.094573	0.188585	-0.154885
C	2.611061	0.462697	1.128349
C	2.867440	0.555797	-1.277317
C	3.861862	1.094481	1.283073
H	2.041348	0.190423	2.021116
C	4.110808	1.195958	-1.118091
H	2.504947	0.341322	-2.286371
C	4.631987	1.473499	0.164816
H	4.244665	1.292719	2.289679
H	4.691718	1.472198	-2.004608
S	1.112696	-2.453862	-0.916806
C	2.403046	-2.983212	0.210749
F	3.655376	-2.451487	-0.008671
F	2.138563	-2.745057	1.545049
F	2.582041	-4.355156	0.107997
H	-3.667196	2.527341	-0.007010
H	-4.553404	0.637279	0.255454
O	-2.657263	4.870372	0.062157
O	-5.721997	-1.632473	0.281691
C	-1.985468	6.153389	0.101072
H	-1.362684	6.288373	-0.797393
H	-2.789042	6.899345	0.120408
H	-1.367530	6.234359	1.009637
C	-6.278914	-2.969102	0.329201
H	-7.353184	-2.828495	0.497987
H	-6.108269	-3.491676	-0.625585
H	-5.832852	-3.538966	1.159749
C	5.975201	2.160114	0.326318
H	6.769718	1.620004	-0.217856
H	5.952047	3.189756	-0.074370
H	6.266732	2.216815	1.387785

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A5_pMe

Ni	-0.172144	-0.437584	0.905754
N	-1.125425	1.268481	0.580901
N	-1.841802	-1.217579	0.205976
C	-0.672960	2.528103	0.773938
C	-1.414982	3.679681	0.491161
C	-2.716876	3.520694	-0.030695
C	-4.365136	-2.043785	-0.760992
C	-3.377315	-2.993895	-0.423054
C	-2.146475	-2.526094	0.048277
C	-2.394100	1.118161	0.070969
C	-3.204165	2.213166	-0.241549
C	-4.063829	-0.673934	-0.606333
C	-2.807959	-0.294937	-0.124963
H	0.339280	2.608105	1.172409
H	-0.976270	4.658790	0.674254
H	-3.542598	-4.065408	-0.519426
H	-1.355052	-3.227025	0.314299
H	2.933755	-2.007859	-1.597533
C	2.572258	-1.573251	-0.663453
C	2.995211	-0.249519	-0.281896
C	1.726087	-2.291581	0.165604
C	2.534304	0.322303	0.903020

C	1.194416	-1.749438	1.403545
H	1.449430	-3.314572	-0.110064
C	1.610137	-0.380930	1.751106
H	2.886366	1.311807	1.205363
H	1.521680	-0.034492	2.789804
S	4.070763	0.693583	-1.354579
C	5.720236	0.106027	-0.800299
F	6.684546	0.766638	-1.510591
F	5.967070	0.333290	0.525980
F	5.923445	-1.233505	-0.993183
H	-4.204162	2.080500	-0.652192
H	-4.818965	0.066828	-0.865686
O	-5.603804	-2.337611	-1.231184
O	-3.557583	4.534603	-0.356620
C	-3.077406	5.888369	-0.188079
H	-2.182405	6.060291	-0.807964
H	-3.899848	6.531729	-0.523958
H	-2.848963	6.088278	0.871574
C	-5.943971	-3.732494	-1.403052
H	-5.889119	-4.264858	-0.439652
H	-6.974465	-3.735764	-1.778741
H	-5.270505	-4.205611	-2.136391
C	0.748958	-2.727789	2.485539
H	0.113549	-3.522884	2.058896
H	1.618934	-3.219937	2.964262
H	0.174712	-2.216104	3.274573

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ADTS_pMe

N	2.400206	0.867251	-0.709371
N	1.836801	-1.643126	-0.058564
C	2.667106	2.167152	-0.983079
C	3.932729	2.749855	-0.927324
C	5.024732	1.941170	-0.519483
C	3.770305	-3.713859	-0.198097
C	2.404626	-4.008592	0.044833
C	1.503553	-2.943270	0.083501
C	3.486051	0.062132	-0.403573
C	4.785341	0.584281	-0.260510
C	4.143133	-2.372200	-0.367554
C	3.172566	-1.358042	-0.263914
H	1.807937	2.771889	-1.272634
H	4.053947	3.799099	-1.188941
H	2.048665	-5.023410	0.210254
H	0.445641	-3.144598	0.261018
Ni	0.585527	0.058806	-0.279296
N	-0.670471	1.702453	-0.368330
N	-0.973144	-0.727891	-1.361196
C	-0.379028	2.981843	-0.044665
C	-1.821487	1.495023	-1.098399
C	-1.139820	-2.008461	-1.765750
C	-2.074916	0.101311	-1.460872
C	-1.162958	4.087524	-0.374898
H	0.527588	3.121703	0.540913
C	-2.662660	2.550602	-1.490018
C	-2.339736	-2.547672	-2.229066
H	-0.249623	-2.634694	-1.731632
C	-3.328933	-0.367847	-1.883592
C	-2.349371	3.866085	-1.116588
H	-0.863516	5.078983	-0.040076
C	-3.479912	-1.708013	-2.266780
H	-2.372635	-3.587556	-2.547883
H	-4.195657	0.291997	-1.887928
H	-3.545891	2.363735	-2.100034
H	5.608735	-0.053539	0.060113
H	5.180755	-2.130527	-0.596138
O	-4.728367	-2.100821	-2.641254
O	-3.212809	4.837851	-1.521850
O	4.762496	-4.639567	-0.296328
O	6.302867	2.381562	-0.354075
C	-4.904602	-3.481648	-3.004333
H	-5.971226	-3.591940	-3.238057
H	-4.300036	-3.739721	-3.890191
H	-4.634934	-4.147705	-2.167213
C	-2.898160	6.193498	-1.158850
H	-3.702618	6.806971	-1.584409
H	-2.875647	6.315185	-0.062682
H	-1.928206	6.502310	-1.584383
C	6.556421	3.777266	-0.593526
H	5.948302	4.410044	0.075285
H	7.622665	3.925480	-0.379356
H	6.346190	4.043450	-1.643319
C	4.395022	-6.023278	-0.147867
H	3.665170	-6.322856	-0.918668
H	5.325980	-6.590497	-0.274228
H	3.973807	-6.214774	0.853359
H	-0.289771	-1.703958	1.647318
C	-0.377542	-0.650548	1.896246
C	-1.615667	-0.093942	2.240298
C	0.784492	0.168468	2.002823
C	-1.751814	1.221213	2.700332
C	0.688338	1.474723	2.561125
H	1.770375	-0.297067	1.972276
C	-0.578492	1.986626	2.874249
H	-0.666677	3.004754	3.263460
I	-3.410865	-1.317576	1.948778
H	-2.728012	1.640759	2.942942
C	1.946712	2.294219	2.735106
H	2.688901	1.766174	3.360657
H	2.434028	2.480931	1.761352
H	1.733408	3.267613	3.205509

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B1T_pMe

N	1.491197	1.165595	-0.201547
N	1.493700	-1.289181	0.699448
C	1.403844	2.386102	-0.772118
C	2.493293	3.114059	-1.255121
C	3.781065	2.518627	-1.161359
C	3.821206	-2.742285	1.381861
C	2.529462	-3.283198	1.629334
C	1.422132	-2.508146	1.275351
C	2.745885	0.580713	-0.114729
C	3.897656	1.243133	-0.594939
C	3.923803	-1.468935	0.806940
C	2.753086	-0.752987	0.471498
H	0.395150	2.792843	-0.855767
H	2.333816	4.096466	-1.694828
H	2.380843	-4.261786	2.081290
H	0.412359	-2.879334	1.460109
Ni	-0.044221	-0.055513	0.274143
N	-1.586858	-1.312905	-0.059267
N	-1.573272	1.204928	0.649611
C	-1.511369	-2.570431	-0.545607
C	-2.841399	-0.726858	0.026643
C	-1.490011	2.463264	1.132259
C	-2.836295	0.645559	0.513862
C	-2.611092	-3.331421	-0.947158
H	-0.504853	-2.984884	-0.621070
C	-4.004114	-1.425346	-0.368876
C	-2.589019	3.252350	1.481236
H	-0.477661	2.856281	1.243584
C	-3.998797	1.375244	0.848584
C	-3.898116	-2.733889	-0.856193
H	-2.460359	-4.341773	-1.321948
C	-3.884376	2.685456	1.330806
H	-2.431231	4.261761	1.855610
H	-4.987475	0.925628	0.760604
H	-4.984005	-0.950315	-0.328893
H	4.876988	0.767057	-0.550622
H	4.910645	-1.036456	0.643799
O	-5.049148	3.326249	1.639795
O	-5.060838	-3.343662	-1.230198
O	4.993510	-3.373688	1.681544
O	4.934425	3.099696	-1.603831
C	-4.959936	4.657081	2.189169
H	-5.996222	4.963948	2.380091
H	-4.388706	4.653545	3.132578
H	-4.489970	5.347465	1.468875
C	-4.973498	-4.667919	-1.794957
H	-6.006902	-4.952359	-2.031153
H	-4.365995	-4.661742	-2.715480
H	-4.545490	-5.377752	-1.067425
C	4.840772	4.411489	-2.195624
H	4.431989	5.138187	-1.473653
H	5.870004	4.685661	-2.460411
H	4.213172	4.389008	-3.102292
C	4.916683	-4.690142	2.266324
H	4.414012	-5.392742	1.580699
H	5.957302	-5.000938	2.424527
H	4.382335	-4.660152	3.230495
C	-1.428377	-0.136483	-7.462715
C	-0.265865	0.209265	-8.180643
C	0.915265	0.465578	-7.450694
C	0.939721	0.382568	-6.047314
C	-0.235086	0.036694	-5.359393
C	-1.422802	-0.225902	-6.056513
H	-2.355433	-0.339303	-8.006536
H	1.831612	0.733916	-7.984793
H	1.864143	0.585615	-5.503058
H	-2.336349	-0.494278	-5.522271

I -0.206010 -0.076314 -3.154140
C -0.276307 0.313304 -9.692509
H -0.056851 1.344348 -10.021214
H 0.491309 -0.339862 -10.142353
H -1.256746 0.025159 -10.103632

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B5_pMe
Ni -0.207556 -0.140878 -0.013765
N 1.635395 -0.971266 -0.137584
N 0.898317 1.531001 -0.202551
C 1.921448 -2.288262 -0.122189
C 3.213537 -2.803820 -0.253704
C 4.280368 -1.891630 -0.412260
C 2.654140 3.728575 -0.305004
C 1.257778 3.926483 -0.220435
C 0.435449 2.797652 -0.173067
C 2.668670 -0.086008 -0.287451
C 3.993859 -0.510813 -0.429030
C 3.149702 2.408617 -0.339135
C 2.253575 1.336731 -0.284016
H 1.068303 -2.956608 -0.000298
H 3.366718 -3.880834 -0.229753
H 0.810916 4.917716 -0.185042
H -0.647737 2.904940 -0.100717
S -1.310375 -0.673114 1.906635
C 0.033949 -0.963022 3.037961
F 0.752329 -2.132365 2.811230
F 1.001612 0.033784 3.068010
F -0.393144 -1.072940 4.357894
H 4.809243 0.200887 -0.551515
H 4.224882 2.243691 -0.390885
O 5.583259 -2.235823 -0.555800
O 3.577558 4.717984 -0.352527
C 5.917270 -3.643648 -0.524932
H 5.421145 -4.176245 -1.352444
H 7.006242 -3.685790 -0.648096
H 5.625633 -4.086872 0.440840
C 3.109773 6.085127 -0.259725
H 4.014693 6.703172 -0.302973
H 2.445114 6.324056 -1.105558
H 2.582896 6.245399 0.694738
C -0.847998 -1.628333 -2.450292
C -1.951166 -2.402777 -2.076740
C -0.829928 -0.242781 -2.093533
C -3.074011 -1.837671 -1.413125
H -1.968935 -3.467508 -2.324177
C -1.931864 0.337087 -1.386975
H -0.081462 0.410296 -2.549588
C -3.054720 -0.483824 -1.096546
H -3.929002 -2.464843 -1.160132
H -1.995745 1.418177 -1.261463
I -4.757146 0.416844 -0.100309
C 0.308068 -2.206165 -3.232814
H 0.345097 -1.776555 -4.250445
H 1.270108 -1.972060 -2.748174
H 0.221071 -3.300185 -3.327190

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B6_pMe
Ni -0.375083 -0.496033 0.091963
N 0.149850 1.394212 -0.314016
N 1.654571 -0.759082 -0.196539
C -0.672038 2.463589 -0.267373
C -0.248161 3.771988 -0.500948
C 1.114018 3.989069 -0.797469
C 4.418400 -0.823675 -0.702086
C 3.724721 -1.999282 -0.344609
C 2.351797 -1.906428 -0.104989
C 1.480226 1.600731 -0.574184
C 1.984066 2.877575 -0.824323
C 3.695650 0.385959 -0.798929
C 2.324140 0.383519 -0.536596
H -1.713054 2.257110 -0.030423
H -0.971185 4.582678 -0.444509
H 4.220893 -2.962312 -0.248109
H 1.777425 -2.789865 0.174559
C -2.246752 -0.161068 -0.170659
C -2.569596 0.096987 -1.512759
C -3.230145 -0.054193 0.824165
C -3.879462 0.490974 -1.854195
H -1.816790 0.010136 -2.300315
C -4.531716 0.349487 0.470322
H -2.994465 -0.274501 1.865389
C -4.878124 0.627546 -0.869790
H -4.119664 0.695398 -2.901782
H -5.291935 0.438068 1.252663
S -0.941118 -2.653822 0.401315
C -1.209991 -3.204126 -1.291516
F -2.507438 -3.092194 -1.739463
F -0.446986 -2.535801 -2.230138
F -0.894450 -4.539781 -1.423589
H 3.039857 3.037897 -1.032245
H 4.226047 1.297262 -1.069018
O 1.671506 5.189727 -1.054254
O 5.740793 -0.750992 -0.962754
C 0.815993 6.360261 -1.019696
H 0.384755 6.487868 -0.014329
H 1.473734 7.203502 -1.261350
H 0.015200 6.272138 -1.770903
C 6.521793 -1.969008 -0.859470
H 7.548787 -1.674497 -1.106002
H 6.473350 -2.366516 0.166696
H 6.156520 -2.719719 -1.577763
I -0.041626 -0.019320 2.855166
C -6.289318 1.047727 -1.232469
H -7.016151 0.256390 -0.978157
H -6.591911 1.954064 -0.679553
H -6.377516 1.257351 -2.310535

49
B7_pMe
Ni 0.187818 0.076104 0.119187
N 1.680321 -1.254904 -0.082043
N 1.721397 1.354116 -0.037916
C 1.561742 -2.597200 -0.082018
C 2.636020 -3.469140 -0.280000
C 3.916269 -2.909296 -0.491118
C 4.033856 2.940436 -0.263865
C 2.769466 3.536476 -0.057844
C 1.656571 2.698414 0.047351
C 2.921519 -0.709563 -0.273168
C 4.051437 -1.504965 -0.485524
C 4.114418 1.533960 -0.341110
C 2.948733 0.771837 -0.223277
H 0.555013 -2.981284 0.088526
H 2.464726 -4.543559 -0.263062
H 2.638403 4.613407 0.023498
H 0.661051 3.114339 0.207670
H 5.034573 -1.063508 -0.641238
H 5.085320 1.062496 -0.485298
O 5.050549 -3.618420 -0.701076
O 5.199696 3.615542 -0.395214
C 4.960696 -5.063189 -0.678100
H 4.287232 -5.421395 -1.473442
H 5.982160 -5.418842 -0.859237
H 4.606060 -5.410680 0.305565
C 5.157438 5.061190 -0.321014
H 6.194835 5.388264 -0.460487
H 4.518631 5.468839 -1.121180
H 4.785863 5.385292 0.664248
C -0.696462 0.046859 -1.825423
C -1.417672 -1.178594 -1.641641
C -1.270140 1.228958 -1.250483
C -2.646648 -1.212009 -0.975916
H -1.001954 -2.100144 -2.054232
C -2.521252 1.197423 -0.596697
H -0.782988 2.190238 -1.422686
C -3.217605 -0.016698 -0.472144
H -3.167972 -2.161552 -0.844250
H -2.934317 2.115975 -0.177866
S -4.758297 -0.071257 0.439262
C -5.942962 0.191393 -0.936134
F -5.892764 -0.781156 -1.896883
F -7.208178 0.192760 -0.424556
F -5.766942 1.377273 -1.594138
I -0.880415 -0.256123 2.574475
C 0.409617 0.136427 -2.860007
H 1.033610 -0.770017 -2.852609
H -0.028739 0.237656 -3.870084
H 1.051045 1.010537 -2.677466

72
HAT_pMe
N 1.454696 1.277603 -0.160329
N 1.437185 -1.237800 0.560404
C 1.381054 2.522391 -0.679734
C 2.487865 3.276995 -1.072471
C 3.771181 2.689370 -0.945514
C 3.735594 -2.678852 1.356227
C 2.446839 -3.258983 1.456979

C 1.350941 -2.494123 1.051465
C 2.701441 0.706138 -0.040599
C 3.868026 1.386118 -0.429863
C 3.847352 -1.367730 0.862658
C 2.691359 -0.670330 0.475582
H 0.374694 2.925843 -0.795716
H 2.340607 4.276916 -1.475377
H 2.288410 -4.266095 1.837681
H 0.342578 -2.903693 1.122147
Ni -0.105376 0.008225 0.136937
N -1.693332 -1.239334 -0.098130
N -1.596720 1.232475 0.754839
C -1.674128 -2.461614 -0.673437
C -2.921798 -0.669723 0.151868
C -1.458894 2.455931 1.313229
C -2.859639 0.677630 0.736207
C -2.815627 -3.196409 -0.998911
H -0.684986 -2.862380 -0.894661
C -4.122254 -1.328317 -0.165745
C -2.512568 3.202287 1.845350
H -0.443060 2.852539 1.333685
C -3.975112 1.357789 1.252634
C -4.079538 -2.609812 -0.739264
H -2.708907 -4.179379 -1.453391
C -3.812194 2.638487 1.807482
H -2.315339 4.183708 2.272349
H -4.965065 0.902751 1.243874
H -5.086864 -0.851875 0.003703
H 4.845473 0.909427 -0.366745
H 4.830459 -0.901640 0.807223
O -4.934495 3.241663 2.284549
O -5.277653 -3.189560 -1.021054
O 4.894683 -3.292714 1.716955
O 4.938252 3.288531 -1.305727
C -4.795246 4.555144 2.868712
H -5.807452 4.845932 3.176289
H -4.128613 4.521614 3.746260
H -4.405720 5.271285 2.126373
C -5.264841 -4.506602 -1.614252
H -6.319693 -4.765602 -1.769404
H -4.732899 -4.493872 -2.579681
H -4.792266 -5.233835 -0.933233
C 4.866470 4.611807 -1.880471
H 4.428660 5.324955 -1.162469
H 5.905041 4.889203 -2.100232
H 4.274266 4.600702 -2.810263
C 4.808386 -4.624852 2.268474
H 4.367600 -5.321978 1.536889
H 5.843314 -4.915411 2.488265
H 4.211972 -4.624002 3.195924
C -0.807777 -1.030206 -7.759727
C 0.102852 -0.225230 -8.477908
C 0.943671 0.645517 -7.751587
C 0.877472 0.715584 -6.343041
C -0.036765 -0.093106 -5.661431
C -0.882312 -0.966951 -6.351347
H -1.463584 -1.716493 -8.306583
H 1.661287 1.272430 -8.292040
H 1.543860 1.394177 -5.801025
H -1.594057 -1.603477 -5.815916
I -0.123498 -0.011658 -3.134440
C 0.158375 -0.276300 -9.992831
H 1.164261 -0.021159 -10.364915
H -0.109807 -1.277173 -10.369421
H -0.550673 0.443861 -10.441038

44
OA1_pMe
Ni -0.108487 -1.528405 -0.849225
N 1.798153 -1.237394 -0.547310
N -0.023270 0.224522 -1.868083
C 2.811972 -2.046604 -0.154666
C 4.082126 -1.587036 0.211576
C 4.334070 -0.196279 0.147740
C -0.338461 2.991058 -1.288134
C -1.298751 2.301216 -2.061973
C -1.090544 0.940178 -2.313664
C 2.062220 0.113664 -0.648850
C 3.308689 0.656723 -0.304052
C 0.788165 2.283760 -0.825950
C 0.925564 0.923923 -1.136268
H 2.575487 -3.110792 -0.105609
H 4.833437 -2.300001 0.546332
H -2.187712 2.791730 -2.456676
H -1.817408 0.377131 -2.903967
C -1.906538 -0.493022 1.159571
C -2.542707 0.700192 0.807906
C -1.007908 -0.571754 2.233064
C -2.256909 1.857870 1.559358
H -3.230800 0.746750 -0.036153
C -0.729260 0.600917 2.957541
H -0.520818 -1.512859 2.489858
C -1.344482 1.830410 2.631524
H -2.748856 2.797854 1.295981
H -0.014700 0.557147 3.784601
I -2.328968 -2.351033 -0.044651
H 3.499133 1.725267 -0.402396
H 1.520778 2.789754 -0.196749
O 5.515218 0.396658 0.477133
O -0.418492 4.306312 -0.928441
C 6.599881 -0.458537 0.897291
H 6.864609 -1.171511 0.098822
H 7.443222 0.214983 1.094848
H 6.330924 -1.006196 1.815694
C -1.562692 5.052581 -1.386168
H -2.497538 4.614210 -0.997950
H -1.431040 6.066822 -0.987721
H -1.594518 5.082268 -2.488378
C -1.004943 3.090934 3.399945
H -0.004664 3.465908 3.117155
H -1.733270 3.891376 3.193421
H -0.988266 2.905436 4.487134

49
OA2_pMe
Ni -0.740620 -0.557399 0.453676
N 1.243356 -0.115077 0.443400
N -0.829815 1.436830 0.016039
C 2.242553 -1.002874 0.591885
C 3.591234 -0.690681 0.396593
C 3.918398 0.629946 0.023698
C -0.678161 4.217146 -0.399231
C -1.930061 3.573294 -0.291225
C -1.943060 2.190298 -0.086392
C 1.556036 1.165617 0.083231
C 2.876706 1.569625 -0.130021
C 0.493645 3.439508 -0.286575
C 0.385336 2.062702 -0.074165
H 1.942142 -2.009000 0.877969
H 4.344080 -1.464382 0.531613
H -2.871997 4.113719 -0.358087
H -2.887156 1.651501 -0.003389
C -0.718277 -1.470711 -1.429644
C -0.115503 -2.718486 -1.160357
C -0.179226 -0.603025 -2.409635
C 1.132230 -3.004053 -1.745035
H -0.581621 -3.422061 -0.471853
C 1.063931 -0.913208 -2.970520
H -0.688437 0.326002 -2.663122
C 1.749958 -2.106671 -2.637052
H 1.632895 -3.942476 -1.492038
H 1.517062 -0.211007 -3.676303
S -1.208586 -1.765071 2.388090
C -0.167671 -0.927737 3.559272
F 1.181557 -1.267659 3.496582
F -0.171785 0.460090 3.465799
F -0.526385 -1.189215 4.876794
H 3.119066 2.589983 -0.422826
H 1.464178 3.928705 -0.350014
O 5.172872 1.084122 -0.211056
O -0.499464 5.543859 -0.599527
C 6.267689 0.148650 -0.066078
H 6.158106 -0.685500 -0.777767
H 7.172101 0.725247 -0.295207
H 6.313107 -0.235934 0.965453
C -1.677720 6.383157 -0.663725
H -1.298127 7.401524 -0.810594
H -2.316280 6.089912 -1.512534
H -2.244290 6.321073 0.279271
I -3.049646 -1.349074 -1.062647
C 3.112306 -2.397732 -3.228821
H 3.851047 -1.642825 -2.904316
H 3.478702 -3.388908 -2.917359
H 3.086820 -2.370003 -4.332199

15
pMePhI
C 0.188465 0.000001 -0.001981
C 0.875386 -1.223203 -0.006029
C 2.282315 -1.209745 -0.011564
C 3.007171 0.000001 -0.011064

C	2.282315	1.209747	-0.011564
C	0.875386	1.223204	-0.006029
H	0.336358	-2.171288	-0.008407
H	2.820715	-2.161243	-0.018649
H	2.820714	2.161245	-0.018649
H	0.336358	2.171289	-0.008407
I	-1.986121	0.000000	0.002501
C	4.521836	-0.000001	0.018046
H	4.930239	0.895391	-0.478221
H	4.892563	-0.000055	1.059231
H	4.930238	-0.895343	-0.478312

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pMePhI_rad

C	0.926808	0.000001	-0.216299
C	1.576408	-1.227071	-0.159034
C	2.985919	-1.215755	-0.036557
C	3.701980	0.000003	0.028068
C	2.985918	1.215757	-0.036556
C	1.576405	1.227072	-0.159035
H	1.033543	-2.175096	-0.207552
H	3.531534	-2.164025	0.008256
H	3.531532	2.164026	0.008257
H	1.033539	2.175096	-0.207555
I	-2.636320	0.000000	0.036163
C	5.209826	-0.000001	0.200173
H	5.664353	0.894575	-0.256285
H	5.486446	-0.000326	1.270515
H	5.664420	-0.894260	-0.256842

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pMePh_rad

C	-1.916743	-0.000001	0.010622
C	-1.282218	-1.231969	0.003167
C	0.133162	-1.216419	-0.009547
C	0.849672	0.000001	-0.012674
C	0.133160	1.216420	-0.009547
C	-1.282221	1.231967	0.003167
H	-1.826513	-2.180047	0.002786
H	0.678622	-2.164967	-0.019675
H	0.678618	2.164969	-0.019675
H	-1.826517	2.180045	0.002785
C	2.366527	0.000001	0.009172
H	2.772145	0.894789	-0.490037
H	2.743472	-0.000053	1.047783
H	2.772146	-0.894737	-0.490128

19

pMePhSCF3

C	0.279089	-0.027960	0.662118
C	0.957437	-1.239308	0.416501
C	2.294649	-1.209857	-0.003489
C	2.977328	0.013385	-0.181780
C	2.282377	1.213938	0.073748
C	0.943705	1.202623	0.496748
H	0.442826	-2.192764	0.546053
H	2.816498	-2.150270	-0.197925
H	2.794710	2.169665	-0.060326
H	0.420741	2.140804	0.689594
S	-1.426556	-0.061030	1.240813
C	-2.302253	0.015299	-0.367838
F	-2.064941	1.165110	-1.065016
F	-1.986241	-1.011620	-1.209541
F	-3.642481	-0.046574	-0.125298
C	4.428372	0.027161	-0.610491
H	5.085745	-0.245033	0.234500
H	4.611898	-0.704500	-1.414203
H	4.731217	1.024647	-0.965107

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RE1_pMe

Ni	0.599167	-0.229407	-0.329746
N	-0.825087	1.149121	-0.552907
N	-0.980387	-1.369709	0.177137
C	-0.661388	2.463169	-0.826541
C	-1.699604	3.397752	-0.835615
C	-3.002781	2.951281	-0.519955
C	-3.403960	-2.776159	0.543194
C	-2.160305	-3.435524	0.672688
C	-0.995686	-2.689621	0.472665
C	-2.094773	0.717658	-0.243025
C	-3.190425	1.588993	-0.213138
C	-3.408110	-1.401304	0.235652
C	-2.191950	-0.727318	0.070163
H	0.362380	2.770930	-1.046023
H	-1.483544	4.436725	-1.078269
H	-2.083691	-4.493720	0.915076
H	-0.018331	-3.167851	0.550044
C	2.379493	0.545976	-0.206215
C	2.391129	0.257162	1.202148
C	2.759673	1.858910	-0.645834
C	2.585602	1.318043	2.116161
H	2.335218	-0.764602	1.576798
C	2.958797	2.869753	0.290440
H	2.838843	2.069766	-1.714855
C	2.849518	2.630118	1.690766
H	2.554277	1.099844	3.188168
H	3.205402	3.877269	-0.059411
S	2.338596	-0.848892	-1.471870
C	3.398808	-2.201850	-0.703515
F	4.600451	-1.750686	-0.235717
F	2.797728	-2.859587	0.334898
F	3.669410	-3.144803	-1.661291
H	-4.185160	1.237287	0.057872
H	-4.360506	-0.886228	0.116875
O	-4.618107	-3.366854	0.684217
O	-4.108265	3.740152	-0.476368
C	-4.649276	-4.778789	0.994420
H	-4.162965	-4.972440	1.964471
H	-5.713114	-5.040930	1.045849
H	-4.153486	-5.359518	0.199453
C	-3.945722	5.140645	-0.794203
H	-3.573561	5.264120	-1.824545
H	-4.947012	5.578574	-0.699567
H	-3.253808	5.620747	-0.082785
C	3.066715	3.756714	2.679899
H	4.056073	4.230461	2.545325
H	2.311502	4.554811	2.556490
H	3.003746	3.390202	3.717491

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RE2_pMe

Ni	-0.059606	-0.683943	0.551276
N	-0.554872	1.277834	0.501043
N	1.786837	0.139043	0.202578
C	-1.808525	1.756547	0.598064
C	-2.143424	3.090532	0.350496
C	-1.109515	3.978218	-0.020359
C	4.209936	1.539072	-0.074290
C	4.204513	0.136275	0.088660
C	2.970606	-0.505273	0.221722
C	0.450739	2.132563	0.148305
C	0.208599	3.482043	-0.119539
C	2.976852	2.226605	-0.069539
C	1.792043	1.502714	0.078037
H	-2.568321	1.029754	0.883901
H	-3.179357	3.408566	0.445738
H	5.119903	-0.450884	0.113524
H	2.922542	-1.586337	0.347679
C	-1.173768	-1.208445	-1.039331
C	-0.739120	-0.557216	-2.211427
C	-2.551931	-1.385430	-0.791862
C	-1.693323	0.002335	-3.077271
H	0.320638	-0.425893	-2.420170
C	-3.485180	-0.816167	-1.671933
H	-2.888488	-1.922657	0.094657
C	-3.077118	-0.114029	-2.826888
H	-1.348086	0.549106	-3.959380
H	-4.551434	-0.928238	-1.455925
S	0.016409	-2.826792	-0.099107
C	1.007512	-3.198102	-1.596899
F	0.245109	-3.485255	-2.695180
F	1.883274	-2.223256	-1.978824
F	1.754741	-4.319246	-1.340841
H	1.013096	4.155437	-0.410150
H	2.970615	3.311464	-0.159865
O	-1.275665	5.291243	-0.299095
O	5.316808	2.299117	-0.225239
C	-2.612412	5.841196	-0.204060
H	-2.998834	5.735943	0.822253
H	-2.507105	6.901774	-0.461812
H	-3.285109	5.340172	-0.918348
C	6.604455	1.633996	-0.209558
H	7.342519	2.433132	-0.347647
H	6.763044	1.130984	0.757571
H	6.670354	0.906233	-1.034042
I	-1.336296	-1.271347	2.956923
C	-4.094539	0.458523	-3.791653
H	-3.686504	1.328710	-4.331156
H	-4.386219	-0.292351	-4.548552
H	-5.012561	0.768630	-3.266344

Substrate: methyl 4-iodobenzoate

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A4_pCO2Me

Ni	0.705891	-0.239881	-0.344251
N	-0.426105	1.354579	-0.079462
N	-1.104180	-1.157525	-0.294643
C	-0.013388	2.642448	-0.013798
C	-0.875178	3.734368	0.103530
C	-2.263387	3.490732	0.153168
C	-3.732318	-2.151536	-0.032827
C	-2.644507	-3.029393	-0.222252
C	-1.365241	-2.480463	-0.343732
C	-1.780957	1.119455	-0.029409
C	-2.709977	2.154761	0.083659
C	-3.474060	-0.765403	0.027966
C	-2.161174	-0.307278	-0.103052
H	1.060469	2.804177	-0.057301
H	-0.455771	4.737081	0.149296
H	-2.768168	-4.109076	-0.273707
H	-0.500158	-3.126636	-0.490965
C	2.310782	0.720459	-0.189415
C	2.783857	1.038428	1.105930
C	2.997914	1.254200	-1.303899
C	3.889711	1.881731	1.281397
H	2.283055	0.631422	1.987847
C	4.097977	2.108070	-1.134566
H	2.670856	1.008588	-2.317217
C	4.557672	2.436014	0.164121
H	4.242844	2.122275	2.286205
H	4.603773	2.515531	-2.011044
S	1.889309	-2.019787	-0.972896
C	2.743729	-2.538667	0.513487
F	3.961354	-1.928288	0.742878
F	2.028005	-2.353281	1.682531
F	3.032258	-3.892296	0.465113
H	-3.778672	1.951675	0.113587
H	-4.303908	-0.078861	0.185118
O	-3.219728	4.438224	0.259765
O	-5.023349	-2.527027	0.103946
C	-2.796702	5.821111	0.357264
H	-2.245637	6.118477	-0.549006
H	-3.723924	6.399786	0.444534
H	-2.169457	5.966669	1.250826
C	-5.327089	-3.942845	0.043051
H	-6.414276	-4.010607	0.168647
H	-5.028884	-4.356881	-0.933339
H	-4.815694	-4.479886	0.857686
C	5.718257	3.337277	0.407663
O	6.151984	3.640190	1.519911
O	6.265455	3.809655	-0.749439
C	7.413190	4.685034	-0.603692
H	7.704695	4.945970	-1.628888
H	7.137516	5.587648	-0.037957
H	8.232033	4.159742	-0.089984

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B1T_pCO2Me

N	1.484746	1.160708	-0.217672
N	1.487408	-1.294563	0.683595
C	1.396906	2.379818	-0.791638
C	2.484966	3.102630	-1.284731
C	3.771653	2.504022	-1.198443
C	3.816086	-2.747177	1.362784
C	2.524952	-3.286448	1.615694
C	1.416922	-2.512094	1.263140
C	2.738177	0.573412	-0.137541
C	3.888250	1.229841	-0.628580
C	3.917242	-1.474837	0.784794
C	2.746020	-0.759719	0.451711
H	0.388998	2.789297	-0.870425
H	2.325266	4.084183	-1.726274
H	2.377294	-4.263573	2.071126
H	0.407766	-2.882222	1.452676
Ni	-0.051894	-0.060184	0.261629
N	-1.600711	-1.315267	-0.052963
N	-1.576061	1.206007	0.642762
C	-1.532124	-2.576616	-0.530964
C	-2.853142	-0.725885	0.038817
C	-1.486106	2.466319	1.119201
C	-2.841263	0.649987	0.516949
C	-2.636557	-3.337514	-0.918697
H	-0.527466	-2.994404	-0.611216
C	-4.020388	-1.424044	-0.343510
C	-2.580709	3.260951	1.468777
H	-0.471936	2.855848	1.225362
C	-3.999728	1.385620	0.851786
C	-3.921482	-2.736230	-0.822483
H	-2.490954	-4.351163	-1.286504
C	-3.878718	2.698389	1.325712
H	-2.417712	4.271188	1.838701
H	-4.990472	0.939478	0.769873
H	-4.998935	-0.946765	-0.298825
H	4.866256	0.750589	-0.589956
H	4.903576	-1.042816	0.617707
O	-5.039736	3.345004	1.635116
O	-5.088245	-3.345489	-1.183625
O	4.988746	-3.378101	1.659799
O	4.923056	3.079883	-1.651081
C	-4.944242	4.684098	2.163486
H	-5.979033	4.999167	2.348915
H	-4.373404	4.692205	3.107088
H	-4.470181	5.360403	1.432694
C	-5.008582	-4.673780	-1.740509
H	-6.044399	-4.956730	-1.967625
H	-4.407480	-4.674909	-2.665240
H	-4.577276	-5.380133	-1.011600
C	4.829175	4.390676	-2.245750
H	4.426781	5.120037	-1.522967
H	5.857424	4.661363	-2.517638
H	4.195759	4.367101	-3.148286
C	4.913582	-4.693899	2.246836
H	4.407751	-5.396982	1.564110
H	5.954669	-5.004924	2.401225
H	4.383145	-4.661943	3.213054
C	-1.422222	-0.148526	-7.436682
C	-0.244637	0.190763	-8.141850
C	0.943897	0.435535	-7.418496
C	0.961401	0.346084	-6.019122
C	-0.219308	0.008329	-5.335996
C	-1.411700	-0.240329	-6.036012
H	-2.349407	-0.340876	-7.976874
H	1.855363	0.695631	-7.958751
H	1.885567	0.538510	-5.471417
H	-2.326870	-0.500673	-5.501374
I	-0.199602	-0.105172	-3.130450
C	-0.199474	0.305834	-9.632339
O	0.802808	0.611684	-10.275887
O	-1.399309	0.032847	-10.210857
C	-1.445862	0.122084	-11.660350
H	-2.477965	-0.135704	-11.927848
H	-1.203607	1.144199	-11.986427
H	-0.738363	-0.591056	-12.108216

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B5_pCO2Me

Ni	-0.219220	-0.225715	-0.062555
N	1.638610	-0.978179	-0.333828
N	0.832754	1.485139	-0.041161
C	1.953113	-2.275256	-0.515171
C	3.247599	-2.727964	-0.782865
C	4.282197	-1.770222	-0.866016
C	2.513357	3.737900	0.044431
C	1.116836	3.876012	0.209454
C	0.332003	2.720843	0.159086
C	2.640105	-0.049167	-0.407643
C	3.964882	-0.409790	-0.670587
C	3.046986	2.448401	-0.162659
C	2.187144	1.347605	-0.202155
H	1.123652	-2.978777	-0.442912
H	3.426011	-3.792541	-0.919715
H	0.640746	4.839831	0.377432
H	-0.749784	2.779021	0.289035
S	-1.354963	-1.072138	1.712629
C	-0.028037	-1.497252	2.824552
F	0.734675	-2.590938	2.431399
F	0.900759	-0.488432	3.042909
F	-0.484290	-1.833401	4.093844
H	4.755700	0.336065	-0.736322
H	4.122457	2.329385	-0.283824
O	5.581617	-2.052005	-1.126385
O	3.403954	4.756956	0.071467
C	5.943895	-3.439013	-1.323900
H	5.400778	-3.859972	-2.185578
H	7.022255	-3.430781	-1.523931
H	5.728840	-4.025929	-0.416206
C	2.892893	6.098386	0.261382
H	3.775254	6.749324	0.242606
H	2.204616	6.365808	-0.556425
H	2.379381	6.180969	1.232645
C	-0.721608	-1.417888	-2.684681

C -1.813658 -2.271064 -2.452693
C -0.748247 -0.081312 -2.171151
C -2.965182 -1.815124 -1.773284
H -1.792617 -3.296984 -2.820491
C -1.892303 0.377371 -1.449729
H -0.002419 0.632971 -2.518703
C -2.993335 -0.502780 -1.294097
H -3.811595 -2.485442 -1.626477
H -1.987823 1.433004 -1.195035
I -4.746728 0.218992 -0.261924
C 0.484137 -1.833407 -3.450489
O 0.548038 -3.181530 -3.637835
O 1.338584 -1.055918 -3.875314
C 1.692694 -3.663276 -4.388601
H 1.674232 -3.261334 -5.412684
H 2.628313 -3.369489 -3.890299
H 1.586056 -4.755205 -4.401631

52
B6_pCO2Me
Ni 0.237254 -0.559730 0.219639
N 0.458839 1.390803 -0.149768
N 2.229471 -0.543748 -0.288326
C -0.473689 2.342846 0.063339
C -0.254327 3.700315 -0.168570
C 1.011328 4.099823 -0.648828
C 4.871212 -0.247817 -1.201427
C 4.398194 -1.502691 -0.761192
C 3.076383 -1.589541 -0.318345
C 1.702226 1.774741 -0.581253
C 2.000626 3.111872 -0.846041
C 3.993493 0.858015 -1.160445
C 2.689506 0.677242 -0.697685
H -1.434403 1.998112 0.437679
H -1.056523 4.407755 0.028627
H 5.023056 -2.392983 -0.754768
H 2.669911 -2.539385 0.028799
C -1.673093 -0.473442 0.170273
C -2.168812 -0.206047 -1.120289
C -2.552227 -0.554846 1.262824
C -3.542673 0.001266 -1.317999
H -1.493479 -0.148978 -1.977300
C -3.925125 -0.342358 1.063392
H -2.179897 -0.779800 2.262063
C -4.436236 -0.063458 -0.224292
H -3.912928 0.211572 -2.321753
H -4.612238 -0.401856 1.909143
S -0.020845 -2.785102 0.475984
C -0.325286 -3.307918 -1.220120
F -1.647523 -3.291808 -1.603809
F 0.333727 -2.550806 -2.168961
F 0.094491 -4.606251 -1.406280
H 2.987782 3.413090 -1.190573
H 4.351522 1.831193 -1.490119
O 1.369212 5.368218 -0.931940
O 6.114738 -0.003688 -1.664528
C 0.382997 6.413827 -0.731619
H 0.087294 6.460487 0.328078
H 0.884501 7.342169 -1.029347
H -0.498134 6.233935 -1.367360
C 7.043109 -1.115427 -1.742738
H 7.970372 -0.686706 -2.140699
H 7.217164 -1.539854 -0.741410
H 6.655595 -1.888644 -2.424887
I 0.791358 -0.154111 2.953701
C -5.908652 0.138637 -0.373591
O -6.723870 0.036469 0.541714
O -6.264126 0.451315 -1.650143
C -7.684660 0.637811 -1.889074
H -8.066026 1.474545 -1.285231
H -7.766315 0.863752 -2.959548
H -8.236677 -0.281618 -1.643845

52
B7_pCO2Me
Ni -0.282221 -0.193893 0.086292
N -1.745228 1.148667 -0.223782
N -1.836884 -1.448541 0.037355
C -1.591521 2.476916 -0.379656
C -2.631140 3.335710 -0.745528
C -3.909824 2.776429 -0.963769
C -4.188815 -2.986328 0.029431
C -2.934728 -3.590311 0.270237
C -1.799457 -2.776041 0.262525
C -2.987410 0.606297 -0.410610
C -4.083540 1.387767 -0.783872
C -4.236894 -1.596298 -0.209268
C -3.050449 -0.859286 -0.196621
H -0.584674 2.859229 -0.206862
H -2.435540 4.400434 -0.853989
H -2.828970 -4.655504 0.464530
H -0.810737 -3.197920 0.446227
H -5.065194 0.945067 -0.945665
H -5.198238 -1.115609 -0.383970
O -5.007080 3.473317 -1.341383
O -5.374430 -3.637781 0.015338
C -4.870070 4.903372 -1.524076
H -4.142589 5.120841 -2.322885
H -5.867435 5.254599 -1.815065
H -4.556028 5.382735 -0.583062
C -5.369958 -5.058388 0.298288
H -6.421781 -5.364971 0.253065
H -4.782426 -5.599599 -0.460280
H -4.961010 -5.247036 1.303807
C 0.660697 -0.263325 -1.839816
C 1.501550 0.894696 -1.725896
C 1.115490 -1.485897 -1.241988
C 2.731086 0.818984 -1.070425
H 1.177269 1.837918 -2.161790
C 2.370722 -1.554472 -0.606356
H 0.528520 -2.392042 -1.385178
C 3.180333 -0.409332 -0.525440
H 3.350268 1.712457 -0.980747
H 2.698633 -2.496753 -0.166216
S 4.729335 -0.477445 0.375413
C 5.877163 -0.808356 -1.017160
F 5.880486 0.174345 -1.967119
F 7.142871 -0.899878 -0.517701
F 5.613575 -1.972973 -1.681331
I 0.842664 0.177896 2.477963
C -0.517355 -0.311307 -2.766641
O -1.096928 -1.342152 -3.101412
O -0.871915 0.925519 -3.204031
C -2.058422 0.989546 -4.036764
H -2.226249 2.058932 -4.213692
H -1.885905 0.462386 -4.987039
H -2.915908 0.544075 -3.513294

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HAT_pCO2Me
N 1.483116 1.260049 -0.145284
N 1.468466 -1.254850 0.578832
C 1.409953 2.505228 -0.664759
C 2.516211 3.260735 -1.055881
C 3.800500 2.673610 -0.928102
C 3.767938 -2.688575 1.385795
C 2.479030 -3.269336 1.489840
C 1.383164 -2.507672 1.078942
C 2.731217 0.689221 -0.023519
C 3.897764 1.371080 -0.412477
C 3.878999 -1.380345 0.886097
C 2.722437 -0.684842 0.494264
H 0.403660 2.908368 -0.782330
H 2.368622 4.260996 -1.457811
H 2.320932 -4.273690 1.877772
H 0.375028 -2.916884 1.153906
Ni -0.074607 -0.015428 0.136592
N -1.656059 -1.270410 -0.110778
N -1.582044 1.215487 0.704418
C -1.622636 -2.502787 -0.663912
C -2.891499 -0.692233 0.087419
C -1.458655 2.444740 1.252934
C -2.845577 0.663011 0.650158
C -2.754372 -3.239009 -1.017280
H -0.628380 -2.912503 -0.841909
C -4.082761 -1.353505 -0.261522
C -2.527168 3.203253 1.735752
H -0.442056 2.835986 1.307653
C -3.976290 1.356929 1.114720
C -4.024940 -2.643649 -0.812115
H -2.635560 -4.230339 -1.449904
C -3.827682 2.644235 1.656715
H -2.340707 4.188708 2.158243
H -4.967219 0.905425 1.078883
H -5.051154 -0.871282 -0.134784
H 4.875510 0.895066 -0.348200
H 4.861593 -0.913146 0.830549
O -4.964024 3.258420 2.084395
O -5.214567 -3.224261 -1.128147
O 4.927136 -3.300221 1.750692
O 4.967250 3.273926 -1.288602

C -4.841072 4.576971 2.660470
H -5.863528 4.875128 2.924078
H -4.211416 4.549803 3.565223
H -4.418706 5.284073 1.927503
C -5.185410 -4.546731 -1.708066
H -6.235191 -4.804605 -1.896142
H -4.621788 -4.544864 -2.655523
H -4.738379 -5.269321 -1.005146
C 4.894462 4.597316 -1.862732
H 4.456254 5.309991 -1.144484
H 5.932811 4.875604 -2.082479
H 4.302296 4.586410 -2.792591
C 4.841259 -4.630167 2.307345
H 4.401072 -5.330376 1.578320
H 5.876269 -4.919397 2.528562
H 4.244701 -4.626210 3.234690
C -1.080028 -0.703142 -7.641352
C 0.004416 -0.135447 -8.352497
C 1.062948 0.466704 -7.632865
C 1.039765 0.501583 -6.227900
C -0.043187 -0.064984 -5.542462
C -1.101596 -0.666349 -6.235600
H -1.904814 -1.169068 -8.182888
H 1.899850 0.903862 -8.181789
H 1.865830 0.968881 -5.683938
H -1.945472 -1.107739 -5.697386
I -0.076552 -0.028512 -3.070124
C 0.079118 -0.141383 -9.844509
O 0.985167 0.369363 -10.501996
O -0.977744 -0.782157 -10.416659
C -0.987601 -0.830255 -11.867547
H -0.090194 -1.346422 -12.239172
H -1.893048 -1.392237 -12.128666
H -1.031295 0.187958 -12.281793

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OA1_pCO2Me
Ni 0.903770 -1.050206 -0.155785
N 2.800050 -0.397432 -0.231508
N 0.485266 0.869970 -0.064595
C 3.953868 -1.106567 -0.224525
C 5.223360 -0.545478 -0.048995
C 5.312372 0.851035 0.140289
C 0.217593 3.684743 -0.130895
C -0.922839 2.852391 -0.118785
C -0.730100 1.468582 -0.090034
C 2.894733 0.965946 -0.056504
C 4.122317 1.607817 0.136928
C 1.491580 3.080196 -0.111265
C 1.595420 1.685917 -0.073993
H 3.845482 -2.182448 -0.371247
H 6.101607 -1.188545 -0.063574
H -1.935731 3.250629 -0.128800
H -1.585775 0.796625 -0.080229
C -1.860240 -1.929327 0.094151
C -2.569645 -1.558929 -1.070985
C -2.261801 -1.470848 1.369470
C -3.672801 -0.708726 -0.955527
H -2.259058 -1.922341 -2.051561
C -3.362132 -0.618033 1.466893
H -1.710742 -1.762997 2.264396
C -4.095933 -0.219293 0.312513
H -4.217676 -0.426835 -1.857048
H -3.676515 -0.253877 2.446494
I -0.120718 -3.283938 -0.086960
H 4.178644 2.683786 0.297357
H 2.378665 3.711615 -0.136329
O 6.466299 1.541898 0.334401
O 0.193420 5.043189 -0.165511
C 7.701686 0.792226 0.338970
H 7.857217 0.298596 -0.634398
H 8.491626 1.532066 0.517571
H 7.695970 0.041078 1.145706
C -1.099091 5.687962 -0.205759
H -1.684817 5.442045 0.695178
H -0.886586 6.763892 -0.234004
H -1.654072 5.387532 -1.109772
C -5.248032 0.682561 0.485024
O -5.636566 1.142043 1.566776
O -5.874129 0.975867 -0.702635
C -7.035299 1.834769 -0.608830
H -6.758814 2.817256 -0.196358
H -7.399657 1.940149 -1.639081
H -7.806794 1.372853 0.026158

52
OA2_pCO2Me
Ni -0.799459 -0.451894 0.327951
N 1.215803 -0.597594 0.050155
N -0.314698 1.534041 0.254900
C 1.898032 -1.736759 -0.160757
C 3.236568 -1.773168 -0.561583
C 3.905170 -0.546221 -0.754726
C 0.657329 4.169726 0.408276
C -0.721031 3.901099 0.557659
C -1.145715 2.572191 0.474715
C 1.862280 0.593276 -0.126815
C 3.199437 0.654565 -0.525294
C 1.535605 3.089610 0.176060
C 1.021233 1.792750 0.105263
H 1.340845 -2.659224 -0.008211
H 3.721808 -2.733747 -0.720308
H -1.451166 4.686621 0.739867
H -2.200556 2.319484 0.584244
C -1.215615 -0.895178 -1.645837
C -0.995987 -2.289245 -1.766807
C -0.593355 0.013792 -2.538136
C 0.007994 -2.743515 -2.629446
H -1.551350 -2.991414 -1.146822
C 0.408216 -0.457021 -3.385807
H -0.831960 1.075273 -2.497165
C 0.745375 -1.834231 -3.424097
H 0.227806 -3.810383 -2.668778
H 0.955268 0.244480 -4.017416
S -1.371742 -1.890857 2.063234
C 0.051618 -1.767460 3.124227
F 1.130987 -2.564484 2.756531
F 0.590759 -0.493163 3.240460
F -0.231561 -2.150497 4.428314
H 3.700291 1.608197 -0.684726
H 2.602908 3.280615 0.076815
O 5.191005 -0.418031 -1.156247
O 1.222139 5.396427 0.477294
C 5.933658 -1.629829 -1.432215
H 5.444669 -2.205035 -2.234601
H 6.925692 -1.293410 -1.756737
H 6.018622 -2.243998 -0.521324
C 0.357803 6.527611 0.747591
H 1.023980 7.397917 0.781349
H -0.382545 6.645847 -0.059937
H -0.151369 6.399380 1.716343
I -3.352400 -0.269040 -0.818332
C 1.877409 -2.256974 -4.290322
O 2.537840 -1.496756 -4.999975
O 2.127336 -3.595397 -4.209222
C 3.209302 -4.090256 -5.040332
H 4.159542 -3.615039 -4.754779
H 3.244282 -5.170330 -4.850291
H 2.998015 -3.889566 -6.101129

18
pCO2MePhI
C -0.836317 0.044420 -0.000032
C -0.080922 -1.139642 0.000320
C 1.319557 -1.053883 0.000218
C 1.962606 0.203938 -0.000155
C 1.178909 1.378154 -0.000453
C -0.221690 1.307664 -0.000428
H -0.566613 -2.115219 0.000657
H 1.905822 -1.972318 0.000533
H 1.670358 2.351715 -0.000684
H -0.815357 2.222183 -0.000689
I -2.997137 -0.083601 0.000043
O 4.042239 1.428199 0.000962
O 4.090481 -0.849517 -0.001345
C 5.544396 -0.801387 0.000366
H 5.904699 -0.283143 0.900921
H 5.863324 -1.850647 0.001256
H 5.906778 -0.284191 -0.899977
C 3.453043 0.349570 -0.000039

18
pCO2MePhI_rad
C -0.280350 0.225889 -0.410638
C 0.385012 -0.995773 -0.439956
C 1.786370 -0.987550 -0.286187
C 2.475734 0.236692 -0.107292
C 1.752745 1.453177 -0.084204
C 0.351567 1.453317 -0.233507
H -0.147906 -1.940512 -0.573234
H 2.336974 -1.929113 -0.304214

H 2.291971 2.392097 0.056769
H -0.204100 2.394223 -0.205678
I -3.675772 -0.106108 0.101282
O 4.608507 1.343557 0.148085
O 4.533323 -0.931837 0.111634
C 5.975353 -0.960176 0.274027
H 6.262274 -0.476153 1.219411
H 6.239751 -2.024830 0.289321
H 6.465836 -0.451122 -0.568919
C 3.959653 0.301988 0.061227

17
pCO2MePh_rad
C -3.006908 -0.311391 -0.000050
C -2.194205 -1.433856 0.000093
C -0.801256 -1.206112 0.000099
C -0.294478 0.114723 0.000034
C -1.182828 1.214755 -0.000075
C -2.577857 1.006690 -0.000154
H -2.588399 -2.452738 0.000156
H -0.119920 -2.057296 0.000189
H -0.782558 2.230051 -0.000126
H -3.266111 1.855202 -0.000251
O 1.660028 1.534260 0.000240
O 1.926380 -0.727010 -0.000064
C 3.368298 -0.539637 -0.000164
H 3.679597 0.008683 0.900787
H 3.785922 -1.553603 -0.000791
H 3.679374 0.009674 -0.900584
C 1.176040 0.405165 0.000085

22
pCO2MePhSCF3
C 0.824187 0.008096 -0.766300
C 0.052801 -1.164521 -0.649930
C -1.314764 -1.068505 -0.357952
C -1.916308 0.196107 -0.177040
C -1.132374 1.363526 -0.296887
C 0.232615 1.275561 -0.597754
H 0.515464 -2.143311 -0.781441
H -1.907281 -1.977846 -0.266378
H -1.598209 2.339396 -0.158439
H 0.830307 2.182139 -0.697670
C -3.375471 0.356253 0.140763
O -3.917839 1.435971 0.357050
O -4.030057 -0.830430 0.160698
C -5.451418 -0.775328 0.470179
H -5.978548 -0.173669 -0.284185
H -5.787513 -1.818557 0.440782
H -5.603816 -0.344252 1.470085
S 2.573433 -0.122518 -1.191918
C 3.289388 -0.072778 0.496341
F 3.063476 1.104282 1.147836
F 2.820037 -1.058219 1.313486
F 4.637144 -0.230330 0.387280

51
RE1_pCO2Me
Ni -0.754731 0.333068 -0.298530
N 0.686719 -1.010094 -0.044827
N 0.752524 1.608988 -0.086561
C 0.562192 -2.352691 0.042942
C 1.621558 -3.220352 0.320068
C 2.901665 -2.663000 0.535027
C 3.096218 3.166349 0.130210
C 1.837535 3.780819 -0.056756
C 0.712453 2.958984 -0.159454
C 1.932351 -0.467573 0.172788
C 3.046805 -1.262473 0.461685
C 3.156146 1.759746 0.200843
C 1.978048 1.012401 0.095535
H -0.445828 -2.740986 -0.109124
H 1.436128 -4.291815 0.366649
H 1.719489 4.860473 -0.121966
H -0.276564 3.394964 -0.307467
C -2.540407 -0.400617 -0.170450
C -2.608277 0.474007 0.985729
C -2.859452 -1.798183 -0.016005
C -2.725560 -0.109822 2.261180
H -2.713558 1.554974 0.889481
C -2.983095 -2.329610 1.255266
H -2.938764 -2.436229 -0.898639
C -2.874651 -1.506169 2.423693
H -2.729527 0.541653 3.135866
H -3.166916 -3.397745 1.381701
S -2.395620 0.316943 -1.843372
C -3.668627 1.705617 -1.841601
F -4.855604 1.349652 -1.275362
F -3.247806 2.836486 -1.197918
F -3.919155 2.060323 -3.137951
H 4.025781 -0.820852 0.643002
H 4.122510 1.276480 0.335711
O 4.275141 3.826204 0.249553
O 4.023644 -3.371548 0.820083
C 4.248407 5.271410 0.186153
H 3.624986 5.681656 0.997284
H 5.291124 5.586939 0.313648
H 3.866997 5.607923 -0.791568
C 3.900633 -4.807832 0.936475
H 3.561158 -5.246201 -0.016042
H 4.908327 -5.166767 1.179288
H 3.199084 -5.069938 1.745167
C -2.980747 -2.153938 3.746081
O -2.867659 -1.266394 4.785636
O -3.145010 -3.365237 3.930381
C -2.973135 -1.831522 6.114709
H -2.169778 -2.563699 6.288688
H -2.868249 -0.979070 6.798332
H -3.951734 -2.316391 6.251944

52
RE2_pCO2Me
Ni 0.802681 -0.737653 0.571674
N -0.125492 0.964708 1.147750
N 2.023153 0.648656 -0.323719
C -1.269806 1.014711 1.853989
C -2.006712 2.187117 2.039268
C -1.523566 3.376721 1.450917
C 3.624220 2.758417 -1.265762
C 4.047796 1.418184 -1.402343
C 3.210372 0.411693 -0.915571
C 0.353461 2.113912 0.584763
C -0.319567 3.330407 0.714426
C 2.394248 3.018335 -0.621773
C 1.626841 1.948510 -0.157792
H -1.600806 0.068706 2.280928
H -2.924929 2.155297 2.621740
H 4.994109 1.148854 -1.866728
H 3.500336 -0.634564 -1.001486
C -0.722226 -1.374197 -0.539633
C -0.975493 -0.519976 -1.635356
C -1.792100 -1.987830 0.152132
C -2.297355 -0.194180 -1.961308
H -0.158444 -0.060600 -2.187058
C -3.106815 -1.659035 -0.189808
H -1.593209 -2.682921 0.967052
C -3.379734 -0.753706 -1.242305
H -2.481773 0.506009 -2.776236
H -3.935287 -2.108577 0.359434
S 1.084726 -2.689418 -0.500595
C 1.383450 -2.613619 -2.311105
F 0.306111 -3.011984 -3.051650
F 1.759278 -1.395930 -2.798286
F 2.399713 -3.485518 -2.602794
H 0.059083 4.239836 0.250918
H 2.075681 4.049297 -0.476074
O -2.128173 4.582750 1.528354
O 4.312684 3.838007 -1.694541
C -3.359313 4.678764 2.287693
H -3.181353 4.407620 3.340451
H -3.662106 5.730029 2.212617
H -4.132017 4.027449 1.849459
C 5.595822 3.617931 -2.332991
H 5.959983 4.617594 -2.598017
H 6.292409 3.130214 -1.632596
H 5.471676 3.004476 -3.239189
I 0.896673 -1.923695 3.065918
C -4.803337 -0.436619 -1.551929
O -5.770512 -0.947413 -0.987742
O -4.925675 0.496123 -2.536667
C -6.281581 0.858535 -2.910340
H -6.811042 1.294935 -2.050408
H -6.168727 1.599673 -3.711380
H -6.825681 -0.025369 -3.274328