SUPPLEMENTARY INFORMATION

Mechanistic Study of the Bismuth Mediated Fluorination of Aarylboronic Esters and Further Rational Design

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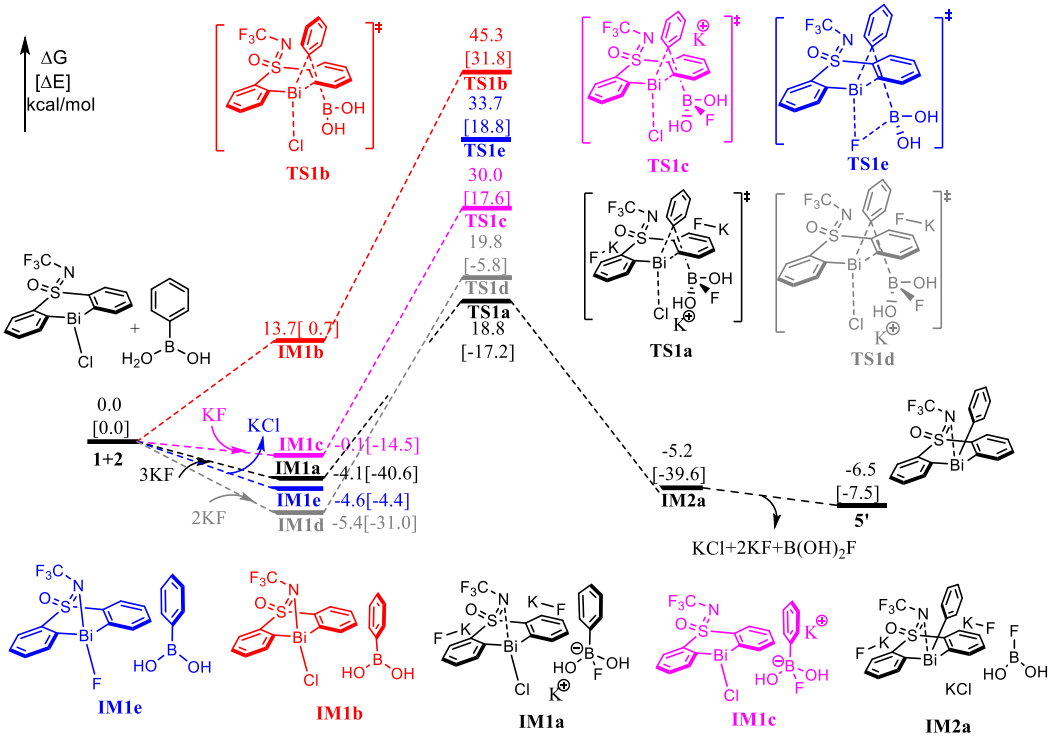
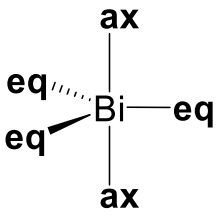


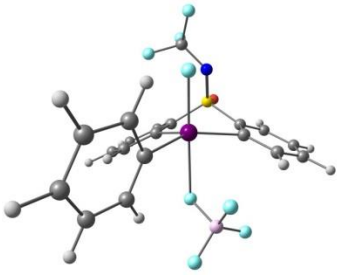
Fig. S1 Computed free energy profiles (in kcal/mol) of the aromatic ring attacking from above the Bi atom for stage I. The electronic energies (in kcal/mol) are given in brackets for reference.

Table S1. Isomers of **IM4A** are evaluated at the BP86+D3/def2-TZVPP (smd, solvent= Chloroform) level. In parenthesis, relative energies given in kcal/mol.



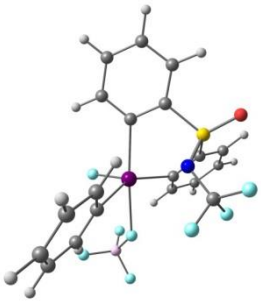
Pentavalent Bi^{V} species

Trans isomers

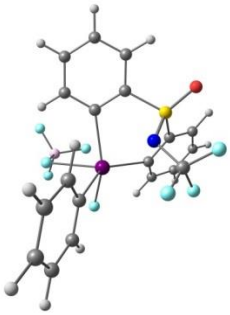


IM4D (4.1)

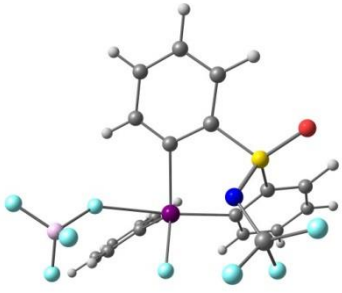
Cis isomers



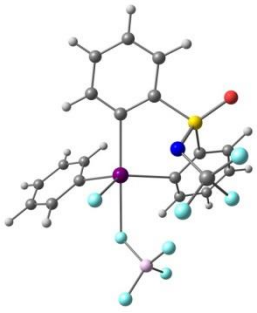
IM4A (10.7)



IM4B (5.7)



IM4C (0.0)



IM4E (9.0)

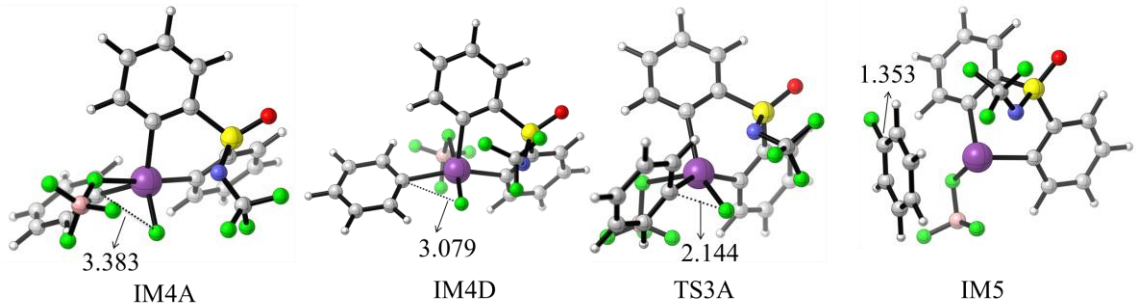


Fig. S2 Key optimized geometries according to the reaction pathway in Fig. 4. Key bond distances are given in Å. Color code, C: gray, H: white, F: green, K: blue, Bi: purple, S: yellow, O: red.

Table S2. Wiberg bond order(P) and Natural Charge(q) of Bi species calculated at the BP86+D3(BJ)/def2-TZVPP level with the NBO program.

Bi species					
	Natural Charge **q**			Wiberg bond orders **P**	
	TS3A	**7**		**TS3A**	**7**
Bi	1.815	1.553	Bi-C1	0.434	
C1	0.006		Bi-C2	0.598	0.711
C2	-0.415	-0.389	Bi-F1	0.388	
F1	-0.529		Bi-F2	0.107	0.184
F2	-0.548	-0.542	C1-F1	0.231	

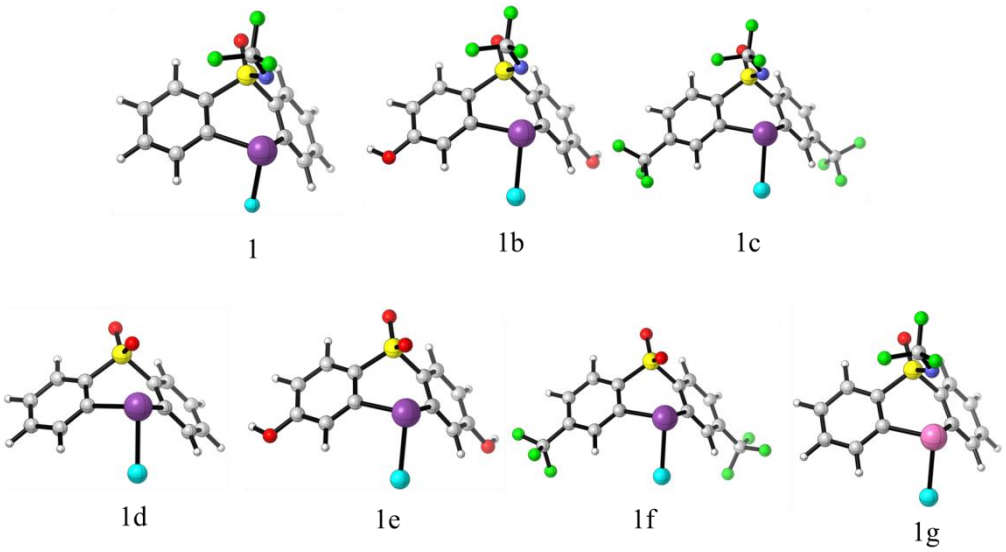


Fig. S3 Structures of several designed catalysts. color code, C: gray, H: white, F: green, Cl: indigo, O: red, S: yellow, N: blue and Sb: pink.

Table S3. Coordinates and energies (in hatree) of the calculated structures at the BP86+D3/def2-TZVPP (smd, solvent = Acetonitrile(TM)/ Chloroform (OA and RE))//BP86+D3/def2-SVP (smd, solvent = Acetonitrile(TM)/ Chloroform (OA and RE))

1

Energy = -2003.4860329

Bi	-1.00200	-0.80387	-0.72411
Cl	-3.24046	-1.2961	0.468976
S	1.545911	1.157403	0.202196
F	2.067177	-1.24606	-2.63056
F	2.863496	-1.4032	-0.59639
F	3.603035	0.148815	-1.93468
O	2.742819	1.98285	0.513825
N	1.422437	0.348216	-1.19536
C	-1.15003	1.450376	-0.23477
C	0.031015	2.120577	0.117344
C	0.090792	3.473804	0.476929
H	1.046576	3.943003	0.756128
C	-1.11387	4.198999	0.458849
H	-1.10862	5.267621	0.722826
C	-2.31865	3.560466	0.111101
H	-3.25846	4.135093	0.111034
C	-2.34181	2.192273	-0.23007
H	-3.29755	1.701734	-0.47549
C	0.167979	-0.94779	1.280034
C	1.22018	-0.04922	1.511215
C	1.978954	-0.01335	2.688547
H	2.789304	0.720685	2.814157
C	1.666496	-0.95272	3.687175
H	2.247669	-0.96703	4.622046
C	0.612003	-1.86462	3.494072
H	0.367424	-2.58954	4.286663
C	-0.141	-1.86021	2.301529
H	-0.98012	-2.56386	2.178114
C	2.46624	-0.50983	-1.56367

2

Energy = -408.4619375

C	-0.55368	-1.21316	-0.01757
C	0.177508	-0.000009	0.000027
C	-0.55366	1.213143	0.017589
C	-1.95898	1.217648	0.018742
C	-2.66496	0.000018	-0.000019
C	-1.95899	-1.21764	-0.01875
H	-0.00683	-2.17004	-0.03176
H	-0.00682	2.170028	0.031803
H	-2.50879	2.172732	0.034309
H	-3.7671	0.000016	-0.000045
H	-2.50883	-2.1727	-0.03433
B	1.7552	0.000009	0.000033
O	2.396939	-1.21695	0.038311
H	3.373766	-1.15143	0.030675
O	2.396978	1.216945	-0.03831
H	3.373804	1.151379	-0.03097

5

Energy = -1774.9193375

Bi	-0.61271	-0.41716	-1.0605
S	2.199954	0.754584	0.603176
F	2.929104	-1.2908	-2.4287
F	4.541732	-0.48736	-1.18949
F	3.119744	-1.90213	-0.33378
O	3.359226	1.258369	1.394042
N	2.365628	0.244005	-0.89898
C	0.198071	-1.12364	0.98613
C	1.335934	-0.5287	1.553295
C	1.846925	-0.87155	2.813568
H	2.741358	-0.36304	3.203682
C	1.187537	-1.87716	3.539502
H	1.568255	-2.17629	4.528375
C	0.044566	-2.49644	3.001922
H	-0.47304	-3.28174	3.575598
C	-0.45189	-2.11857	1.738855
H	-1.3619	-2.60198	1.347516
C	-0.23176	1.728966	-0.31012
C	0.958821	2.036835	0.367031
C	1.240352	3.295988	0.917344
H	2.188078	3.468487	1.449754
C	0.283047	4.311444	0.756584
H	0.47693	5.314087	1.167815

C	-0.91727	4.043169	0.074401
H	-1.66828	4.840399	-0.04455
C	-1.17656	2.761539	-0.44996
H	-2.13441	2.567307	-0.9595
C	-2.74973	-0.35903	-0.21559
C	-3.03585	0.178998	1.057239
H	-2.22457	0.588281	1.68173
C	-4.35633	0.19753	1.540297
H	-4.57055	0.619764	2.535815
C	-5.4032	-0.32152	0.755015
H	-6.43751	-0.30622	1.134505
C	-5.12645	-0.85916	-0.51371
H	-5.94309	-1.2668	-1.13177
C	-3.8028	-0.87727	-0.99665
H	-3.60198	-1.30374	-1.995
C	3.214525	-0.8214	-1.1843

5′

Energy = -1774.905813

Bi	0.377322	1.320042	1.232784
S	0.856492	-1.55214	-1.11541
F	-2.70694	-1.17952	-2.14994
F	-1.59085	-3.05606	-1.99006
F	-2.10213	-1.93854	-0.18947
O	1.506417	-2.72445	-1.77616
N	-0.53252	-1.00733	-1.64414
C	0.398819	-0.94512	1.608189
C	0.74268	-1.92616	0.661727
C	0.873974	-3.28641	0.988568
H	1.144572	-4.01013	0.205483
C	0.644357	-3.68824	2.314146
H	0.73727	-4.75118	2.585734
C	0.296673	-2.73321	3.283788
H	0.11328	-3.04529	4.3242
C	0.191727	-1.37309	2.934623
H	-0.05756	-0.63677	3.71766
C	1.733243	1.08682	-0.5978
C	1.907022	-0.0986	-1.33363
C	2.869421	-0.23321	-2.3481
H	2.970345	-1.1913	-2.87969
C	3.676178	0.871817	-2.66391
H	4.42858	0.786229	-3.46306
C	3.519602	2.07612	-1.95843
H	4.150811	2.944821	-2.20392
C	2.567741	2.174472	-0.92577
H	2.480777	3.120469	-0.36484
C	-1.59227	1.440551	0.085459
C	-2.78138	1.044571	0.725189
H	-2.75757	0.599923	1.734266
C	-4.01635	1.191127	0.065975
H	-4.94427	0.864734	0.563205
C	-4.06436	1.744615	-1.22512
H	-5.0308	1.855254	-1.74233
C	-2.87565	2.147201	-1.85975
H	-2.90819	2.57038	-2.8769
C	-1.63942	1.995028	-1.20702
H	-0.71171	2.289144	-1.72428
C	-1.67894	-1.77353	-1.49255

$B(OH)_2Cl$

Energy = -637.0071191

B	-0.48575	-7.8E-05	-2.1E-05
O	-1.18226	-1.16723	-6.2E-05
H	-0.61133	-1.9611	0.000195
O	-1.18035	1.16885	0.000115
H	-0.60528	1.959946	-0.00065
Cl	1.326251	-0.00067	0.000008

IM1A

Energy = -4511.8734344

Bi	0.69716	0.911194	0.000173
Cl	1.814491	3.125617	-0.96398
S	2.328637	-1.91596	0.644268
F	-0.85864	-0.98786	2.27439
F	0.94482	-1.91888	3.094952
F	-0.50585	-3.13212	2.010946
O	2.873742	-3.25977	0.97134
N	0.726306	-1.62601	0.783963
C	1.895385	-0.31735	-1.54384
C	2.508291	-1.4973	-1.09405
C	3.246651	-2.36753	-1.91101
H	3.710437	-3.27718	-1.49965
C	3.349508	-2.03134	-3.27276
H	3.90663	-2.6929	-3.95345
C	2.741586	-0.86025	-3.76176
H	2.827953	-0.60926	-4.83061
C	2.020013	-0.00369	-2.9052
H	1.556049	0.911704	-3.30462

C	2.573351	0.683482	1.382974
C	3.142452	-0.58811	1.547408
C	4.285173	-0.86106	2.311401
H	4.684461	-1.88332	2.391774
C	4.883921	0.224762	2.973274
H	5.776214	0.057571	3.595854
C	4.345344	1.518562	2.838122
H	4.825089	2.363243	3.357569
C	3.203784	1.751407	2.043705
H	2.813093	2.776531	1.938069
C	0.109231	-1.91493	2.014072
C	-1.91957	0.213125	-1.96757
C	-2.66945	0.216395	-0.75756
C	-2.8921	1.477505	-0.14723
C	-2.44899	2.685375	-0.72285
C	-1.72605	2.661375	-1.93157
C	-1.44922	1.417858	-2.53506
H	-1.65856	-0.73024	-2.50514
H	-3.43905	1.512121	0.811006
H	-2.70357	3.643934	-0.23586
H	-1.38746	3.595528	-2.41005
H	-0.86834	1.381778	-3.47164
B	-3.38568	-1.11057	-0.11447
O	-2.56344	-2.31531	-0.26406
H	-2.90462	-2.95203	0.396157
O	-3.81222	-0.9206	1.289405
H	-3.02145	-0.79515	1.844838
F	-4.66824	-1.29364	-0.83956
K	0.076215	5.22821	0.213492
F	-0.76082	-2.10011	-3.46164
K	-0.42861	-3.18908	-1.44126
K	-6.22712	0.004943	0.82075
F	-8.19696	-0.10057	1.967829

TS1A

Energy = -4511.8301021

Bi	0.061156	-0.33312	-0.81784
Cl	0.030817	-2.98113	-1.14857
S	2.895453	1.102138	0.687591
F	1.003711	2.714842	-1.95832
F	3.093549	2.987984	-1.36056
F	1.506129	4.129701	-0.37477
O	3.960577	1.853942	1.411524
N	1.61788	1.892088	0.083497
C	0.855588	-0.67189	1.340988
C	2.02329	-0.02486	1.785616
C	2.616303	-0.24347	3.041669
H	3.531831	0.295957	3.328012
C	2.0045	-1.16981	3.903485
H	2.441934	-1.36194	4.895099
C	0.839327	-1.84531	3.49439
H	0.362946	-2.57484	4.168066
C	0.271214	-1.59515	2.229287
H	-0.63692	-2.13806	1.926611
C	2.6127	-0.69364	-1.3285
C	3.569967	0.046827	-0.62437
C	4.961832	0.01754	-0.81628
H	5.640975	0.631844	-0.20495
C	5.438661	-0.83334	-1.82878
H	6.519881	-0.89474	-2.02833
C	4.530008	-1.60481	-2.58304
H	4.913422	-2.27266	-3.37225
C	3.140675	-1.53599	-2.33543
H	2.458468	-2.16913	-2.93136
C	1.826982	2.889505	-0.8655
C	-2.77478	-0.90951	1.287716
C	-2.36536	-0.70987	-0.05959
C	-3.06214	-1.43299	-1.06489
C	-4.12542	-2.3073	-0.76238
C	-4.51582	-2.48756	0.582529
C	-3.84262	-1.78126	1.600819
H	-2.27157	-0.34411	2.10866
H	-2.77809	-1.31145	-2.12826
H	-4.65108	-2.84957	-1.56679
H	-5.34564	-3.16983	0.83161
H	-4.15497	-1.91352	2.651773
B	-2.68464	1.733496	-0.40473
O	-1.3743	2.202327	-0.47564
H	-1.08594	2.495771	-1.36447
O	-3.5549	1.64889	-1.47482
H	-3.12546	1.439909	-2.32882
F	-3.29365	1.916942	0.807666
K	2.476062	-3.32874	0.606934
F	-1.30912	0.78516	3.270618
K	-0.34389	2.511605	2.057978
K	-5.75338	0.635381	-0.23863
F	-7.5702	0.141747	-1.48631

IM2A

Energy = -4511.8691711

Bi	-0.04534	-0.55483	-1.07788
Cl	0.275852	2.248885	2.967657
S	2.455007	-0.22248	1.416337
F	1.852492	-3.27833	0.281961
F	3.555449	-2.93064	1.600573
F	3.84933	-3.0551	-0.57492
O	3.412325	0.011308	2.531551
N	2.874027	-1.19291	0.19854
C	1.333939	1.253888	-0.65023
C	2.219924	1.277426	0.436487
C	3.065242	2.357307	0.738003
H	3.724102	2.31871	1.617881
C	3.04175	3.469018	-0.1225
H	3.703118	4.326041	0.076438
C	2.182689	3.478566	-1.2409
H	2.176685	4.345075	-1.92118
C	1.322172	2.386844	-1.49194
H	0.642071	2.420712	-2.3595
C	-0.16689	-1.0624	1.161776
C	0.881596	-0.81748	2.058717
C	0.812682	-1.08978	3.433309
H	1.669927	-0.86475	4.083759
C	-0.37406	-1.64195	3.937526
H	-0.45834	-1.86753	5.011734
C	-1.45225	-1.89918	3.070385
H	-2.38594	-2.3312	3.46401
C	-1.34748	-1.6103	1.697195
H	-2.20026	-1.82441	1.035686
C	3.021564	-2.5594	0.39695
C	-2.49919	1.313131	-2.04683
C	-1.84549	0.872497	-0.87622
C	-2.26448	1.374861	0.377458
C	-3.32003	2.311866	0.453378
C	-3.96309	2.753989	-0.72199
C	-3.55196	2.249149	-1.97052
H	-2.19485	0.927017	-3.03386
H	-1.74864	1.074441	1.306378
H	-3.6415	2.69435	1.437249
H	-4.78723	3.481925	-0.66057
H	-4.05454	2.583487	-2.89229
B	-3.31857	-2.55936	-1.4826
O	-2.16541	-3.04425	-2.01397
H	-1.74625	-3.7622	-1.49389
O	-3.95446	-2.92108	-0.32117
H	-3.5415	-3.66113	0.172599
F	-3.92457	-1.54669	-2.15027
K	-0.50556	3.911471	0.817026
F	5.852337	1.249831	-2.47815
K	4.054513	-0.02273	-2.02449
K	-5.0014	-0.40458	0.350562
F	-6.98637	0.404416	1.032015

IM1B

Energy = -2411.9700448

Bi	0.929685	-1.64666	0.096804
Cl	-0.98991	-2.66613	1.577725
S	1.230814	1.502168	-0.92591
F	4.203214	-0.77603	-1.2762
F	3.95082	0.837638	0.180786
F	4.177548	1.312274	-1.93306
O	1.483888	2.873058	-1.44147
N	2.219563	0.263714	-1.29947
C	-0.56687	-0.54824	-1.26079
C	-0.30315	0.798873	-1.5476
C	-1.11423	1.600788	-2.36042
H	-0.86506	2.65671	-2.54351
C	-2.23815	0.992054	-2.94656
H	-2.89782	1.586186	-3.59679
C	-2.51181	-0.3667	-2.71274
H	-3.39041	-0.8333	-3.1833
C	-1.688	-1.13588	-1.86581
H	-1.93266	-2.19181	-1.67673
C	0.991364	0.223012	1.467068
C	1.140427	1.484538	0.874337
C	1.276911	2.681252	1.588725
H	1.388779	3.641646	1.063722
C	1.277354	2.595703	2.991999
H	1.398031	3.509697	3.593331
C	1.114952	1.348123	3.624079
H	1.106827	1.292754	4.724079
C	0.959096	0.166388	2.869626
H	0.815844	-0.79803	3.382684
C	3.595324	0.420077	-1.0803
C	-3.96695	1.833514	-0.23052
C	-3.59533	0.622336	0.403411
C	-2.6114	0.686162	1.418032

C	-2.03112	1.908257	1.793216
C	-2.40257	3.096269	1.139588
C	-3.37373	3.056983	0.122035
H	-4.72911	1.807984	-1.02552
H	-2.2815	-0.23555	1.925084
H	-1.28178	1.933465	2.596698
H	-1.93441	4.052328	1.424573
H	-3.66747	3.983604	-0.39739
B	-4.27056	-0.73786	-0.02498
O	-3.82585	-1.98423	0.33519
H	-2.93924	-2.01669	0.770618
O	-5.40492	-0.6605	-0.80688
H	-5.72458	-1.5563	-1.04059

TS1B

Energy = -2411.9036442

Bi	0.382987	-0.37637	0.672282
Cl	2.145384	-2.85701	-0.53056
S	-2.73127	0.704379	-0.10047
F	-2.37761	-2.15079	2.296171
F	-3.07529	-2.23144	0.221408
F	-4.32343	-1.31118	1.752343
O	-4.13615	1.107264	-0.38581
N	-2.37332	-0.20826	1.180041
C	-0.31292	1.857011	0.520129
C	-1.65969	2.107699	0.209127
C	-2.22311	3.383901	0.067408
H	-3.28657	3.50262	-0.19052
C	-1.38206	4.49032	0.274517
H	-1.78699	5.509672	0.180775
C	-0.02922	4.28744	0.60062
H	0.630356	5.155437	0.759385
C	0.500243	2.986356	0.721788
H	1.565312	2.860512	0.966134
C	-0.69439	-0.62378	-1.40154
C	-1.99211	-0.10173	-1.54139
C	-2.75647	-0.18138	-2.71375
H	-3.7691	0.248269	-2.74866
C	-2.18977	-0.83565	-3.82049
H	-2.76202	-0.92273	-4.75695
C	-0.89981	-1.3852	-3.71924
H	-0.45797	-1.90728	-4.58282
C	-0.16013	-1.2835	-2.52299
H	0.83741	-1.74489	-2.46572
C	-3.02473	-1.4332	1.341081
C	3.274991	1.075831	0.835676
C	2.632422	0.20714	-0.0965
C	2.692227	0.566648	-1.47219
C	3.396035	1.700606	-1.90111
C	4.067953	2.506693	-0.96075
C	4.012578	2.190764	0.410246
H	3.226771	0.833839	1.910609
H	2.197531	-0.06913	-2.2231
H	3.431229	1.957752	-2.97186
H	4.633228	3.390038	-1.29879
H	4.533164	2.825375	1.145118
B	3.248492	-1.62113	0.418895
O	4.547653	-1.66902	-0.09596
H	5.162299	-1.24999	0.540031
O	3.027453	-1.64518	1.819106
H	2.620098	-2.48808	2.097308

IM1C

Energy = -3111.9484495

Bi	0.117333	0.653429	-0.92827
Cl	0.731194	3.15427	-1.24667
S	-2.30079	-0.54336	1.298854
F	-1.13857	-3.30473	-0.99869
F	-2.75938	-1.9119	-1.46661
F	-2.98135	-3.31328	0.186053
O	-3.32636	-1.02381	2.265089
N	-1.43835	-1.59812	0.434531
C	0.041947	0.946446	1.359419
C	-0.9769	0.355949	2.123797
C	-1.07212	0.467542	3.51921
H	-1.90101	-0.01044	4.06283
C	-0.07694	1.202372	4.185934
H	-0.11385	1.298313	5.281862
C	0.951663	1.820853	3.451896
H	1.722062	2.407787	3.976488
C	1.008643	1.699226	2.048661
H	1.810979	2.200801	1.486455
C	-2.1793	1.194335	-0.83111
C	-3.02499	0.6415	0.142764
C	-4.38333	0.960878	0.289785
H	-4.9875	0.494789	1.082705
C	-4.93238	1.888381	-0.61195
H	-5.99705	2.158404	-0.53615

C	-4.11941	2.471425	-1.60182
H	-4.55298	3.205226	-2.30016
C	-2.75455	2.133791	-1.70634
H	-2.13196	2.624628	-2.47264
C	-2.08522	-2.48435	-0.42069
C	4.051412	0.551326	1.149349
C	3.363289	-0.30443	0.25839
C	3.4212	0.029407	-1.11901
C	4.106636	1.168219	-1.58244
C	4.76737	2.008828	-0.6683
C	4.74469	1.691772	0.702679
H	4.023527	0.3228	2.228609
H	2.910663	-0.61356	-1.85796
H	4.117135	1.407189	-2.65859
H	5.297504	2.907711	-1.02283
H	5.262193	2.343358	1.426441
B	2.485621	-1.5687	0.80187
O	2.198915	-1.57319	2.215915
H	1.878532	-0.69183	2.484523
O	1.232212	-1.64883	-0.03202
H	0.441251	-1.81796	0.536728
F	3.205821	-2.83656	0.516121
K	1.664074	-3.8298	-1.3251

TS1C

Energy = -3111.8933397

Bi	0.214693	0.169956	-0.76231
Cl	1.388953	2.516917	-1.12222
S	-2.67459	-0.32465	1.057178
F	-1.8747	-2.5974	-1.78066
F	-3.72162	-1.54009	-1.26542
F	-3.16006	-3.34232	-0.18004
O	-3.8731	-0.72382	1.845861
N	-1.88223	-1.45533	0.178695
C	-0.12294	0.622427	1.487555
C	-1.34259	0.278523	2.091679
C	-1.65274	0.50373	3.441689
H	-2.63387	0.213977	3.847586
C	-0.67178	1.113171	4.24142
H	-0.87299	1.295901	5.308075
C	0.553741	1.501215	3.670308
H	1.313258	2.000849	4.292366
C	0.823282	1.258842	2.308891
H	1.788823	1.57732	1.889741
C	-1.94153	1.442268	-0.87685
C	-3.01494	1.052651	-0.06805
C	-4.28392	1.650242	-0.02655
H	-5.07079	1.279926	0.648536
C	-4.49778	2.735849	-0.89315
H	-5.47786	3.237659	-0.91034
C	-3.45584	3.178004	-1.73275
H	-3.62978	4.034439	-2.40502
C	-2.1959	2.543033	-1.72021
H	-1.39608	2.925724	-2.37801
C	-2.65792	-2.19787	-0.72009
C	3.208304	-0.71894	1.229643
C	2.568524	-0.85086	-0.03071
C	3.414224	-0.81993	-1.17133
C	4.816494	-0.68636	-1.07233
C	5.418772	-0.56445	0.199531
C	4.607329	-0.57988	1.355983
H	2.599436	-0.76575	2.149929
H	2.967979	-0.92485	-2.17946
H	5.444819	-0.68299	-1.97969
H	6.513221	-0.46646	0.289256
H	5.072738	-0.49298	2.352892
B	1.343791	-2.80781	0.054448
O	0.500471	-2.68248	1.14473
H	-0.39142	-2.31805	0.91409
O	0.912781	-2.86513	-1.27861
H	-0.05793	-2.91543	-1.36644
F	2.509813	-3.50024	0.307381
K	4.216311	2.355222	-0.22511

TS1D

Energy = -3811.8639432

Bi	-0.21258	0.955816	-0.50344
Cl	0.647521	3.101808	0.771918
S	-2.66385	-1.18211	0.543583
F	-1.84341	-0.90034	-3.12515
F	-3.70149	-0.38811	-2.08582
F	-3.14906	-2.47575	-2.3491
O	-3.66903	-2.23659	0.845967
N	-1.8676	-1.21755	-0.89395
C	-0.21889	-0.29867	1.434196
C	-1.25864	-1.22053	1.651291
C	-1.29201	-2.13774	2.711765
H	-2.13738	-2.83279	2.828832

C	-0.19782	-2.14473	3.597682
H	-0.17013	-2.87645	4.41999
C	0.852642	-1.22316	3.429266
H	1.745989	-1.26192	4.067632
C	0.825042	-0.29326	2.368987
H	1.662982	0.408522	2.255325
C	-2.46861	1.524042	0.33841
C	-3.33917	0.487501	0.697115
C	-4.6419	0.638202	1.196085
H	-5.25952	-0.23391	1.460512
C	-5.11673	1.95387	1.333504
H	-6.13599	2.130383	1.710875
C	-4.28593	3.039026	0.990961
H	-4.66434	4.067867	1.107511
C	-2.97813	2.826577	0.505948
H	-2.3464	3.698358	0.263158
C	-2.6435	-1.24673	-2.06168
C	3.365332	-0.17974	0.139972
C	2.387727	0.125587	-0.85101
C	2.847211	0.908461	-1.94549
C	4.187326	1.329659	-2.08549
C	5.139663	0.96276	-1.11043
C	4.71995	0.204248	0.003171
H	3.140878	-0.77067	1.05487
H	2.133936	1.178027	-2.74881
H	4.496548	1.92995	-2.95838
H	6.194881	1.263342	-1.21861
H	5.446494	-0.09662	0.778618
B	1.461767	-1.84306	-1.77234
O	0.629846	-2.41796	-0.8157
H	-0.31677	-2.10894	-0.85632
O	1.043409	-1.34423	-2.99484
H	0.075846	-1.22683	-3.05251
F	2.730606	-2.40787	-1.77124
K	3.605348	2.880587	0.94631
F	3.493768	-2.04463	2.595885
K	2.397091	-3.31593	0.961175

IM1D

Energy = -3811.8394326

Bi	-0.49532	0.919753	-0.71413
Cl	0.237893	3.336045	0.1415
S	-2.42092	-1.29325	0.898517
F	-1.95631	-1.75404	-2.81665
F	-3.74038	-1.03169	-1.77726
F	-3.1016	-3.0992	-1.52802
O	-3.27262	-2.37222	1.463401
N	-1.76507	-1.46083	-0.59464
C	0.005928	-0.0962	1.314368
C	-0.90756	-1.03567	1.815038
C	-0.64972	-1.89226	2.896657
H	-1.40896	-2.61242	3.238041
C	0.626767	-1.82857	3.480975
H	0.883071	-2.52107	4.297986
C	1.586462	-0.92075	2.991648
H	2.637844	-0.98918	3.313798
C	1.256465	-0.03999	1.94431
H	2.046601	0.60036	1.527039
C	-2.59749	1.344009	0.238922
C	-3.27357	0.293287	0.876557
C	-4.51645	0.41353	1.513928
H	-4.98896	-0.45228	2.001955
C	-5.12882	1.678431	1.491031
H	-6.11144	1.817051	1.967747
C	-4.48535	2.761855	0.863198
H	-4.97001	3.751213	0.855189
C	-3.22701	2.600892	0.2476
H	-2.73226	3.468747	-0.21775
C	-2.63118	-1.82538	-1.63928
C	3.751877	-0.12138	-0.13452
C	2.804291	-0.15318	-1.19608
C	2.7599	0.988105	-2.03906
C	3.616857	2.094302	-1.86887
C	4.577479	2.081365	-0.83927
C	4.631582	0.969105	0.030717
H	3.827295	-0.94112	0.617003
H	2.036394	0.992897	-2.87123
H	3.549143	2.958356	-2.5507
H	5.285963	2.920448	-0.72408
H	5.373974	0.945172	0.848475
B	1.865203	-1.46363	-1.55397
O	1.167184	-2.09179	-0.41555
H	0.194362	-2.04096	-0.5273
O	0.925394	-1.05242	-2.59796
H	0.301556	-1.77931	-2.78698
F	2.800218	-2.51523	-2.03479
K	2.889469	3.289604	1.464198
F	4.078646	-2.13663	2.124476

K	2.922077	-3.59701	0.65148

TS1F

Energy = -5211.7987588

Bi	-0.46041	-0.53045	-0.55473
S	2.681344	0.491653	-0.12057
F	2.08101	-2.73555	-1.94186
F	2.848932	-2.49179	0.094009
F	4.075025	-1.89749	-1.60603
O	4.119031	0.853277	0.001402
N	2.189263	-0.63303	-1.17789
C	0.30152	1.627685	-0.92043
C	1.663447	1.863917	-0.67588
C	2.289002	3.110895	-0.8176
H	3.361652	3.229777	-0.60121
C	1.497048	4.185327	-1.25596
H	1.951528	5.179077	-1.38862
C	0.131058	3.985753	-1.52772
H	-0.48563	4.831439	-1.87106
C	-0.46506	2.719803	-1.3606
H	-1.5389	2.599901	-1.56703
C	0.660593	-0.43863	1.482928
C	1.990921	0.00933	1.477718
C	2.798047	0.101708	2.620095
H	3.833854	0.466494	2.548223
C	2.235097	-0.30122	3.842909
H	2.838859	-0.2565	4.76247
C	0.904218	-0.75637	3.887491
H	0.465541	-1.05979	4.851562
C	0.115999	-0.8216	2.720292
H	-0.94025	-1.1191	2.792185
C	2.789763	-1.89701	-1.14448
C	-3.28852	-1.45189	0.504159
C	-2.86814	-0.1534	0.085562
C	-3.43764	0.328536	-1.13361
C	-4.3734	-0.41589	-1.86738
C	-4.76841	-1.69004	-1.41211
C	-4.22537	-2.20682	-0.22042
H	-2.87163	-1.87033	1.435986
H	-3.14986	1.325891	-1.50447
H	-4.79923	-0.00709	-2.79804
H	-5.50073	-2.27934	-1.98715
H	-4.53474	-3.20101	0.140892
B	-2.67915	1.156726	1.546945
O	-2.76405	0.368785	2.733956
H	-3.67006	0.030802	2.86214
O	-3.71224	2.084256	1.22293
H	-4.58126	1.642543	1.185955
F	-1.43153	1.796455	1.480973

IM3A

Energy = -3467.0853791

C	2.388561	-0.92402	2.224202
C	1.186107	-1.5689	2.515785
C	0.781136	-2.65628	1.724641
C	1.568722	-3.09078	0.649735
C	2.788483	-2.4603	0.384528
H	0.569611	-1.18476	3.338934
H	-0.18037	-3.14654	1.926354
H	1.250341	-3.91352	-0.00384
N	3.152688	-1.42028	1.199128
F	4.342235	-0.83469	0.97296
Cl	3.857084	-2.91976	-0.84667
Cl	2.970292	0.448229	3.049158
B	2.74887	0.426094	-2.42174
F	1.360335	0.645095	-2.69849
F	3.19783	-0.68978	-3.1328
F	3.483188	1.571511	-2.7382
F	2.876796	0.167861	-1.00759
Bi	-0.00389	0.393652	-0.25482
S	-3.09073	-1.07247	0.521935
F	-1.33461	-4.15198	-0.4199
F	-3.0165	-3.14292	-1.40667
F	-0.96566	-2.46954	-1.75571
O	-4.45394	-1.59056	0.833289
N	-1.86825	-2.08882	0.335452
C	-2.00553	0.656618	-1.36615
C	-3.17677	0.018487	-0.92431
C	-4.42095	0.144997	-1.56269
H	-5.30159	-0.38228	-1.16621
C	-4.49161	0.950836	-2.71037
H	-5.45127	1.066347	-3.23769
C	-3.33789	1.603174	-3.18355
H	-3.39678	2.23323	-4.0854
C	-2.10552	1.460444	-2.51737
H	-1.21302	1.979635	-2.90158
C	-1.2465	0.611211	1.71449
C	-2.46997	-0.05578	1.872071

C	-3.28254	0.033909	3.013919
H	-4.2424	-0.50285	3.058462
C	-2.82195	0.822057	4.081395
H	-3.42656	0.908063	4.997545
C	-1.59622	1.50593	3.97039
H	-1.24518	2.134948	4.804412
C	-0.82301	1.408343	2.797247
H	0.11858	1.976975	2.722722
C	0.398832	2.645887	-0.15569
C	1.737737	3.087273	-0.14986
H	2.559155	2.360792	-0.2526
C	2.030113	4.459494	-0.02505
H	3.079634	4.796736	-0.02618
C	0.987975	5.395973	0.088961
H	1.21731	6.469901	0.181478
C	-0.35015	4.959023	0.080573
H	-1.1705	5.690457	0.16791
C	-0.64351	3.58842	-0.03849
H	-1.69497	3.256814	-0.03751
C	-1.82216	-2.91999	-0.77652

TS2A

Energy = -3467.0628954

C	1.984483	-2.48718	-1.24458
C	2.87177	-3.36908	-0.61945
C	2.377214	-4.2774	0.327106
C	1.009653	-4.29435	0.638621
C	0.157201	-3.39452	-0.00762
H	3.936353	-3.32105	-0.88565
H	3.061249	-4.98374	0.819477
H	0.584385	-4.98415	1.380696
N	0.679101	-2.47106	-0.86263
F	-0.32097	-2.14534	-2.10679
Cl	-1.51424	-3.27229	0.321276
Cl	2.490005	-1.38498	-2.45296
B	-3.37938	-0.75894	1.94862
F	-1.93513	-0.63562	1.93667
F	-3.76015	-1.30462	3.178722
F	-3.9269	0.530829	1.779851
F	-3.76018	-1.5985	0.884993
Bi	-0.45504	0.105837	-0.19333
S	2.525469	1.591108	0.525553
F	3.648264	-1.46938	1.838308
F	2.678346	0.156729	2.929989
F	1.48279	-1.47698	2.087115
O	3.803641	2.276483	0.860982
N	2.394365	-0.00331	0.6107
C	-0.11785	1.765094	1.356166
C	1.168208	2.313981	1.489302
C	1.455985	3.37697	2.356699
H	2.481502	3.769157	2.429221
C	0.402441	3.900592	3.126185
H	0.599186	4.729678	3.823406
C	-0.89054	3.357705	3.019399
H	-1.70895	3.764439	3.6342
C	-1.15664	2.284476	2.144508
H	-2.16481	1.844286	2.08912
C	0.842399	1.340404	-1.64824
C	2.059957	1.864063	-1.18691
C	2.936747	2.616939	-1.98013
H	3.873203	3.011293	-1.5573
C	2.572996	2.840089	-3.31982
H	3.243003	3.416136	-3.97648
C	1.357505	2.333586	-3.81537
H	1.076772	2.518992	-4.86439
C	0.493969	1.591001	-2.98548
H	-0.45384	1.199651	-3.39002
C	-2.41369	0.669297	-1.22909
C	-2.98975	-0.27968	-2.08158
H	-2.54338	-1.28128	-2.20184
C	-4.15295	0.066116	-2.7968
H	-4.61622	-0.6699	-3.47319
C	-4.72279	1.340937	-2.63538
H	-5.63896	1.605855	-3.18687
C	-4.13539	2.276083	-1.7647
H	-4.58302	3.275027	-1.63737
C	-2.97306	1.942612	-1.04348
H	-2.51801	2.676232	-0.36065
C	2.552656	-0.65271	1.835095

TS2E

Energy = -3467.0565978

C	1.984483	-2.48718	-1.24458
C	2.87177	-3.36908	-0.61945
C	2.377214	-4.2774	0.327106
C	1.009653	-4.29435	0.638621
C	0.157201	-3.39452	-0.00762
H	3.936353	-3.32105	-0.88565

H	3.061249	-4.98374	0.819477
H	0.584385	-4.98415	1.380696
N	0.679101	-2.47106	-0.86263
F	-0.32097	-2.14534	-2.10679
Cl	-1.51424	-3.27229	0.321276
Cl	2.490005	-1.38498	-2.45296
B	-3.37938	-0.75894	1.94862
F	-1.93513	-0.63562	1.93667
F	-3.76015	-1.30462	3.178722
F	-3.9269	0.530829	1.779851
F	-3.76018	-1.5985	0.884993
Bi	-0.45504	0.105837	-0.19333
S	2.525469	1.591108	0.525553
F	3.648264	-1.46938	1.838308
F	2.678346	0.156729	2.929989
F	1.48279	-1.47698	2.087115
O	3.803641	2.276483	0.860982
N	2.394365	-0.00331	0.6107
C	-0.11785	1.765094	1.356166
C	1.168208	2.313981	1.489302
C	1.455985	3.37697	2.356699
H	2.481502	3.769157	2.429221
C	0.402441	3.900592	3.126185
H	0.599186	4.729678	3.823406
C	-0.89054	3.357705	3.019399
H	-1.70895	3.764439	3.6342
C	-1.15664	2.284476	2.144508
H	-2.16481	1.844286	2.08912
C	0.842399	1.340404	-1.64824
C	2.059957	1.864063	-1.18691
C	2.936747	2.616939	-1.98013
H	3.873203	3.011293	-1.5573
C	2.572996	2.840089	-3.31982
H	3.243003	3.416136	-3.97648
C	1.357505	2.333586	-3.81537
H	1.076772	2.518992	-4.86439
C	0.493969	1.591001	-2.98548
H	-0.45384	1.199651	-3.39002
C	-2.41369	0.669297	-1.22909
C	-2.98975	-0.27968	-2.08158
H	-2.54338	-1.28128	-2.20184
C	-4.15295	0.066116	-2.7968
H	-4.61622	-0.6699	-3.47319
C	-4.72279	1.340937	-2.63538
H	-5.63896	1.605855	-3.18687
C	-4.13539	2.276083	-1.7647
H	-4.58302	3.275027	-1.63737
C	-2.97306	1.942612	-1.04348
H	-2.51801	2.676232	-0.36065
C	2.552656	-0.65271	1.835095

TS2C

Energy = -3467.0628954

C	-3.67775	1.129877	0.807236
C	-4.99516	0.801279	0.489585
C	-5.48481	-0.46693	0.834707
C	-4.64529	-1.40377	1.456324
C	-3.33243	-1.04126	1.750898
H	-5.61147	1.541537	-0.03695
H	-6.52652	-0.73254	0.603938
H	-4.98242	-2.42065	1.700884
N	-2.8725	0.189618	1.382103
F	-1.89366	0.809657	2.406459
Cl	-2.1853	-2.12037	2.425907
Cl	-2.96001	2.632606	0.414457
B	-3.0286	-0.43232	-2.219
F	-2.93056	-1.22664	-3.36703
F	-4.20595	0.322446	-2.2209
F	-2.98451	-1.2708	-1.06167
F	-1.89471	0.446093	-2.14011
Bi	-0.24189	-0.10315	0.023911
S	3.254121	-1.09372	-0.23843
F	3.607626	1.719678	0.930889
F	5.258921	1.172498	-0.38317
F	3.688667	2.506758	-1.11072
O	4.556156	-1.82322	-0.18529
N	3.151081	0.342398	-0.90283
C	0.735088	-1.64049	-1.37351
C	2.083796	-2.01696	-1.2475
C	2.636707	-3.09914	-1.95014
H	3.699919	-3.34867	-1.81339
C	1.811696	-3.8234	-2.82593
H	2.229093	-4.67054	-3.39169
C	0.463633	-3.46146	-2.97494
H	-0.18769	-4.02417	-3.66207
C	-0.07881	-2.38643	-2.24313
H	-1.14508	-2.14792	-2.35857
C	1.301582	-0.52819	1.707749

C	2.588741	-1.0367	1.453068
C	3.481261	-1.40155	2.473499
H	4.477341	-1.78907	2.211677
C	3.07666	-1.24604	3.809247
H	3.763058	-1.52381	4.624024
C	1.801156	-0.73342	4.096512
H	1.481733	-0.60362	5.142712
C	0.917414	-0.39303	3.053184
H	-0.08765	-0.01825	3.30356
C	0.449258	1.983864	-0.54554
C	0.733542	2.865489	0.508973
H	0.715861	2.525537	1.556894
C	1.062323	4.200694	0.211118
H	1.303093	4.898031	1.029671
C	1.085657	4.638718	-1.1245
H	1.339398	5.685743	-1.35476
C	0.785396	3.744176	-2.16755
H	0.807335	4.086281	-3.2148
C	0.454046	2.407043	-1.88289
H	0.205654	1.712255	-2.69823
C	3.901382	1.38908	-0.37649

TS2B

Energy = -3467.0582716

C	3.501045	1.698376	-0.4306
C	4.744801	1.715163	0.198662
C	5.503748	0.536418	0.229747
C	5.003593	-0.64269	-0.34394
C	3.757204	-0.61906	-0.9665
H	5.086841	2.643701	0.675891
H	6.489002	0.531733	0.717242
H	5.553992	-1.59189	-0.30044
N	3.021326	0.531337	-0.94822
F	2.232871	0.729175	-2.27433
Cl	3.040324	-1.99148	-1.69543
Cl	2.444311	3.046557	-0.46873
B	2.698127	-0.78443	2.36644
F	2.161897	-0.98283	3.643371
F	1.938302	-1.53171	1.400784
F	2.580408	0.592439	2.007555
F	4.038792	-1.1848	2.316489
Bi	0.212032	0.147504	-0.0973
S	-3.34276	0.896819	0.055968
F	-2.89488	-1.90813	1.415838
F	-4.94314	-1.50835	0.782447
F	-3.6509	-2.78479	-0.43833
O	-4.68065	1.534706	0.235988
N	-3.21363	-0.58814	-0.47838
C	-1.06415	1.510311	-1.47102
C	-2.41573	1.793673	-1.2035
C	-3.15951	2.738487	-1.92729
H	-4.21264	2.920231	-1.6643
C	-2.53308	3.4173	-2.98531
H	-3.09984	4.15803	-3.5702
C	-1.19017	3.144094	-3.29115
H	-0.69621	3.670578	-4.12306
C	-0.46023	2.209177	-2.53054
H	0.600364	2.033988	-2.76998
C	-1.09204	0.661462	1.735429
C	-2.43293	1.070151	1.616169
C	-3.18231	1.521565	2.714237
H	-4.23156	1.818636	2.566402
C	-2.56855	1.568575	3.976443
H	-3.14261	1.915523	4.849545
C	-1.22901	1.172961	4.115779
H	-0.7419	1.205911	5.103038
C	-0.4861	0.736439	3.000215
H	0.567228	0.455726	3.135715
C	-0.42087	-1.88631	-0.90121
C	-0.24087	-3.03652	-0.11866
H	0.137047	-2.96755	0.911269
C	-0.54989	-4.29086	-0.67766
H	-0.42914	-5.20043	-0.06735
C	-1.00557	-4.38331	-2.00433
H	-1.23915	-5.36868	-2.43816
C	-1.16552	-3.22024	-2.7789
H	-1.53023	-3.28915	-3.8165
C	-0.87145	-1.95953	-2.22863
H	-1.01443	-1.0492	-2.83219
C	-3.66235	-1.64941	0.301879

IM4A

Energy = -2299.402171

S	2.766059	0.412017	-0.48236
C	0.29408	0.888154	-1.68824
C	1.689661	0.896432	-1.8398
C	2.288876	1.363713	-3.01629
H	3.385886	1.370242	-3.10497

C	1.455171	1.84033	-4.04449
H	1.907374	2.222928	-4.97196
C	0.059806	1.849592	-3.88591
C	-0.53821	1.365758	-2.70242
H	-1.62994	1.382705	-2.5733
C	1.182218	-1.75485	0.219378
C	2.466442	-1.35365	-0.19057
C	3.538387	-2.25092	-0.26927
H	4.530755	-1.89562	-0.58596
C	3.30708	-3.5935	0.082951
H	4.135957	-4.3164	0.037542
C	2.032329	-4.00853	0.502228
C	0.959823	-3.09316	0.564821
H	-0.03568	-3.43164	0.892608
C	-2.40037	-1.45527	-0.11148
C	-3.57166	-1.0036	0.505334
H	-3.60571	-0.0544	1.061928
C	-4.72153	-1.80453	0.366775
H	-5.6599	-1.47701	0.841238
C	-4.67646	-2.99986	-0.37262
H	-5.58493	-3.61365	-0.47543
C	-3.48162	-3.41635	-0.98462
H	-3.44718	-4.35014	-1.5676
C	-2.31274	-2.64077	-0.85534
H	-1.37382	-2.96544	-1.33002
O	4.191854	0.601362	-0.85672
F	-1.70342	3.360884	1.269851
H	-0.58414	2.24203	-4.68809
H	1.86278	-5.05778	0.789883
C	2.547207	1.13403	1.998355
F	-3.53236	3.408984	-0.14405
B	-2.74886	2.643767	0.713423
F	-3.5227	1.992019	1.681466
F	-2.14627	1.567933	-0.14678
F	-0.59327	0.455812	2.016297
Bi	-0.51945	-0.24212	0.086413
N	2.040368	1.210751	0.687371
F	3.869007	1.47306	2.083743
F	1.862297	1.982191	2.7847
F	2.452477	-0.11148	2.568304

IM4B

Energy = -2299.4101457

S	-2.43886	0.272123	0.823413
C	-0.10869	-1.02832	1.603549
C	-1.47089	-0.81688	1.87397
C	-2.11544	-1.38489	2.981088
H	-3.18486	-1.19215	3.156857
C	-1.34744	-2.17573	3.853104
H	-1.82479	-2.63064	4.734246
C	0.020891	-2.37618	3.607244
C	0.649336	-1.80977	2.477845
H	1.712927	-1.99812	2.281675
C	-1.26943	-0.5973	-1.50546
C	-2.48093	-0.50043	-0.80514
C	-3.69249	-0.9337	-1.35944
H	-4.62822	-0.83589	-0.78859
C	-3.66305	-1.47292	-2.65812
H	-4.60048	-1.81324	-3.12375
C	-2.45025	-1.57611	-3.36257
C	-1.23511	-1.1491	-2.78618
H	-0.27853	-1.24093	-3.32096
C	1.858893	1.737134	0.058113
C	1.778949	2.27488	1.345707
H	1.109914	1.853327	2.111411
C	2.579512	3.399057	1.622971
H	2.540847	3.853572	2.625411
C	3.41659	3.9354	0.627929
H	4.037811	4.815687	0.855526
C	3.471244	3.355906	-0.6519
H	4.132564	3.775001	-1.42663
C	2.686047	2.226791	-0.95597
H	2.724648	1.742547	-1.94206
O	-3.81823	0.451969	1.339312
F	2.619834	-1.47035	0.200938
H	0.619057	-2.99168	4.297008
H	-2.44171	-1.9991	-4.37921
C	-1.76209	2.641837	-0.01196
F	3.113359	-3.1202	-1.37813
B	2.293532	-2.82211	-0.31568
F	0.91857	-2.69759	-0.72486
F	2.406587	-3.72057	0.732283
F	1.683255	-0.41339	-2.17597
Bi	0.636428	-0.09876	-0.36942
F	-0.79703	3.575946	0.129798
F	-2.92947	3.187316	0.424359
F	-1.92019	2.447074	-1.36239

N	-1.38444	1.48672	0.703917

IM4C

Energy = -2299.4183907

S	2.601598	-0.07745	-0.76572
C	1.44541	-1.05918	1.528808
C	2.652096	-0.90108	0.827873
C	3.891849	-1.3148	1.330529
H	4.813203	-1.16349	0.747894
C	3.902909	-1.93117	2.595069
H	4.857215	-2.2804	3.017615
C	2.70847	-2.09657	3.318517
C	1.475449	-1.652	2.796072
H	0.549467	-1.76434	3.380912
C	0.740428	1.795024	0.080111
C	2.048405	1.606565	-0.39615
C	2.906159	2.692492	-0.61428
H	3.922902	2.523349	-1.00014
C	2.417792	3.983725	-0.34439
H	3.06844	4.854202	-0.51829
C	1.10973	4.167774	0.134563
C	0.250639	3.069055	0.357724
H	-0.77669	3.213006	0.728356
C	-1.74307	-1.75406	-0.16258
C	-1.09925	-2.94378	-0.51298
H	-0.00359	-3.04454	-0.50351
C	-1.92386	-4.01811	-0.89978
H	-1.45777	-4.97285	-1.18996
C	-3.32183	-3.86852	-0.9171
H	-3.95638	-4.71526	-1.22192
C	-3.91625	-2.64946	-0.54844
H	-5.01143	-2.53384	-0.55822
C	-3.12221	-1.55093	-0.16048
H	-3.57554	-0.59423	0.138865
O	3.921814	-0.05356	-1.43974
F	-1.24775	0.348818	2.397982
H	2.733512	-2.5716	4.311614
H	0.735592	5.183224	0.337595
F	-3.94731	2.793367	-0.81073
B	-3.34736	2.148593	0.263667
F	-2.80126	3.057943	1.180517
F	-4.22188	1.257324	0.896968
F	-2.22629	1.347512	-0.28566
Bi	-0.38696	-0.11342	0.567819
N	1.313398	-0.81666	-1.40288
C	0.967926	-0.52317	-2.74183
F	0.793778	0.809415	-3.00453
F	1.896291	-0.96349	-3.63008
F	-0.19927	-1.13852	-3.02847

IM4D

Energy = -2299.413225

Bi	-0.58069	-0.11955	-0.44938
S	2.807006	0.303682	0.257372
C	0.540108	-0.90594	1.336606
C	1.857545	-0.48623	1.58372
C	2.51603	-0.79595	2.781072
H	3.552193	-0.46023	2.937095
C	1.823538	-1.54426	3.749806
H	2.324757	-1.80073	4.695626
C	0.504115	-1.96553	3.514296
C	-0.15149	-1.63468	2.310657
H	-1.19419	-1.94733	2.140236
C	0.623558	1.76446	-0.81604
C	1.921362	1.787487	-0.27259
C	2.659018	2.97903	-0.2461
H	3.67295	2.972069	0.182767
C	2.092779	4.142666	-0.79514
H	2.667029	5.081308	-0.78239
C	0.811981	4.105509	-1.3643
C	0.057052	2.913964	-1.36548
H	-0.96648	2.904096	-1.76179
C	-2.62363	-1.09001	-0.45842
C	-2.86187	-1.97627	-1.51231
H	-2.12341	-2.12368	-2.31321
C	-4.08351	-2.67802	-1.49299
H	-4.3078	-3.38209	-2.30973
C	-4.99995	-2.48109	-0.44605
H	-5.95195	-3.03434	-0.44135
C	-4.71128	-1.58117	0.594385
H	-5.42924	-1.42373	1.414585
C	-3.50213	-0.85786	0.602852
H	-3.28528	-0.14156	1.405415
F	-1.45778	1.310992	1.39759
O	4.13373	0.688176	0.811277
N	2.63587	-0.55532	-1.05867
C	3.059605	-1.88794	-1.10276
F	3.035775	-2.31797	-2.38272

F	4.332432	-2.08733	-0.63479
F	2.271516	-2.75529	-0.38504
H	-0.02965	-2.55506	4.275724
H	0.371563	5.014383	-1.80209
F	-0.02325	-1.27512	-2.09689
B	-2.40962	2.334036	0.88912
F	-2.59989	1.990072	-0.48037
F	-1.8243	3.578011	1.02195
F	-3.58838	2.203627	1.605538

IM4E

Energy = -2299.4013121

S	-2.57114	0.959617	0.156018
C	-0.16741	2.215599	-0.4211
C	-1.51142	2.395367	-0.0532
C	-2.07931	3.663103	0.120765
H	-3.13552	3.761763	0.413593
C	-1.26351	4.787227	-0.10563
H	-1.68761	5.795876	0.013296
C	0.078935	4.627746	-0.48759
C	0.63714	3.3404	-0.63759
H	1.69604	3.224695	-0.91969
C	-0.59582	-0.55801	1.428069
C	-1.86529	0.027172	1.548982
C	-2.63539	-0.1688	2.703152
H	-3.63529	0.285623	2.773111
C	-2.10604	-0.96346	3.735884
H	-2.70257	-1.13783	4.644232
C	-0.83378	-1.54431	3.609003
C	-0.0563	-1.34073	2.449102
H	0.928615	-1.81569	2.340225
C	2.870748	0.540307	0.015858
C	3.826598	-0.03135	-0.83065
H	3.541954	-0.70667	-1.65062
C	5.177655	0.280896	-0.5892
H	5.954019	-0.15354	-1.23848
C	5.533282	1.132088	0.47252
H	6.594242	1.36435	0.654204
C	4.546133	1.685503	1.306182
H	4.825781	2.348657	2.139892
C	3.186164	1.393669	1.081846
H	2.409293	1.826229	1.732584
O	-3.95689	1.36447	0.510942
F	0.889583	-4.02629	1.032987
H	0.706926	5.513553	-0.67027
H	-0.43221	-2.17842	4.414435
N	-2.19196	0.160165	-1.16576
C	-2.92138	-1.0055	-1.47741
F	-0.4109	-2.86097	-0.48403
B	0.870746	-3.34135	-0.1813
F	1.415158	-4.08218	-1.21791
F	0.656235	-0.55345	-2.24872
F	1.720446	-2.12786	0.000375
Bi	0.692505	0.114874	-0.31078
F	-2.28778	-1.67708	-2.45372
F	-3.10281	-1.86434	-0.42593
F	-4.17819	-0.71991	-1.93448

TS3C

Energy = -2299.3820467

Bi	0.433896	0.107458	-0.356
S	-2.59337	-0.17231	0.809292
C	-1.13156	-1.4429	-1.08912
C	-2.3963	-1.41771	-0.48352
C	-3.47099	-2.22447	-0.87572
H	-4.44679	-2.1547	-0.37169
C	-3.24071	-3.12592	-1.93173
H	-4.05178	-3.79341	-2.26115
C	-1.9878	-3.16882	-2.57135
C	-0.93423	-2.3237	-2.16192
H	0.035017	-2.33684	-2.68547
C	-1.17393	1.728104	-0.62839
C	-2.4098	1.399101	-0.05096
C	-3.52735	2.239656	-0.13468
H	-4.48095	1.94967	0.332979
C	-3.37382	3.459787	-0.81779
H	-4.22897	4.148726	-0.89137
C	-2.13809	3.806332	-1.39028
C	-1.02337	2.944931	-1.29528
H	-0.05229	3.23017	-1.72443
C	2.597256	-1.0901	-0.5093
C	3.740805	-0.3394	-0.33217
H	3.778403	0.752281	-0.44605
C	4.873105	-1.09521	0.051826
H	5.816501	-0.55548	0.232137
C	4.796536	-2.4908	0.198266
H	5.693505	-3.05911	0.487921
C	3.586783	-3.16735	-0.02908

H	3.515252	-4.26064	0.086418
C	2.425327	-2.45827	-0.41653
H	1.468467	-2.96822	-0.59973
F	1.529609	-0.36051	-2.23115
O	-3.89287	-0.29637	1.512682
N	-1.18242	-0.16614	1.623355
C	-0.92801	-1.21488	2.532415
F	-1.69246	-1.14041	3.648518
F	-1.12507	-2.47537	2.023134
F	0.368641	-1.1445	2.909103
H	-1.82815	-3.86917	-3.4065
H	-2.02772	4.768225	-1.91491
F	1.508934	1.846786	1.422141
B	2.170301	2.759526	0.531386
F	3.539407	2.766846	0.784262
F	1.600026	4.019395	0.613356
F	1.95483	2.222466	-0.80813

TS3B

Energy = -2299.37770787

S	-2.58569	0.671602	0.519658
C	-1.15662	-1.67258	0.878815
C	-2.4108	-1.05593	0.975656
C	-3.55805	-1.73573	1.409918
H	-4.52558	-1.21368	1.466984
C	-3.41431	-3.08416	1.778236
H	-4.29194	-3.64533	2.133539
C	-2.15917	-3.71139	1.698188
C	-1.01879	-3.01208	1.245463
H	-0.05224	-3.53168	1.173959
C	-0.94799	0.420503	-1.6436
C	-2.25552	0.743064	-1.25342
C	-3.2554	1.116617	-2.15933
H	-4.26899	1.364928	-1.80999
C	-2.90084	1.175361	-3.52019
H	-3.65596	1.476183	-4.26251
C	-1.59248	0.862161	-3.9342
C	-0.60792	0.480101	-2.9984
H	0.423003	0.237927	-3.30547
C	2.486242	1.145924	0.126062
C	3.554378	0.642355	0.851402
H	3.652922	-0.42286	1.100349
C	4.506184	1.602028	1.261144
H	5.366322	1.262787	1.860264
C	4.362195	2.955247	0.908768
H	5.119819	3.687012	1.228232
C	3.266646	3.376966	0.136683
H	3.152104	4.433402	-0.15402
C	2.294928	2.450658	-0.30174
H	1.443262	2.765017	-0.91982
O	-3.92861	1.213301	0.840651
F	2.218917	-2.1904	0.705683
H	-2.05464	-4.76885	1.987729
H	-1.33168	0.918823	-5.00273
C	-1.04672	2.638479	1.259538
F	3.161871	-3.08983	-1.22099
B	2.039545	-3.07752	-0.42824
F	0.906145	-2.49785	-1.15167
F	1.67881	-4.33796	0.032675
F	2.091701	-0.07447	-1.62073
Bi	0.516081	-0.28314	-0.03021
F	0.114864	2.899918	1.897718
F	-2.03578	3.299561	1.913641
F	-0.96098	3.229465	0.019332
N	-1.23779	1.242957	1.231106

TS3D

Energy = -2299.3781235

F	-0.89395	1.421888	-1.83566
B	-2.28211	-2.62416	0.575897
F	-1.93847	-2.29706	-0.78568
F	-1.80378	-3.87699	0.901309
F	-1.55957	-1.61772	1.38644
F	-3.63697	-2.46975	0.78223
Bi	-0.50193	-0.03554	-0.18571
S	2.725938	0.747594	0.32856
F	1.771678	0.333617	-2.78795
F	1.637005	2.511609	-2.75604
F	3.532234	1.525544	-2.29772
O	4.153811	1.096059	0.539356
N	1.790217	1.473174	-0.75929
C	1.300319	-1.51889	-0.35217
C	2.561652	-1.02635	0.008649
C	3.689203	-1.85535	0.08706
H	4.665081	-1.43105	0.368994
C	3.526149	-3.21879	-0.21562
H	4.395704	-3.8923	-0.17161
C	2.263753	-3.72086	-0.57458

H	2.143487	-4.79011	-0.80932
C	1.134715	-2.87515	-0.63958
H	0.148135	-3.27873	-0.90844
C	0.359054	0.888762	1.737495
C	1.747666	1.072387	1.800245
C	2.419252	1.482983	2.958612
H	3.512657	1.608599	2.956155
C	1.642795	1.737005	4.103658
H	2.135627	2.0735	5.028551
C	0.248335	1.561945	4.069551
H	-0.34893	1.758014	4.973831
C	-0.39829	1.129367	2.892534
H	-1.48852	0.974524	2.890023
C	-2.62384	1.057689	-0.6821
C	-3.60155	0.288891	-1.29553
H	-3.38015	-0.63724	-1.84152
C	-4.92708	0.738897	-1.11006
H	-5.74614	0.144587	-1.54539
C	-5.19658	1.908687	-0.37899
H	-6.23625	2.248113	-0.25481
C	-4.14642	2.654621	0.183778
H	-4.34867	3.580077	0.746158
C	-2.80616	2.245193	0.015645
H	-1.97	2.832208	0.422587
C	2.18002	1.458565	-2.1153

IM5

Energy = -2299.476826

Bi	0.46988	0.186874	0.424385
S	-2.72957	-0.25564	0.120752
C	-0.60241	-0.42005	-1.55384
C	-1.99084	-0.60215	-1.48757
C	-2.79855	-0.96602	-2.57204
H	-3.88583	-1.08953	-2.45396
C	-2.15272	-1.17565	-3.8034
H	-2.74233	-1.47818	-4.68242
C	-0.76116	-0.99636	-3.91261
C	0.015656	-0.61461	-2.79884
H	1.100562	-0.47496	-2.91102
C	-1.08819	1.888215	0.524939
C	-2.42638	1.491291	0.39486
C	-3.52034	2.36498	0.413558
H	-4.54932	1.98986	0.303388
C	-3.23841	3.731411	0.59083
H	-4.06604	4.456523	0.621948
C	-1.90827	4.168483	0.729329
C	-0.83197	3.257067	0.69938
H	0.201751	3.618425	0.803226
C	2.722002	-2.14408	-0.77842
C	3.571948	-1.07208	-0.47006
H	4.024616	-0.47917	-1.27683
C	3.81845	-0.77849	0.884158
H	4.472207	0.06918	1.135338
C	3.218196	-1.54464	1.900147
H	3.412788	-1.30733	2.95698
C	2.355658	-2.60508	1.563005
H	1.869422	-3.19697	2.352393
C	2.093692	-2.91135	0.214189
H	1.414585	-3.72618	-0.07528
F	2.489234	-2.44091	-2.07854
O	-4.16169	-0.63192	0.185839
N	-1.65127	-0.86538	1.206239
C	-1.6869	-2.25327	1.45949
F	-2.88486	-2.67175	1.934681
F	-1.41563	-3.04197	0.369629
F	-0.74845	-2.53883	2.392361
H	-0.26791	-1.15598	-4.88448
H	-1.70045	5.241864	0.862958
F	2.235331	2.255273	0.988938
B	2.595215	2.499646	-0.37106
F	3.928352	2.204204	-0.59621
F	2.245722	3.782404	-0.74976
F	1.764586	1.542817	-1.14621

7

Energy = -1967.8245672

Bi	-0.63383	-0.69187	-0.59404
S	2.077308	0.94155	0.063046
C	0.502902	-0.78825	1.436355
C	1.678733	-0.03049	1.530742
C	2.480841	0.052582	2.675273
H	3.390972	0.671308	2.687875
C	2.073555	-0.69756	3.792861
H	2.679653	-0.67731	4.711508
C	0.896374	-1.467	3.739607
C	0.106262	-1.51176	2.571845
H	-0.82026	-2.10633	2.558382
C	-0.54492	1.593005	-0.32594

C	0.730313	2.118406	-0.07048	F	-4.63997	-1.49615	0.171785
C	0.999171	3.476637	0.136036	F	-4.26927	0.702861	0.786156
H	2.022756	3.829936	0.333768	F	-2.53632	-0.84413	0.920916
C	-0.09401	4.359028	0.065714				
H	0.069737	5.437489	0.212979	**3**			
C	-1.38652	3.868092	-0.19301	Energy = -331.6361266			
C	-1.62015	2.491156	-0.3924	C	-1.14298	-1.21726	0.000006
H	-2.63748	2.122558	-0.58884	C	0.262969	-1.22676	0.000000
O	3.421394	1.561336	0.128274	C	0.940817	-0.000011	-0.000029
N	1.668506	-0.03687	-1.19569	C	0.262969	1.226748	-0.000009
C	2.585553	-1.04259	-1.57582	C	-1.14296	1.217275	0.000015
F	3.696811	-0.53958	-2.16318	C	-1.84851	0.000002	-0.000007
F	3.023163	-1.83444	-0.54832	H	-1.68923	-2.17381	0.000015
F	1.971866	-1.85383	-2.46973	H	0.838043	-2.16501	0.000001
H	0.583801	-2.04254	4.625234	H	0.838096	2.164964	-0.000009
H	-2.23461	4.569122	-0.24112	H	-1.68924	2.173807	0.000025
F	-3.28749	-0.13951	-1.1332	H	-2.94946	0.000023	-0.00001
B	-3.76235	-0.43223	0.183131	F	2.295326	0.000005	0.000014