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Supporting Information

Is the R_3Si Moiety in Metal–Silyl Complexes a Z ligand? An Answer from the Interaction Energy

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Author Contributions

D.H. data curation: equal; formal analysis: equal; methodology: supporting; writing – review and editing: supporting
M.M. data curation: equal; formal analysis: equal; methodology: equal; writing – review and editing: supporting
J.P. investigation: supporting; methodology: supporting; writing – review and editing: supporting
M.H. conceptualisation: equal; data curation: equal; formal analysis: equal; investigation: equal; methodology: supporting; writing – original draft: supporting; writing – review and editing: supporting
S.Z. conceptualisation: equal; formal analysis: supporting; funding acquisition: equal; investigation: equal; methodology: equal; supervision: equal; validation: equal; writing – review and editing: equal
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NCI plots

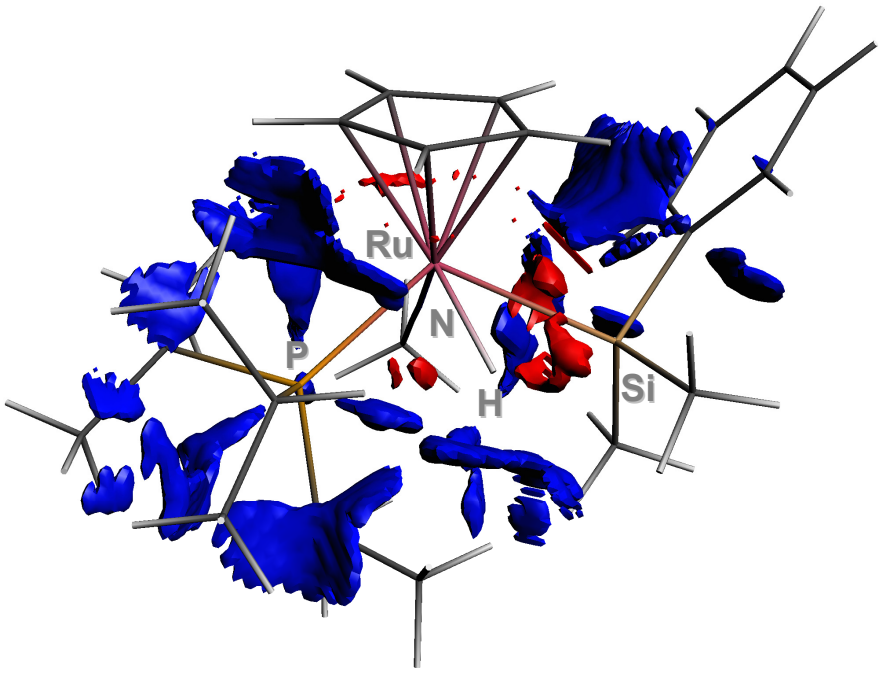

Figure S1. ADFview plots of non-covalent interaction (NCI) regions materialized by reduced density gradient isosurfaces (cut-off value s= 0.02 a.u., ρ= 0.05 a.u.) colored according to the sign of the signed density $\lambda_2\rho$ for a gas-phase relaxed singlet ground state model of cation DVGGIN optimized at the ZORA-PBE0-dDsC/all electron TZP level: red and blue colors are associated to negatively (attractive) and positively (repulsive or van der Waals) signed terms respectively.

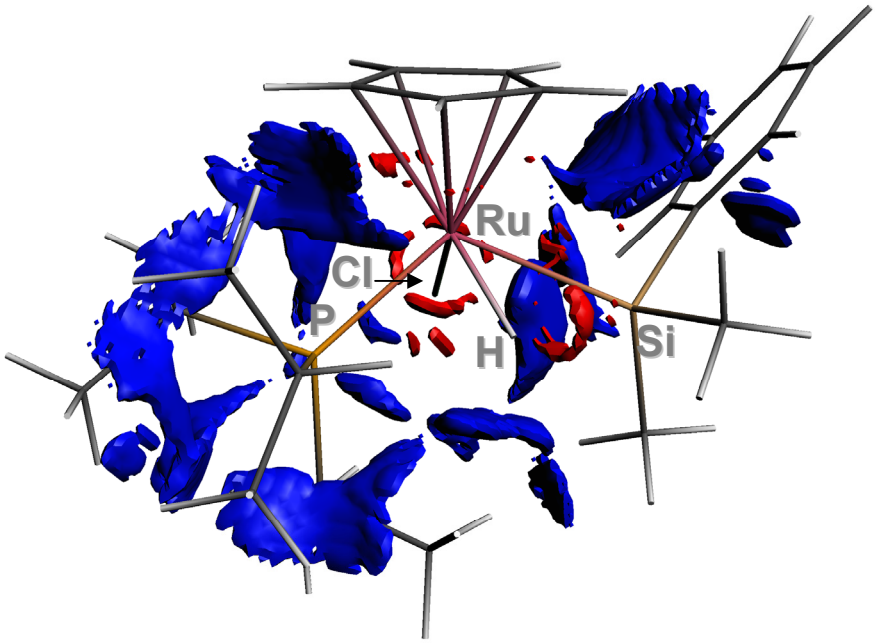

Figure S2. ADFview plots of non-covalent interaction (NCI) regions materialized by reduced density gradient isosurfaces (cut-off value s= 0.02 a.u., ρ= 0.05 a.u.) colored according to the sign of the signed density $\lambda_2\rho$ for a gas-phase relaxed singlet ground state model of neutral Cl-DVGGIN optimized at the ZORA-PBE0-dDsC/all electron TZP level: red and blue colors are associated to negatively (attractive) and positively (repulsive or van der Waals) signed terms respectively. Interatomic distances (Å): Ru-Si 2.486, Ru-H 1.626, H-Si 1.888.

Cartesian coordinates and total bonding energies

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62
Et-YINJOV ZORA-PBE-D3(BJ)/all electron TZP
Si      7.793171    2.900454   11.172725
Li      7.297553    5.468440   10.693148
O       8.978813    6.574366   10.744484
C       9.972651    5.961812   11.626765
H       9.468360    5.124131   12.130441
H      10.292858    6.711262   12.367593
C      11.128760    5.475758   10.736583
H      11.999075    6.142028   10.828640
H      11.443241    4.459131   11.006009
C      10.540290    5.548027    9.318015
H       9.969740    4.634062    9.100197
H      11.305425    5.690223    8.542006
C       9.586789    6.728018    9.436448
H      10.125622    7.692582    9.391204
H       8.769702    6.732600    8.703148
O       6.011654    6.093949   12.108451
C       6.666490    6.135276   13.410124
H       6.977984    7.173370   13.588459
H       7.553622    5.480458   13.381028
C       5.642306    5.601878   14.402737
H       6.115415    5.198382   15.308316
H       4.937231    6.394360   14.697505
C       4.938158    4.525052   13.565353
H       3.938922    4.265729   13.939682
H       5.550309    3.612862   13.533461
C       4.889074    5.158247   12.177959
H       5.018252    4.414067   11.377278
H       3.963329    5.734953   12.014353
O       6.409785    5.852176    8.945617
C       5.182381    6.616812    8.861024
H       5.292939    7.408643    8.097684
H       5.020521    7.082901    9.842027
C       4.118346    5.605890    8.454274
H       3.803149    5.019027    9.329294
H       3.231001    6.077709    8.010451
C       4.891834    4.723954    7.461342
H       4.473396    3.712950    7.370272
H       4.887648    5.185890    6.462815
C       6.309615    4.700554    8.044792
H       6.515287    3.810539    8.657151
H       7.090872    4.790739    7.274828
C       6.258425    1.702553   10.938011
H       5.914438    1.811207    9.891614
H       9.316863    0.946021   10.529235
C       9.175903    1.972351   10.147212
H      10.140986    2.483613   10.318581
C       6.439615    0.213295   11.259245
H       6.683199    0.066192   12.322436
H       7.265145   -0.223092   10.675995
H       5.536010   -0.384335   11.045826
H       5.428598    2.106739   11.548337
H       8.784124    2.918709    8.207851
H       7.404460    2.389858   13.614020
H       8.788610    3.450975   13.462408
C       8.336754    2.535638   13.036115
C       9.287885    1.360958   13.307133
H       8.868850    0.409894   12.948071
H       9.513428    1.239411   14.380949
H      10.247414    1.500003   12.785788
```

C	8.891351	1.910201	8.641027
H	7.948791	1.376711	8.437948
H	9.684879	1.393195	8.075388

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	103.377967843043606	2813.0576	64870.66	271418.82
Delta V^Pauli Coulomb:	-49.026146462403524	-1334.0693	-30764.37	-128718.13
Delta V^Pauli LDA-XC:	-14.451661454244375	-393.2497	-9068.56	-37942.83
Delta V^Pauli GGA-Exchange:	0.701249409784992	19.0820	440.04	1841.13
Delta V^Pauli GGA-Correlation:	-0.163276859977632	-4.4430	-102.46	-428.68
Total Pauli Repulsion:	40.438132476203066	1100.3776	25375.31	106170.30
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	40.438132476203066	1100.3776	25375.31	106170.30
Electrostatic Interaction:	-8.078221858448327	-219.8196	-5069.16	-21209.37
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	32.359910617754736	880.5580	20306.15	84960.93
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-44.559504566812350	-1212.5258	-27961.51	-116990.96
Total Orbital Interactions:	-44.563701321042032	-1212.6400	-27964.15	-117001.98
Alternative Decomposition Orb.Int.				
Kinetic:	-92.167062505534986	-2507.9934	-57835.71	-241984.59
Coulomb:	44.810144653177893	1219.3461	28118.79	117649.02
XC:	2.793216531315074	76.0073	1752.77	7333.59
Total Orbital Interactions:	-44.563701321042018	-1212.6400	-27964.15	-117001.98
Residu (E=Steric+OrbInt+Res):	0.000010143487667	0.0003	0.01	0.03
Dispersion Energy:	-0.076837217433647	-2.0908	-48.22	-201.74
Total Bonding Energy:	-12.280617777233278	-334.1726	-7706.20	-32242.76

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-8.078221858448327	-219.8196	-5069.16	-21209.37
Kinetic Energy:	11.210905337508621	305.0643	7034.95	29434.23
Coulomb (Steric+OrbInt) Energy:	-4.215991665737967	-114.7230	-2645.57	-11069.08
XC Energy:	-11.120472373121942	-302.6034	-6978.20	-29196.80
Dispersion Energy:	-0.076837217433647	-2.0908	-48.22	-201.74
Total Bonding Energy:	-12.280617			

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71
RICNUQ  ZORA-PBE-D3(BJ)/all electron TZP
H       1.034209   -1.079446    1.853190
H       1.545993   -0.711466    4.256908
H       5.773607   -1.150232    3.418220
H       5.258985   -1.437843    0.995502
H       5.050946   -0.283971    5.535159
H       3.645620    1.650232    1.116013
H       3.590246    1.949285    3.351836
Ru      3.520822    0.656533    2.384129
Si      5.563893    1.942503    2.192956
Si      1.644634    2.162799    2.084040
C       2.070361   -1.118679    2.189040
C       3.708298   -0.940157    4.046370
C       2.364442   -0.906371    3.567559
C       4.442654   -1.313630    1.706087
C       3.096157   -1.326116    1.234165
C       4.733922   -1.156972    3.090825
C       0.900119    2.016701    0.318660
H       0.511439    0.990068    0.189984
H       0.016325    2.678976    0.282214
C       1.921306    4.029413    2.385580
H       2.690568    4.397668    1.689229
H       0.982835    4.534050    2.092640
C       0.212900    1.664071    3.273616
H      -0.078139    0.622861    3.051228
H       0.611238    1.650732    4.302860
C       2.285644    4.406954    3.827192
H       1.491401    4.113827    4.531538
H       2.446725    5.490008    3.945029
H       3.206405    3.900042    4.154591
C      -1.029470    2.565177    3.202667
H      -0.786543    3.606092    3.463534
H      -1.820694    2.230717    3.892533
H      -1.461167    2.576518    2.190504
C       1.855089    2.366844   -0.830131
H       2.250376    3.388843   -0.721559
H       1.364511    2.308187   -1.814676
H       2.721917    1.688970   -0.844634
C       6.721842    1.150004    0.881694
H       7.670165    1.716419    0.898581
H       6.984463    0.129094    1.211266
C       6.594138    1.896492    3.813932
H       6.780753    0.841665    4.081815
H       7.586867    2.321420    3.579489
C       6.151796    1.125466   -0.541885
H       5.199717    0.573809   -0.574946
H       6.840089    0.661407   -1.265855
H       5.936704    2.144193   -0.899297
C       5.973712    2.641912    5.001814
H       5.839882    3.710393    4.773984
H       6.593810    2.575564    5.909836
H       4.979313    2.239043    5.245630
C       5.395905    3.785601    1.711610
H       4.839595    3.841250    0.759920
H       4.753374    4.279884    2.457259
C       6.727777    4.540949    1.590837
H       7.290862    4.519867    2.536950
H       6.573993    5.599288    1.327230
H       7.376260    4.102413    0.816615
```

C	4.056913	-0.758092	5.513388
C	3.082943	0.162471	6.255609
H	2.944815	1.108209	5.713911
H	3.467490	0.385738	7.260468
H	2.097563	-0.311409	6.380524
C	4.167362	-2.125545	6.208425
H	3.196943	-2.645197	6.197454
H	4.475174	-1.998931	7.256707
H	4.903087	-2.771416	5.708639
C	2.777679	-1.557785	-0.218468
H	3.588078	-1.193878	-0.862547
H	1.852704	-1.042016	-0.504913
H	2.645299	-2.632116	-0.416575

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	122.686998837287632	3338.4831	76987.26	322114.67
Delta V^Pauli Coulomb:	-58.406025161918357	-1589.3088	-36650.34	-153345.00
Delta V^Pauli LDA-XC:	-16.906748811230578	-460.0560	-10609.15	-44388.66
Delta V^Pauli GGA-Exchange:	0.855226794564771	23.2719	536.66	2245.40
Delta V^Pauli GGA-Correlation:	-0.218143714496579	-5.9360	-136.89	-572.74
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	48.011307944206898	1306.4542	30127.55	126053.67
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	48.011307944206898	1306.4542	30127.55	126053.67
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-9.724026938322014	-264.6042	-6101.92	-25530.43
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	38.287281005884886	1041.8499	24025.63	100523.24
Orbital Interactions				
A:	-52.487624956180142	-1428.2609	-32936.49	-137806.24
Total Orbital Interactions:	-52.499415547068551	-1428.5818	-32943.88	-137837.20
Alternative Decomposition Orb.Int.				
Kinetic:	-109.616644277777297	-2982.8207	-68785.49	-287798.46
Coulomb:	53.564818547565949	1457.5729	33612.43	140634.41
XC:	3.552410183142797	96.6660	2229.17	9326.85
Total Orbital Interactions:	-52.499415547068551	-1428.5818	-32943.88	-137837.20
Residu (E=Steric+OrbInt+Res):	0.000005970039233	0.0002	0.00	0.02
Dispersion Energy:	-0.106691723815478	-2.9032	-66.95	-280.12
Total Bonding Energy:	-14.318820294959911	-389.6349	-8985.20	-37594.06

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-9.724026938322014	-264.6042	-6101.92	-25530.43
Kinetic Energy:	13.070354559510335	355.6624	8201.77	34316.21
Coulomb (Steric+OrbInt) Energy:	-4.841200644313176	-131.7358	-3037.90	-12710.57
XC Energy:	-12.717255548019589	-346.0541	-7980.20	-33389.15
Dispersion Energy:	-0.106691723815478	-2.9032	-66.95	-280.12
Total Bonding Energy:	-14.318820294959922	-389.6349	-8985.20	-37594.06

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71
IMOLOM  ZORA-PBE-D3(BJ)/all electron TZP
W       3.118278    4.465701    0.218918
Si      4.617061    2.264667    0.065043
O       4.998037    4.444757    2.724434
O       4.716413    4.626391   -2.465623
N       3.586987    6.643897    0.326256
N       4.106932   10.835364    0.570612
C       4.344790    4.408469    1.735565
C       4.207590    4.535617   -1.397480
C       4.210114    0.853361    1.319651
H       3.183603    0.478557    1.172842
H       4.863478    0.015705    1.016095
C       4.445953    1.161734    2.803278
H       5.494243    1.433105    2.990806
H       4.208967    0.294569    3.441193
H       3.834669    2.006922    3.146663
C       6.491109    2.528983    0.382183
H       6.632237    2.753976    1.451481
H       6.951686    1.536053    0.219434
C       7.214406    3.583718   -0.461769
H       7.114184    3.385004   -1.539326
H       8.291112    3.620370   -0.230164
H       6.799253    4.586145   -0.277659
C       4.530804    1.449537   -1.685643
H       3.535038    1.622268   -2.123185
H       5.225192    2.020768   -2.323027
C       4.879634   -0.042496   -1.752599
H       5.867643   -0.249087   -1.312105
H       4.904522   -0.409840   -2.791733
H       4.147431   -0.656192   -1.205585
C       3.606069    7.302951    1.513095
H       3.496787    6.681382    2.398654
C       3.767683    8.670134    1.643091
H       3.776249    9.093673    2.645497
C       3.938736    9.478725    0.491798
C       3.930372    8.788630   -0.746299
H       4.069075    9.309674   -1.691541
C       3.756760    7.417955   -0.776664
H       3.760102    6.892147   -1.728730
C       4.193069   11.479920    1.870822
H       3.271158   11.328372    2.453966
H       4.330697   12.555952    1.728351
H       5.042699   11.097635    2.460532
C       4.350527   11.606852   -0.637303
H       5.277222   11.291254   -1.144794
H       4.446661   12.664232   -0.373014
H       3.515689   11.507952   -1.348540
C       1.274233    3.020997   -0.208870
C       1.079499    4.181673   -1.035667
C       0.925137    5.310789   -0.179442
C       1.030121    4.867625    1.192868
C       1.235295    3.441444    1.170562
C       1.175287    1.607838   -0.696570
H       0.134171    1.258798   -0.600664
H       1.811095    0.921232   -0.129013
H       1.455030    1.524428   -1.752665
C       0.963142    4.179230   -2.530390
H      -0.062523    3.923438   -2.841314
H       1.645983    3.450617   -2.985208
```

H	1.203104	5.162694	-2.953719
C	0.568203	6.697464	-0.617204
H	0.955792	6.922990	-1.618771
H	0.955292	7.459410	0.071222
H	-0.526835	6.809940	-0.653870
C	0.723272	5.691960	2.407742
H	0.989438	6.746723	2.260407
H	1.268001	5.328938	3.288891
H	-0.352629	5.657912	2.645955
C	1.132630	2.539976	2.362638
H	1.556545	3.005278	3.261291
H	1.654683	1.591212	2.200815
H	0.074008	2.312396	2.572543

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	148.986239341021815	4054.1218	93490.29	391163.32
Delta V^Pauli Coulomb:	-73.681570403795874	-2004.9775	-46235.89	-193450.94
Delta V^Pauli LDA-XC:	-19.530679547302078	-531.4568	-12255.69	-51277.79
Delta V^Pauli GGA-Exchange:	0.963955035630111	26.2306	604.89	2530.86
Delta V^Pauli GGA-Correlation:	-0.229694508495088	-6.2503	-144.14	-603.06
Total Pauli Repulsion:	56.508249917058883	1537.6677	35459.47	148362.39
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	56.508249917058883	1537.6677	35459.47	148362.39
Electrostatic Interaction:	-11.615152507465197	-316.0644	-7288.62	-30495.58
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	44.893097409593686	1221.6033	28170.85	117866.81
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-60.246201660695689	-1639.3826	-37805.07	-158176.38
Total Orbital Interactions:	-60.246201660695689	-1639.3826	-37805.07	-158176.38
Alternative Decomposition Orb.Int.				
Kinetic:	-133.665056687448185	-3637.2113	-83876.10	-350937.56
Coulomb:	68.541186329780629	1865.1006	43010.25	179954.86
XC:	4.877668696971945	132.7281	3060.78	12806.32
Total Orbital Interactions:	-60.246201660695611	-1639.3826	-37805.07	-158176.38
Residu (E=Steric+OrbInt+Res):	0.000001729467385	0.0000	0.00	0.00
Dispersion Energy:	-0.111390007286984	-3.0311	-69.90	-292.45
Total Bonding Energy:	-15.464492528921602	-420.8103	-9704.12	-40602.02

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.615152507465197	-316.0644	-7288.62	-30495.58
Kinetic Energy:	15.321182653573629	416.9106	9614.19	40225.76
Coulomb (Steric+OrbInt) Energy:	-5.140382344547859	-139.8769	-3225.64	-13496.07
XC Energy:	-13.918750323195111	-378.7485	-8734.15	-36543.67
Dispersion Energy:	-0.111390007286984	-3.0311	-69.90	-292.45
Total Bonding Energy:	-15.464492528921522	-420.8103	-9704.12	-40602.02

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46
KIGJEG  ZORA-PBE-D3(BJ)/all electron TZP
Fe       8.759596    3.655987    8.957475
C       12.007613    3.283926   10.245701
O        7.300318    1.251475    8.280779
N        8.155003    3.894380   10.778587
C        8.460174    5.728582    8.499726
H        7.904439    6.409215    9.140274
C        7.904364    4.932815    7.467215
H        6.863510    4.913366    7.160084
C        8.963940    4.123375    6.928830
H        8.864676    3.391169    6.132925
C       10.169953    4.441827    7.627556
H       11.150982    4.031991    7.417742
C        9.862834    5.441490    8.602474
H       10.573752    5.916556    9.270743
C        7.901388    2.211020    8.614707
C        7.033241    3.294087   11.267111
H        6.521108    2.624598   10.581818
C        6.546529    3.512890   12.549108
H        5.645322    2.986258   12.863898
C        7.206236    4.401121   13.402657
H        6.841760    4.594344   14.411772
C        8.357792    5.024868   12.914586
H        8.931848    5.719552   13.528402
C        8.801631    4.742394   11.630428
H        9.716748    5.181604   11.244169
C       11.051580    0.902834    8.505925
H       11.749924    0.259087    9.071563
H       10.186163    0.262167    8.265701
C       11.719924    1.372103    7.208211
H       11.009115    1.908270    6.562827
H       12.115414    0.528554    6.621003
H       12.564893    2.050867    7.406818
C       10.009879    1.263302   11.325629
H       10.954214    0.805010   11.670613
H        9.719047    1.973718   12.118478
C        8.945411    0.167503   11.184863
H       14.071764    3.089865   10.982194
H        8.795196   -0.376839   12.130637
H        9.225660   -0.572036   10.420108
C       13.216855    2.453479   10.702719
H       12.972106    1.832527   11.576746
H        7.971019    0.579289   10.887230
H       12.305137    3.937108    9.409020
H       11.699413    3.963880   11.060074
Si      10.456665    2.247464    9.739279
H       13.559472    1.774158    9.907557
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	1.521363475119805	41.3984	954.67	3994.34
Delta V^Pauli Coulomb:	-1.041845827913953	-28.3501	-653.77	-2735.37
Delta V^Pauli LDA-XC:	-0.295787143840488	-8.0488	-185.61	-776.59
Delta V^Pauli GGA-Exchange:	0.040002250932282	1.0885	25.10	105.03
Delta V^Pauli GGA-Correlation:	-0.017050387277770	-0.4640	-10.70	-44.77
Total Pauli Repulsion:	0.206682367019877	5.6241	129.70	542.64
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	0.206682367019877	5.6241	129.70	542.64
Electrostatic Interaction:	-0.282072534556990	-7.6756	-177.00	-740.58
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	-0.075390167537113	-2.0515	-47.31	-197.94

(Total Steric Interaction =
Delta E^0 in the BB paper)

Orbital Interactions				
A:	-0.261451351394835	-7.1145	-164.06	-686.44
Total Orbital Interactions:	-0.261451351394835	-7.1145	-164.06	-686.44
Alternative Decomposition Orb.Int.				
Kinetic:	-1.278646419705923	-34.7937	-802.36	-3357.09
Coulomb:	0.880879742097682	23.9700	552.76	2312.75
XC:	0.136315326213405	3.7093	85.54	357.90
Total Orbital Interactions:	-0.261451351394835	-7.1145	-164.06	-686.44
Residu (E=Steric+OrbInt+Res):	-0.000000005626931	-0.0000	-0.00	-0.00
Dispersion Energy:	-0.017150518136680	-0.4667	-10.76	-45.03
Total Bonding Energy:	-0.353992042695560	-9.6326	-222.13	-929.41

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-0.282072534556990	-7.6756	-177.00	-740.58
Kinetic Energy:	0.242717055413882	6.6047	152.31	637.25
Coulomb (Steric+OrbInt) Energy:	-0.160966091443202	-4.3801	-101.01	-422.62
XC Energy:	-0.136519953972570	-3.7149	-85.67	-358.43
Dispersion Energy:	-0.017150518136680	-0.4667	-10.76	-45.03
Total Bonding Energy:	-0.353992042695560	-9.6326	-222.13	-929.41

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ZUJNAT  ZORA-PBE-D3(BJ)/all electron TZP
Ir       3.146497   13.188573   -0.004201
P        2.717122   15.007383    1.230437
Si       2.129760   11.536028    1.268560
O        5.240853   13.574854    0.089872
O        3.542104   11.799061   -1.503757
C        6.146321   12.978713   -0.605614
C        7.566508   13.429202   -0.325083
C        5.932361   11.980418   -1.561851
C        4.691604   11.466724   -1.966106
C        4.654216   10.402484   -3.049247
C        1.735530   10.025727    0.150389
C        1.047422    8.875806    0.911530
C        3.359260   10.874574    2.561015
C        4.746854   10.504159    1.990926
C        0.504828   11.923152    2.176913
C       -0.697408   12.149033    1.229931
C        3.347088   15.170105    2.978579
C        4.829884   14.766916    3.066520
C        5.362862   15.005633    4.479419
C        4.547094   14.240239    5.526574
C        3.069505   14.640878    5.445699
C        2.529678   14.394371    4.026009
C        0.931248   15.542964    1.342850
C        0.311611   15.785599   -0.040716
C       -1.205801   16.006363    0.047355
C       -1.543871   17.153591    0.992633
C       -0.927698   16.913259    2.382570
C        0.598971   16.718779    2.262623
C        3.691836   16.351330    0.378124
C        3.580952   16.302197   -1.170427
C        4.672970   17.176675   -1.794031
C        4.632138   18.624166   -1.295332
C        4.681401   18.687870    0.244532
C        3.570339   17.813967    0.860527
H        1.665363   13.064759   -0.359387
H        7.547623   14.191841    0.416674
H        8.147920   12.607400    0.025427
H        8.008796   13.811779   -1.216705
H        6.827150   11.551036   -1.980858
H        3.640995   10.132251   -3.229642
H        5.086939   10.780714   -3.947317
H        5.200102    9.542922   -2.733676
H        2.729673    9.731982   -0.174013
H        1.157438   10.400078   -0.658443
H        0.136632    9.212294    1.342596
H        0.819890    8.071031    0.250238
H        1.625507    8.487725    1.735948
H        3.492757   11.569227    3.368282
H        2.995934   10.005193    3.073132
H        5.313469    9.924658    2.676296
H        5.268282   11.309389    1.577986
H        4.553469    9.721116    1.276682
H        0.301256   11.053832    2.780807
H        0.600474   12.841005    2.792877
H       -0.472102   12.953167    0.550523
H       -1.593997   12.307865    1.814589
H       -0.836382   11.286526    0.608745
H        3.229180   16.218685    3.150158
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H	5.489311	15.270393	2.389574
H	4.849904	13.716683	2.791991
H	5.364592	16.061008	4.780195
H	6.395448	14.770936	4.620496
H	4.668411	13.182636	5.319155
H	4.894184	14.284854	6.532922
H	2.985428	15.681327	5.719159
H	2.491518	14.008626	6.116034
H	2.502101	13.355497	3.854781
H	1.523479	14.725903	3.964405
H	0.598571	14.580951	1.658186
H	0.605142	15.052162	-0.740415
H	0.735873	16.677461	-0.438136
H	-1.716370	15.105870	0.332827
H	-1.549845	16.171477	-0.959641
H	-2.604683	17.252062	1.085410
H	-1.159397	18.067678	0.587948
H	-1.323022	15.976960	2.825313
H	-1.054548	17.795439	2.955816
H	1.001604	17.625996	1.873099
H	1.056707	16.643316	3.222143
H	4.732368	16.190532	0.431137
H	2.616812	16.676207	-1.401459
H	3.693599	15.306366	-1.536460
H	4.570744	17.213646	-2.855149
H	5.632780	16.716600	-1.527169
H	3.740979	19.096390	-1.644859
H	5.422794	19.167492	-1.782125
H	5.613574	18.207764	0.448215
H	4.562306	19.682667	0.705373
H	2.651803	18.136019	0.359451
H	3.575754	17.906380	1.945134

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	166.463787468796852	4529.7101	104457.61	437050.61
Delta V^Pauli Coulomb:	-81.237344053452020	-2210.5806	-50977.21	-213288.62
Delta V^Pauli LDA-XC:	-22.610233328920589	-615.2558	-14188.14	-59363.16
Delta V^Pauli GGA-Exchange:	1.162518313751178	31.6337	729.49	3052.19
Delta V^Pauli GGA-Correlation:	-0.293899573455327	-7.9974	-184.42	-771.63
Total Pauli Repulsion:	63.484828826720097	1727.5101	39837.34	166679.39
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	63.484828826720097	1727.5101	39837.34	166679.39
Electrostatic Interaction:	-13.067012671106671	-355.5715	-8199.68	-34307.44
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	50.417816155613423	1371.9386	31637.66	132371.96
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-68.832380716262122	-1873.0244	-43192.98	-180719.39
Total Orbital Interactions:	-68.832380716262122	-1873.0244	-43192.98	-180719.39
Alternative Decomposition Orb.Int.				
Kinetic:	-148.410738550129452	-4038.4617	-93129.15	-389652.34
Coulomb:	74.644773355330187	2031.1876	46840.31	195979.82
XC:	4.933584478537140	134.2497	3095.87	12953.12
Total Orbital Interactions:	-68.832380716262122	-1873.0244	-43192.98	-180719.39
Residu (E=Steric+OrbInt+Res):	0.000010729262531	0.0003	0.01	0.03
Dispersion Energy:	-0.140259665513765	-3.8167	-88.01	-368.25
Total Bonding Energy:	-18.554813496899932	-504.9022	-11643.32	-48715.66

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.067012671106671	-355.5715	-8199.68	-34307.44
Kinetic Energy:	18.053048918667400	491.2485	11328.46	47398.27
Coulomb (Steric+OrbInt) Energy:	-6.592559968859305	-179.3927	-4136.89	-17308.76
XC Energy:	-16.808030110087596	-457.3698	-10547.20	-44129.48

Dispersion Energy:	-0.140259665513765	-3.8167	-88.01	-368.25
Total Bonding Energy:	-18.554813496899936	-504.9022	-11643.32	-48715.66

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CONFEQ01  ZORA-PBE-D3(BJ)/all electron TZP
Rh      1.528218    2.919152    4.415250
Si      1.798882    1.551463    6.375196
C       2.500549   -0.203020    6.093292
C       2.767104   -0.991084    7.384856
C       2.981613    2.377448    7.635789
C       4.432141    2.501046    7.153885
C       0.139898    1.297066    7.303056
C      -0.977221    0.647972    6.477006
C      -0.217389    4.454764    4.415250
C       0.586854    4.710633    5.578437
C       1.903385    5.073202    5.136081
C      -1.687026    4.157740    4.415250
C       0.078950    4.827936    6.980560
C       2.999222    5.624484    5.994951
H       0.717180    1.551164    4.415250
H       2.974141    2.265482    4.415250
H      -2.274335    5.090064    4.415250
H      -1.981969    3.580260    3.530002
H      -0.141985    5.882657    7.210797
H       0.808530    4.476702    7.719523
H      -0.846948    4.260290    7.124915
H       2.973210    5.211578    7.009337
H       3.990323    5.414603    5.574852
H       2.900327    6.719340    6.078478
H       3.427630   -0.123812    5.503785
H       1.796907   -0.761901    5.456209
H       3.511789   -0.488981    8.021606
H       1.852079   -1.110799    7.985403
H       3.149634   -2.001298    7.169516
H       2.936049    1.767374    8.555974
H       2.585255    3.365301    7.921706
H       4.486992    3.063625    6.209770
H       5.075723    3.009216    7.889347
H       4.870809    1.509915    6.962181
H      -0.202680    2.258299    7.716398
H       0.374555    0.667730    8.180595
H      -1.260312    1.285367    5.626236
H      -1.884059    0.462516    7.074147
H      -0.658429   -0.318494    6.056662
Si      1.798882    1.551463    2.455304
C       0.586854    4.710633    3.252063
C       1.903385    5.073202    3.694419
H      -1.981969    3.580260    5.300498
C       2.500549   -0.203020    2.737208
C       2.981613    2.377448    1.194711
C       0.139898    1.297066    1.527444
C       0.078950    4.827936    1.849940
C       2.999222    5.624484    2.835549
C       2.767104   -0.991084    1.445644
H       3.427630   -0.123812    3.326715
H       1.796907   -0.761901    3.374291
C       4.432141    2.501046    1.676615
H       2.936049    1.767374    0.274526
H       2.585255    3.365301    0.908794
C      -0.977221    0.647972    2.353494
H      -0.202680    2.258299    1.114102
H       0.374555    0.667730    0.649905
H      -0.141985    5.882657    1.619703
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H	0.808530	4.476702	1.110977
H	-0.846948	4.260290	1.705585
H	2.973210	5.211578	1.821163
H	3.990323	5.414603	3.255648
H	2.900327	6.719340	2.752022
H	3.511789	-0.488981	0.808894
H	1.852079	-1.110799	0.845097
H	3.149634	-2.001298	1.660984
H	4.486992	3.063625	2.620730
H	5.075723	3.009216	0.941153
H	4.870809	1.509915	1.868319
H	-1.260312	1.285367	3.204264
H	-1.884059	0.462516	1.756353
H	-0.658429	-0.318494	2.773838

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	123.067200813823547	3348.8289	77225.84	323112.89
Delta V^Pauli Coulomb:	-58.455571291142874	-1590.6570	-36681.43	-153475.08
Delta V^Pauli LDA-XC:	-17.014706088113805	-462.9937	-10676.89	-44672.10
Delta V^Pauli GGA-Exchange:	0.854498050082057	23.2521	536.21	2243.48
Delta V^Pauli GGA-Correlation:	-0.215087770655636	-5.8528	-134.97	-564.71
Total Pauli Repulsion:	48.236333713993290	1312.5774	30268.76	126644.48
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	48.236333713993290	1312.5774	30268.76	126644.48
Electrostatic Interaction:	-9.703732741953871	-264.0520	-6089.18	-25477.15
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	38.532600972039418	1048.5254	24179.57	101167.33
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
AA:	-27.922056474959660	-759.7978	-17521.36	-73309.35
AAA:	-24.899374399787323	-677.5465	-15624.59	-65373.30
Total Orbital Interactions:	-52.832286611528751	-1437.6397	-33152.76	-138711.15
Alternative Decomposition Orb.Int.				
Kinetic:	-109.802501822238042	-2987.8781	-68902.12	-288286.43
Coulomb:	53.415595402832317	1453.5123	33518.80	140242.63
XC:	3.554619807876961	96.7261	2230.56	9332.65
Total Orbital Interactions:	-52.832286611528765	-1437.6397	-33152.76	-138711.15
Residu (E=Steric+OrbInt+Res):	-0.000007814512376	-0.0002	-0.00	-0.02
Dispersion Energy:	-0.109335454458913	-2.9752	-68.61	-287.06
Total Bonding Energy:	-14.409028908460622	-392.0896	-9041.80	-37830.90

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-9.703732741953871	-264.0520	-6089.18	-25477.15
Kinetic Energy:	13.264698991585504	360.9508	8323.73	34826.46
Coulomb (Steric+OrbInt) Energy:	-5.039983702822930	-137.1449	-3162.64	-13232.48
XC Energy:	-12.820676000810423	-348.8683	-8045.10	-33660.68
Dispersion Energy:	-0.109335454458913	-2.9752	-68.61	-287.06
Total Bonding Energy:	-14.409028908460632	-392.0896	-9041.80	-37830.90

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CIWJAT10  ZORA-PBE-D3(BJ)/all electron TZP
Ir      1.530283    2.919840    4.415250
Si      1.792931    1.564916    6.402514
C       2.507583   -0.186257    6.120492
C       2.758498   -0.982968    7.409419
C       2.962747    2.379876    7.684587
C       4.420651    2.494576    7.222065
C       0.135854    1.287681    7.328005
C      -0.965755    0.610866    6.503147
C      -0.218457    4.465136    4.415250
C       0.589938    4.712031    5.580226
C       1.915911    5.064607    5.137939
C      -1.687041    4.167955    4.415250
C       0.082758    4.829368    6.982754
C       3.011823    5.617266    5.995728
H       0.659064    1.574798    4.415250
H       2.997919    2.285658    4.415250
H      -2.273327    5.100650    4.415250
H      -1.979604    3.589724    3.530133
H      -0.134469    5.885618    7.209947
H       0.812308    4.476298    7.720529
H      -0.844582    4.264030    7.127047
H       2.985520    5.206023    7.010679
H       4.001896    5.404484    5.575309
H       2.912784    6.712310    6.075276
H       3.442772   -0.098405    5.544056
H       1.816434   -0.743954    5.468336
H       3.482148   -0.476537    8.066356
H       1.832907   -1.118607    7.989530
H       3.158571   -1.986542    7.195432
H       2.903076    1.774426    8.606860
H       2.570789    3.371880    7.963288
H       4.491112    3.052673    6.276136
H       5.057783    3.002864    7.963347
H       4.856791    1.500416    7.040826
H      -0.227293    2.246819    7.729436
H       0.374189    0.671850    8.213982
H      -1.253156    1.232678    5.641899
H      -1.874358    0.419101    7.095727
H      -0.628817   -0.355903    6.098044
Si      1.792931    1.564916    2.427986
C       0.589938    4.712031    3.250274
C       1.915911    5.064607    3.692561
H      -1.979604    3.589724    5.300367
C       2.507583   -0.186257    2.710008
C       2.962747    2.379876    1.145913
C       0.135854    1.287681    1.502495
C       0.082758    4.829368    1.847746
C       3.011823    5.617266    2.834772
C       2.758498   -0.982968    1.421081
H       3.442772   -0.098405    3.286444
H       1.816434   -0.743954    3.362164
C       4.420651    2.494576    1.608435
H       2.903076    1.774426    0.223640
H       2.570789    3.371880    0.867212
C      -0.965755    0.610866    2.327353
H      -0.227293    2.246819    1.101064
H       0.374189    0.671850    0.616518
H      -0.134469    5.885618    1.620553
```

H	0.812308	4.476298	1.109971
H	-0.844582	4.264030	1.703453
H	2.985520	5.206023	1.819821
H	4.001896	5.404484	3.255191
H	2.912784	6.712310	2.755224
H	3.482148	-0.476537	0.764144
H	1.832907	-1.118607	0.840970
H	3.158571	-1.986542	1.635068
H	4.491112	3.052673	2.554364
H	5.057783	3.002864	0.867153
H	4.856791	1.500416	1.789674
H	-1.253156	1.232678	3.188601
H	-1.874358	0.419101	1.734773
H	-0.628817	-0.355903	2.732456

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	127.071512104625270	3457.7918	79738.59	333626.21
Delta V^Pauli Coulomb:	-61.889233527944640	-1684.0917	-38836.08	-162490.16
Delta V^Pauli LDA-XC:	-17.170453528723431	-467.2318	-10774.62	-45081.02
Delta V^Pauli GGA-Exchange:	0.873454653782886	23.7679	548.10	2293.25
Delta V^Pauli GGA-Correlation:	-0.223806937800061	-6.0901	-140.44	-587.61
Total Pauli Repulsion:	48.661472763940026	1324.1460	30535.54	127760.68
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	48.661472763940026	1324.1460	30535.54	127760.68
Electrostatic Interaction:	-9.913565471121142	-269.7618	-6220.86	-26028.06
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	38.747907292818880	1054.3842	24314.68	101732.62
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
AA:	-28.104239798747610	-764.7553	-17635.68	-73787.67
AAA:	-25.020560874079429	-680.8441	-15700.64	-65691.47
Total Orbital Interactions:	-53.124800672826979	-1445.5994	-33336.32	-139479.14
Alternative Decomposition Orb.Int.				
Kinetic:	-112.714287375852194	-3067.1118	-70729.29	-295931.32
Coulomb:	56.054909568149995	1525.3317	35174.99	147172.14
XC:	3.534577134875255	96.1807	2217.98	9280.03
Total Orbital Interactions:	-53.124800672826943	-1445.5994	-33336.32	-139479.14
Residu (E=Steric+OrbInt+Res):	0.000010129676641	0.0003	0.01	0.03
Dispersion Energy:	-0.110132332229304	-2.9969	-69.11	-289.15
Total Bonding Energy:	-14.487015582560762	-394.2118	-9090.74	-38035.65

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-9.913565471121142	-269.7618	-6220.86	-26028.06
Kinetic Energy:	14.357224728773076	390.6800	9009.30	37694.89
Coulomb (Steric+OrbInt) Energy:	-5.834313830118006	-158.7598	-3661.09	-15317.99
XC Energy:	-12.986228677865352	-353.3733	-8148.98	-34095.34
Dispersion Energy:	-0.110132332229304	-2.9969	-69.11	-289.15
Total Bonding Energy:	-14.487015582560728	-394.2118	-9090.74	-38035.65

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45
Et-NAVQUW  ZORA-PBE-D3(BJ)/all electron TZP
Hg     -0.459564   -2.187037    5.642473
Si      0.480133   -2.337001    3.273799
C       1.391760   -3.991997    2.995756
H       0.660550   -4.812996    3.090017
H      -1.235602   -2.608241   11.048341
C      -2.663630   -3.386408    8.353424
H       0.340714   -1.911026   11.469637
C       2.570414   -4.215143    3.954823
H       2.238932   -4.209066    5.005503
H       3.326327   -3.421875    3.850262
H       3.075678   -5.176027    3.772441
H       1.747413   -4.023200    1.950682
H      -0.963385   -0.865943   10.873905
C      -0.492202   -1.853123   10.751684
H       0.477169   -3.053345    9.212311
C      -0.962350   -2.204797    2.021263
H      -1.767599   -2.871783    2.376139
H      -0.922438    0.917415    7.046233
H      -1.966102    1.855216    8.134413
H      -2.120910   -4.347317    8.347887
H      -1.375334   -1.183131    2.091367
H      -4.415307   -2.500226    7.379838
H      -3.142803   -0.275976    7.458163
C      -3.836212   -3.435694    7.362035
C      -0.630337   -2.542088    0.558039
H      -0.237061   -3.565096    0.463007
H       0.128808   -1.862564    0.145199
H      -1.520943   -2.470768   -0.085934
C       1.729540   -0.903822    3.045204
H       1.166509    0.043798    3.113583
H      -2.808659   -0.299695    9.187342
H       0.752371   -1.324990    9.044831
C      -0.017469   -2.071147    9.306108
H       2.401041   -0.908016    3.922106
H      -4.533352   -4.257701    7.585618
H      -3.479766   -3.576062    6.328807
H      -3.047048   -3.259651    9.381650
C       2.570230   -0.929812    1.758113
H       1.942529   -0.826561    0.861489
H       3.124932   -1.875440    1.659489
H       3.308044   -0.112303    1.739127
Si     -1.413719   -1.985226    8.003038
C      -2.322764   -0.315074    8.194956
C      -1.411103    0.909932    8.033826
H      -0.611147    0.916395    8.789659
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	67.409502481114473	1834.3059	42300.11	176983.62
Delta V^Pauli Coulomb:	-31.921357281998372	-868.6243	-20030.96	-83809.51
Delta V^Pauli LDA-XC:	-9.297848555397081	-253.0073	-5834.49	-24411.50
Delta V^Pauli GGA-Exchange:	0.462485562920971	12.5849	290.21	1214.26
Delta V^Pauli GGA-Correlation:	-0.111455656229976	-3.0329	-69.94	-292.63
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	26.541326550410020	722.2262	16654.94	69684.24
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	26.541326550410020	722.2262	16654.94	69684.24
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-5.173062273184123	-140.7662	-3246.15	-13581.87
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	21.368264277225897	581.4601	13408.79	56102.37

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Orbital Interactions
  A:                                -29.792293793372426       -810.6896        -18694.95        -78219.66
                                    --------------------      -----------      -----------      -----------
  Total Orbital Interactions:       -29.794640766318260       -810.7534        -18696.42        -78225.82

Alternative Decomposition Orb.Int.
  Kinetic:                          -58.717507450169521      -1597.7847        -36845.80       -154162.79
  Coulomb:                           27.585020995249334        750.6266         17309.86         72424.46
  XC:                                 1.337845688601924         36.4046           839.51          3512.51
                                    --------------------      -----------      -----------      -----------
  Total Orbital Interactions:       -29.794640766318263       -810.7534        -18696.42        -78225.82

  Residu (E=Steric+OrbInt+Res):      -0.000064812562250         -0.0018           -0.04            -0.17
  Dispersion Energy:                 -0.050301374233041         -1.3688          -31.56           -132.07

Total Bonding Energy:                -8.476742675887653       -230.6639        -5319.24        -22255.68


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
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  Electrostatic Energy:              -5.173062273184123       -140.7662        -3246.15        -13581.87
  Kinetic Energy:                     8.691995030944952        236.5212         5454.31         22820.83
  Coulomb (Steric+OrbInt) Energy:    -4.336401099311288       -117.9995        -2721.13        -11385.22
  XC Energy:                         -7.608972960104161       -207.0507        -4774.70        -19977.36
  Dispersion Energy:                 -0.050301374233041         -1.3688          -31.56           -132.07
                                    --------------------      -----------      -----------      -----------
  Total Bonding Energy:              -8.476742675887662       -230.6639        -5319.24        -22255.68
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89
KOSVIZ  ZORA-PBE-D3(BJ)/all electron TZP
Ir      4.627955    3.965212    5.031643
H       3.326604    3.068750    4.690898
Si      4.405659    2.253841    3.247987
P       3.870919    5.905998    4.015252
P       5.495438    2.687114    6.757662
O       4.611907    7.181521    4.858555
O       6.253625    3.786384    7.813097
C       5.517388    5.423984    6.219451
C       5.352131    6.795270    5.958384
C       5.879861    7.801241    6.775757
H       5.728698    8.849771    6.518941
C       6.577634    7.422334    7.926936
H       6.997048    8.191299    8.577277
C       6.721433    6.075338    8.273708
H       7.231554    5.772956    9.188396
C       6.170095    5.108502    7.424862
C       4.349533    6.542690    2.275024
C       5.663571    5.812954    1.940690
H       6.042900    6.173012    0.970474
H       5.526690    4.727290    1.882759
H       6.429696    6.010394    2.704141
C       7.622458    1.094523    7.857567
H       3.337791    3.942154    8.231515
H       8.614092    0.658742    7.651451
H       7.008793    0.306012    8.314253
C       3.278278    6.255226    1.209719
H       3.717857    6.441933    0.216447
H       2.414606    6.925072    1.315897
H       2.917701    5.222185    1.221393
C       2.060878    6.290279    4.422877
C       1.649634    7.723384    4.056836
H       2.293540    2.573329    8.697753
H       1.624699    7.891400    2.972125
C       3.042188    2.917764    7.965584
C       1.142280    5.264582    3.737923
H       0.108798    5.430889    4.082967
H       1.429611    4.238209    4.005398
H       1.147967    5.355654    2.644241
C       1.944608    6.112878    5.949158
H       0.896559    6.282704    6.244884
H       2.577130    6.827850    6.491961
H       2.242391    5.100145    6.248956
H       0.633318    7.907591    4.442063
C       4.628518    8.057717    2.275433
H       4.887827    8.349143    1.244190
H       5.466817    8.317830    2.930800
H       7.753890    1.912297    8.577556
H       6.343113    0.694403    4.654238
H       6.034276   -0.322044    6.081280
H       7.682531   -0.155284    5.446143
H       2.581967    2.946619    6.969176
C       8.043913    2.521782    5.840770
H       8.371499    3.318455    6.520232
H       7.615492    2.994093    4.946221
H       8.925683    1.933999    5.538923
C       4.246291    1.957110    7.995384
C       4.780437    1.902593    9.436331
H       3.956314    1.576116   10.091665
```

H	5.120667	2.888064	9.777175
H	5.603278	1.189120	9.557664
H	3.755749	8.647306	2.581758
C	7.028146	1.586902	6.529638
H	2.322823	8.460393	4.515486
C	6.739556	0.384612	5.625261
C	3.794025	0.559565	7.550490
H	2.953043	0.240245	8.187159
H	4.592812	-0.186487	7.661685
H	3.444879	0.551398	6.510201
C	3.661586	0.554242	3.755293
H	3.805038	-0.142051	2.910955
H	4.217613	0.115708	4.596900
C	2.167838	0.639829	4.101535
H	1.755705	-0.333454	4.411858
H	1.574749	0.989008	3.243132
H	1.983595	1.350049	4.924358
C	3.305304	2.735456	1.745680
H	2.339062	3.120276	2.111451
H	3.802595	3.580696	1.248493
C	3.063904	1.637767	0.697223
H	2.422000	1.998167	-0.123018
H	2.574000	0.752536	1.129715
H	4.006980	1.299507	0.243205
C	6.159239	1.983949	2.458778
H	6.228575	2.724268	1.642946
H	6.947812	2.265916	3.171057
C	6.441549	0.580614	1.896199
H	7.435645	0.533343	1.423223
H	5.701844	0.285495	1.138556
H	6.417478	-0.188887	2.682158

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	166.707446052150374	4536.3404	104610.51	437690.34
Delta V^Pauli Coulomb:	-82.051501631247433	-2232.7350	-51488.10	-215426.19
Delta V^Pauli LDA-XC:	-22.566898545542131	-614.0766	-14160.94	-59249.38
Delta V^Pauli GGA-Exchange:	1.171875393268550	31.8884	735.36	3076.76
Delta V^Pauli GGA-Correlation:	-0.303264862811170	-8.2523	-190.30	-796.22
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	62.957656405818192	1713.1650	39506.53	165295.30
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	62.957656405818192	1713.1650	39506.53	165295.30
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-12.940979279350458	-352.1420	-8120.59	-33976.54
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	50.016677126467734	1361.0230	31385.94	131318.77
Orbital Interactions				
A:	-68.135809214645064	-1854.0697	-42755.87	-178890.54
Total Orbital Interactions:	-68.140512341069282	-1854.1977	-42758.82	-178902.89
Alternative Decomposition Orb.Int.				
Kinetic:	-148.807206840579994	-4049.2501	-93377.94	-390693.27
Coulomb:	75.509559208936949	2054.7197	47382.97	198250.32
XC:	5.157135290573776	140.3328	3236.15	13540.06
Total Orbital Interactions:	-68.140512341069268	-1854.1977	-42758.82	-178902.89
Residu (E=Steric+OrbInt+Res):	0.000001001738631	0.0000	0.00	0.00
Dispersion Energy:	-0.152705673967333	-4.1553	-95.82	-400.93
Total Bonding Energy:	-18.276539886830250	-497.3300	-11468.70	-47985.05

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-12.940979279350458	-352.1420	-8120.59	-33976.54
Kinetic Energy:	17.900239211570380	487.0903	11232.57	46997.07
Coulomb (Steric+OrbInt) Energy:	-6.541941420571860	-178.0153	-4105.13	-17175.86
XC Energy:	-16.541152724510972	-450.1077	-10379.73	-43428.79
Dispersion Energy:	-0.152705673967333	-4.1553	-95.82	-400.93
Total Bonding Energy:	-18.276539886830243	-497.3300	-11468.70	-47985.05

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90
POBMUP  ZORA-PBE-D3(BJ)/all electron TZP
Ir      5.295349    8.060915    3.938487
H       5.058555    6.304402    3.595604
H       6.050885    8.033768    2.596423
P       3.523887    9.193300    2.905064
P       7.292473    7.716723    5.079353
Si      4.188743    4.970166    3.609373
O       3.788690   10.800459    3.322708
C       4.991651   11.054401    3.967399
C       5.821203    9.972483    4.319101
C       7.042692   10.290385    4.945975
O       7.910635    9.261643    5.293707
C       5.331984   12.379697    4.241200
H       4.655455   13.184147    3.953614
C       6.549489   12.639394    4.878522
H       6.829334   13.669724    5.096751
C       7.416317   11.602156    5.238603
H       4.281970    1.995243    3.038153
C       1.827656    8.958383    3.689351
C       2.148896    8.669871    5.171272
H       2.674325    9.515439    5.636973
H       2.767049    7.766215    5.286775
H       1.211277    8.508988    5.725580
C       1.113993    7.761169    3.043102
H       0.249568    7.477313    3.662805
H       1.763649    6.880455    2.956119
H       0.735358    8.008698    2.042938
C       0.939799   10.210089    3.617757
H       0.640182   10.455795    2.592836
H       1.438115   11.083163    4.056082
H       0.022741   10.012716    4.195315
C       3.503990    9.351314    1.026926
C       3.371965    7.967585    0.377933
H       2.395178    7.504891    0.568760
H       4.162134    7.287341    0.721974
H       3.475796    8.078542   -0.712397
C       2.382122   10.282321    0.541788
H       2.412350   11.257945    1.044439
H       1.387729    9.837385    0.679774
H       2.516993   10.454870   -0.537297
C       4.868989    9.955322    0.644245
H       4.905321   10.053614   -0.451208
H       5.704110    9.311484    0.952738
H       5.018394   10.949898    1.082521
C       7.013884    7.213959    6.875724
C       5.685487    7.912504    7.238535
H       4.864578    7.594748    6.571214
H       5.767447    9.006219    7.183414
H       5.397930    7.640089    8.265951
C       8.112927    7.711265    7.824904
H       7.793363    7.509490    8.859559
H       8.276191    8.791172    7.723063
H       9.067215    7.195595    7.666698
C       6.850134    5.692438    6.986662
H       7.793149    5.161415    6.800114
H       6.086959    5.312677    6.295514
H       6.524736    5.441583    8.008168
C       8.754573    6.905333    4.225952
C       9.041492    7.769277    2.982961
```

H	9.335130	8.790634	3.252699
H	8.170117	7.821140	2.315012
H	9.867544	7.305673	2.423049
C	10.000002	6.861113	5.124836
H	10.852518	6.512138	4.521723
H	9.879209	6.158307	5.959993
H	10.254234	7.851734	5.524425
C	8.366081	5.490337	3.773081
H	7.500464	5.513488	3.097296
H	8.136785	4.823379	4.613228
H	9.213016	5.052860	3.222774
C	2.789070	4.932487	4.877916
H	2.080400	5.753499	4.703555
H	2.235582	4.014547	4.603189
C	3.187617	4.865524	6.358041
H	3.880683	4.035908	6.556318
H	2.305531	4.715014	6.995748
H	3.677998	5.789957	6.690602
C	3.547880	4.740263	1.853234
H	2.899118	3.846632	1.888496
H	2.886855	5.573375	1.577534
C	4.652711	4.546392	0.803817
H	5.368922	5.381746	0.804649
H	4.233724	4.471959	-0.209018
H	5.224086	3.626945	0.991185
C	5.446349	3.606593	3.988214
H	6.241721	3.628431	3.228585
H	5.941239	3.789059	4.952803
C	4.765952	2.222965	3.999570
H	3.998058	2.149666	4.783613
H	5.502890	1.429390	4.188604
H	8.366980	11.798501	5.733695

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	167.401588475445834	4555.2290	105046.09	439512.81
Delta V^Pauli Coulomb:	-82.258902965835659	-2238.3786	-51618.25	-215970.72
Delta V^Pauli LDA-XC:	-22.630484120301478	-615.8068	-14200.84	-59416.33
Delta V^Pauli GGA-Exchange:	1.173511855991585	31.9329	736.39	3081.05
Delta V^Pauli GGA-Correlation:	-0.302282085673488	-8.2255	-189.68	-793.64
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	63.383431159626795	1724.7509	39773.71	166413.17
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	63.383431159626795	1724.7509	39773.71	166413.17
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-13.034942497640099	-354.6988	-8179.55	-34223.24
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	50.348488661986693	1370.0521	31594.16	132189.94
Orbital Interactions				
A:	-68.405063781751579	-1861.3965	-42924.83	-179597.47
Total Orbital Interactions:	-68.412825736342739	-1861.6077	-42929.70	-179617.85
Alternative Decomposition Orb.Int.				
Kinetic:	-149.381703013945327	-4064.8830	-93738.44	-392201.61
Coulomb:	75.624546022938830	2057.8486	47455.12	198552.22
XC:	5.344331254663741	145.4267	3353.62	14031.54
Total Orbital Interactions:	-68.412825736342754	-1861.6077	-42929.70	-179617.85
Residu (E=Steric+OrbInt+Res):	-0.000010577029242	-0.0003	-0.01	-0.03
Dispersion Energy:	-0.150911712949263	-4.1065	-94.70	-396.22
Total Bonding Energy:	-18.215259364334553	-495.6624	-11430.25	-47824.16

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.034942497640099	-354.6988	-8179.55	-34223.24
Kinetic Energy:	18.019885461500508	490.3460	11307.65	47311.20
Coulomb (Steric+OrbInt) Energy:	-6.634367519926073	-180.5303	-4163.13	-17418.53

XC Energy:	-16.414923095319644	-446.6728	-10300.52	-43097.37
Dispersion Energy:	-0.150911712949263	-4.1065	-94.70	-396.22
Total Bonding Energy:	-18.215259364334571	-495.6624	-11430.25	-47824.16

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90
pro-POBMUP  ZORA-PBE-D3(BJ)/all electron TZP
Ir      4.605781    3.969526    5.061217
H       3.600849    3.275740    4.090350
Si      4.428655    2.406033    3.204467
P       3.788646    5.881462    4.052291
P       5.617029    2.754705    6.746148
O       4.354830    7.131555    4.980850
O       6.508475    3.835240    7.630183
C       5.519297    5.468521    6.207598
C       5.245806    6.803622    5.996982
C       5.798877    7.828082    6.741529
H       5.606197    8.738594    6.553083
C       6.648349    7.467315    7.777984
H       7.067464    8.148097    8.291592
C       6.899932    6.148294    8.082823
H       7.452165    5.911842    8.818133
C       6.317193    5.171877    7.279155
C       4.422942    6.607708    2.442369
C       5.935251    6.389431    2.514422
H       6.362705    6.817642    1.745857
H       6.124099    5.427754    2.503337
H       6.279100    6.780716    3.343955
C       7.938648    1.096627    7.633756
H       3.359826    3.933351    8.117926
H       8.634617    0.429492    7.460090
H       7.449871    0.843798    8.454051
C       3.886669    5.938096    1.174975
H       4.323688    6.331119    0.389783
H       2.919807    6.076603    1.115855
H       4.079629    4.977395    1.208231
C       1.971031    6.160885    4.315746
C       1.337460    7.540164    4.127300
H       2.572075    2.671644    8.709130
H       1.474061    7.841000    3.205391
C       3.177370    2.976594    8.003380
C       1.144713    5.105085    3.560114
H       0.220738    5.111888    3.892666
H       1.535057    4.218269    3.704219
H       1.146305    5.311987    2.603102
C       1.737695    5.982376    5.821468
H       0.788348    6.097187    6.022847
H       2.260412    6.652904    6.312907
H       2.026155    5.085474    6.091205
H       0.639409    7.696382    3.868648
C       4.349836    8.111153    2.150462
H       4.709653    8.287488    1.252571
H       4.867850    8.602865    2.813719
H       8.349337    1.974465    7.764929
H       5.401165    0.001437    5.801146
H       5.622322   -0.214071    7.371531
H       6.704967   -0.761700    6.327687
H       2.766526    2.826000    7.127659
C       7.222242    0.507269    5.330073
H       8.044156    0.420079    4.807227
H       6.458458    0.618499    4.720394
H       7.089450   -0.295724    5.873241
C       4.468742    2.211924    8.086518
C       5.075992    1.880251    9.440745
H       4.368932    1.597082   10.055966
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H	5.524536	2.673268	9.799162
H	5.728377	1.155382	9.335437
H	3.539292	8.823217	2.101644
C	6.817021	1.285664	6.595576
H	1.280038	8.274429	4.917210
C	6.070760	-0.036760	6.517980
C	3.204707	1.437586	7.724406
H	2.711418	1.227081	8.541006
H	3.456026	0.610337	7.264375
H	2.650640	1.986892	7.133202
C	4.207620	0.551971	3.519468
H	4.366764	0.074448	2.665918
H	4.909176	0.261667	4.155012
C	2.873203	0.111860	4.062637
H	2.944914	-0.800215	4.413664
H	2.203293	0.131642	3.343955
H	2.593978	0.717100	4.781319
C	2.999852	2.657259	1.963863
H	2.165052	2.307093	2.366621
H	2.876114	3.627607	1.814215
C	3.225761	1.970189	0.609637
H	2.389105	1.986563	0.092333
H	3.498007	1.041137	0.755590
H	3.922963	2.444082	0.112656
C	6.069656	2.622380	2.265008
H	5.910276	3.265917	1.529698
H	6.717475	3.037044	2.883924
C	6.720827	1.380241	1.666414
H	7.595958	1.616686	1.298759
H	6.150579	1.024629	0.951426
H	6.829670	0.700512	2.362926
H	3.159245	3.962153	5.833925

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	167.823659276447216	4566.7141	105310.95	440620.96
Delta V^Pauli Coulomb:	-82.542286760328011	-2246.0899	-51796.07	-216714.74
Delta V^Pauli LDA-XC:	-22.699420985906638	-617.6827	-14244.10	-59597.32
Delta V^Pauli GGA-Exchange:	1.179914388703132	32.1071	740.41	3097.86
Delta V^Pauli GGA-Correlation:	-0.305749663985672	-8.3199	-191.86	-802.75
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	63.456116254930024	1726.7288	39819.32	166604.01
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	63.456116254930024	1726.7288	39819.32	166604.01
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-13.062411283831921	-355.4463	-8196.79	-34295.36
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	50.393704971098103	1371.2825	31622.53	132308.65
Orbital Interactions				
A:	-68.450606885157768	-1862.6358	-42953.41	-179717.04
Total Orbital Interactions:	-68.456918331568048	-1862.8075	-42957.37	-179733.61
Alternative Decomposition Orb.Int.				
Kinetic:	-149.809422869603281	-4076.5218	-94006.84	-393324.58
Coulomb:	75.945472363950003	2066.5815	47656.51	199394.81
XC:	5.407032174085223	147.1328	3392.96	14196.16
Total Orbital Interactions:	-68.456918331568062	-1862.8075	-42957.37	-179733.61
Residu (E=Steric+OrbInt+Res):	-0.000009617429956	-0.0003	-0.01	-0.03
Dispersion Energy:	-0.153170999534619	-4.1680	-96.12	-402.15
Total Bonding Energy:	-18.216393977434521	-495.6933	-11430.96	-47827.14

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.062411283831921	-355.4463	-8196.79	-34295.36
Kinetic Energy:	18.014236406843935	490.1923	11304.11	47296.37
Coulomb (Steric+OrbInt) Energy:	-6.596824013807961	-179.5087	-4139.57	-17319.96
XC Energy:	-16.418224087103958	-446.7626	-10302.59	-43106.04
Dispersion Energy:	-0.153170999534619	-4.1680	-96.12	-402.15
Total Bonding Energy:	-18.216393977434524	-495.6933	-11430.96	-47827.14

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91
pro-H-POBMUP  ZORA-PBE-D3(BJ)/all electron TZP
Ir      4.494063    3.965954    5.118712
H       3.169493    3.061923    4.811710
Si      4.222428    2.277955    3.254604
P       3.926986    5.927356    3.980576
P       5.501968    2.661702    6.781111
O       4.602267    7.179312    4.891984
O       6.111974    3.777221    7.892633
C       5.426252    5.437772    6.311937
C       5.312706    6.796384    6.021266
C       5.866499    7.797222    6.828613
H       5.755816    8.845731    6.550915
C       6.543562    7.414501    7.990957
H       6.984853    8.177159    8.633512
C       6.646205    6.066001    8.347678
H       7.149451    5.753754    9.263075
C       6.068173    5.109412    7.504734
C       4.782833    6.441521    2.341974
C       6.248264    5.989639    2.480787
H       6.800100    6.329664    1.590033
H       6.336590    4.901090    2.553310
H       6.724108    6.432391    3.366679
C       7.811456    1.217838    7.677883
H       3.124826    3.363527    8.360473
H       8.829958    0.884331    7.420865
H       7.271292    0.345878    8.069479
C       4.157969    5.779038    1.108741
H       4.681290    6.146480    0.211393
H       3.092731    6.025270    0.992283
H       4.267128    4.689209    1.129720
C       2.099692    6.468499    4.065732
C       1.801165    7.785944    3.336109
H       2.448206    1.775854    8.809629
H       1.893152    7.688455    2.246031
C       3.057810    2.308522    8.062140
C       1.198803    5.357907    3.510211
H       0.147443    5.641707    3.677986
H       1.383404    4.403021    4.018657
H       1.335234    5.208069    2.431047
C       1.784758    6.665218    5.560651
H       0.716481    6.916589    5.654262
H       2.374761    7.482577    5.993673
H       1.979284    5.752742    6.137622
H       0.758469    8.069582    3.553127
C       4.793717    7.971671    2.146046
H       5.487999    8.193214    1.319728
H       5.152718    8.493617    3.040470
H       7.894763    1.975800    8.467675
H       6.582974    1.068057    4.426789
H       6.393834   -0.153823    5.711029
H       8.011200    0.284192    5.127531
H       2.547479    2.265200    7.093242
C       8.091842    2.880712    5.845768
H       8.285069    3.670803    6.582526
H       7.673766    3.345066    4.943677
H       9.052448    2.409430    5.584253
C       4.446903    1.648459    8.012930
C       5.022955    1.685425    9.441599
H       4.321639    1.144797   10.097772
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H	5.115745	2.713832	9.809972
H	5.999971	1.198072	9.525291
H	3.814453	8.373585	1.867725
C	7.160488	1.790437	6.408353
H	2.448724	8.602606	3.681545
C	7.010381	0.683059	5.359138
C	4.297722	0.191380	7.551960
H	3.589581	-0.317697	8.225214
H	5.247350	-0.358017	7.597508
H	3.895551	0.117814	6.534580
C	3.800873	0.496688	3.841793
H	3.943671	-0.172985	2.976182
H	4.532371	0.162173	4.589936
C	2.374463	0.329729	4.382745
H	2.214836	-0.665610	4.826839
H	1.626684	0.453467	3.586450
H	2.142402	1.074987	5.160794
C	2.741938	2.636004	2.082919
H	1.821992	2.484446	2.672465
H	2.722125	3.695223	1.799014
C	2.698265	1.768311	0.817673
H	1.796149	1.967470	0.217236
H	2.699101	0.693839	1.057661
H	3.568104	1.957831	0.170251
C	5.805404	2.169615	2.141762
H	5.696259	2.943474	1.361085
H	6.673207	2.487067	2.740777
C	6.105010	0.815441	1.482014
H	6.995433	0.872920	0.836009
H	5.270095	0.463721	0.859684
H	6.297695	0.036684	2.235325
H	3.289036	4.302824	6.184664
H	5.915511	3.926582	4.299179

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	170.322641114600714	4634.7149	106879.08	447182.03
Delta V^Pauli Coulomb:	-84.487864022326889	-2299.0318	-53016.94	-221822.86
Delta V^Pauli LDA-XC:	-22.947628607751689	-624.4367	-14399.86	-60248.99
Delta V^Pauli GGA-Exchange:	1.197836756401585	32.5948	751.65	3144.92
Delta V^Pauli GGA-Correlation:	-0.314075824513125	-8.5464	-197.09	-824.61
Total Pauli Repulsion:	63.770909416410596	1735.2947	40016.85	167430.50
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	63.770909416410596	1735.2947	40016.85	167430.50
Electrostatic Interaction:	-13.183620551013195	-358.7446	-8272.85	-34613.59
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	50.587288865397397	1376.5502	31744.01	132816.91
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-68.979204291111472	-1877.0197	-43285.11	-181104.88
Total Orbital Interactions:	-68.979204291111472	-1877.0197	-43285.11	-181104.88
Alternative Decomposition Orb.Int.				
Kinetic:	-151.989931508548949	-4135.8565	-95375.13	-399049.51
Coulomb:	77.677772763900009	2113.7197	48743.54	203942.96
XC:	5.332954453537395	145.1171	3346.48	14001.67
Total Orbital Interactions:	-68.979204291111543	-1877.0197	-43285.11	-181104.88
Residu (E=Steric+OrbInt+Res):	-0.000003375623307	-0.0001	-0.00	-0.01
Dispersion Energy:	-0.157484212249789	-4.2854	-98.82	-413.47
Total Bonding Energy:	-18.549403013587174	-504.7549	-11639.93	-48701.45

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.183620551013195	-358.7446	-8272.85	-34613.59
Kinetic Energy:	18.332709606051765	498.8584	11503.95	48132.52
Coulomb (Steric+OrbInt) Energy:	-6.810094634050188	-185.3121	-4273.40	-17879.90
XC Energy:	-16.730913222325835	-455.2713	-10498.81	-43927.01
Dispersion Energy:	-0.157484212249789	-4.2854	-98.82	-413.47
Total Bonding Energy:	-18.549403013587245	-504.7549	-11639.93	-48701.45

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69
UVAWIZ  ZORA-PBE-D3(BJ)/all electron TZP
C      -1.877616   -2.334984    0.420598
C      -2.713004   -3.404364    0.785472
C      -2.280116   -4.712804    0.636151
C      -1.003477   -4.952814    0.108316
C      -0.215984   -3.869115   -0.240000
N      -0.632478   -2.591887   -0.081257
H      -3.703086   -3.191382    1.184491
H      -2.927233   -5.543298    0.918885
H      -0.625489   -5.963072   -0.040473
H       0.774526   -3.994603   -0.671519
H      -4.553632    1.325411    1.515753
C      -2.191052   -0.924292    0.512720
C      -1.187717   -0.046896    0.026475
C      -1.444255    1.328816    0.095578
C      -2.638157    1.816561    0.631066
C      -3.621643    0.939009    1.103990
C      -3.398043   -0.430744    1.040803
H      -4.161015   -1.117607    1.407895
H      -0.713921    2.038925   -0.283101
H      -2.807649    2.893708    0.672739
Ir      0.593089   -0.967593   -0.506961
H       1.824292    0.828835    3.257928
C       2.213339   -1.470652    1.137021
C       2.796957   -1.506127   -0.175763
C       2.657974   -0.180324   -0.760222
C       1.966194    0.654415    0.195320
C       1.675393   -0.159209    1.368630
H       3.113456   -2.632283    2.679411
H       3.530203   -2.646917   -1.857546
H       3.502612   -0.510216   -2.718214
H       2.821501    2.582798    0.452748
C       1.863486    2.144669    0.132862
H       1.657173    2.506426   -0.880664
H       1.088567    2.526680    0.805193
C       3.334409    0.302657   -2.003534
H       2.755905    1.086116   -2.505791
H       4.316092    0.726316   -1.742090
C       3.569140   -2.647883   -0.761902
H       4.626712   -2.581176   -0.465346
H       3.196883   -3.617133   -0.406992
C       1.061152    0.333960    2.637787
H       0.261126    1.058576    2.440547
H       0.633729   -0.486217    3.225897
C       2.178435   -2.611885    2.098671
H       1.347879   -2.522580    2.808007
H       2.093539   -3.579074    1.586660
Si     -0.328749   -0.380793   -2.785057
C      -0.320223    1.507715   -3.039337
H      -1.335376    1.474538   -4.986015
H      -1.158325    1.927417   -2.463599
H       0.597275    1.938323   -2.606953
C       0.763570   -1.143090   -4.163436
H       1.761614   -0.677283   -4.174282
H       0.281330   -0.834534   -5.106910
H       1.438137   -3.022103   -3.247321
C      -2.063042   -1.123282   -3.059572
H      -3.318900    0.221368   -1.859454
H      -2.054340   -1.516834   -4.091907
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H	-2.185941	-2.008381	-2.413248
C	-3.257093	-0.173265	-2.883407
H	-3.193416	0.687450	-3.565422
H	-4.204489	-0.689489	-3.098043
C	-0.443961	1.916624	-4.516746
H	-0.529429	3.008435	-4.618548
H	0.428962	1.596781	-5.102828
C	0.885240	-2.672378	-4.135692
H	-0.102743	-3.154934	-4.110390
H	1.419373	-3.059584	-5.015125
H	0.704625	-1.816531	-1.853254

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	1.554546203373072	42.3014	975.49	4081.46
Delta V^Pauli Coulomb:	-1.096380029498097	-29.8340	-687.99	-2878.55
Delta V^Pauli LDA-XC:	-0.272541245834450	-7.4162	-171.02	-715.56
Delta V^Pauli GGA-Exchange:	0.046694489230180	1.2706	29.30	122.60
Delta V^Pauli GGA-Correlation:	-0.020464623501800	-0.5569	-12.84	-53.73
Total Pauli Repulsion:	0.211854793768905	5.7649	132.94	556.22
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	0.211854793768905	5.7649	132.94	556.22
Electrostatic Interaction:	-0.165440071007786	-4.5019	-103.82	-434.36
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	0.046414722761119	1.2630	29.13	121.86
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-0.212902230835287	-5.7934	-133.60	-558.97
Total Orbital Interactions:	-0.212902230835287	-5.7934	-133.60	-558.97
Alternative Decomposition Orb.Int.				
Kinetic:	-0.982811342228749	-26.7437	-616.72	-2580.37
Coulomb:	0.677030198002013	18.4229	424.84	1777.54
XC:	0.092878913391448	2.5274	58.28	243.85
Total Orbital Interactions:	-0.212902230835287	-5.7934	-133.60	-558.97
Residu (E=Steric+OrbInt+Res):	-0.000000021579373	-0.0000	-0.00	-0.00
Dispersion Energy:	-0.022886577998930	-0.6228	-14.36	-60.09
Total Bonding Energy:	-0.189374107652471	-5.1531	-118.83	-497.20

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-0.165440071007786	-4.5019	-103.82	-434.36
Kinetic Energy:	0.571734861144323	15.5577	358.77	1501.09
Coulomb (Steric+OrbInt) Energy:	-0.419349853075458	-11.4111	-263.15	-1101.00
XC Energy:	-0.153432466714621	-4.1751	-96.28	-402.84
Dispersion Energy:	-0.022886577998930	-0.6228	-14.36	-60.09
Total Bonding Energy:	-0.189374107652472	-5.1531	-118.83	-497.20

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69
QUHNEM  ZORA-PBE-D3(BJ)/all electron TZP
Pt     -0.000044   -0.042751   -0.004714
Si     -0.722802    0.535983    2.186965
B      -0.359079    1.254072   -2.948930
N      -1.847890    0.340932   -1.124140
N      -1.738838    0.984112   -2.327197
C      -2.960196    1.085161   -2.917803
C      -3.881603    0.488064   -2.063645
C      -3.146412    0.020625   -0.958384
C      -3.178629    1.721009   -4.252436
C      -3.660024   -0.755422    0.205623
N       0.706365   -0.820278   -2.013668
N       0.400393   -0.077762   -3.115845
C       0.875298   -0.691250   -4.236660
C       1.502686   -1.865908   -3.829347
C       1.371594   -1.910169   -2.424176
C       0.709526   -0.128546   -5.611455
C       1.837164   -2.950811   -1.460465
N       0.837678    1.837052   -0.796353
N       0.463104    2.204386   -2.062675
C       1.137629    3.323988   -2.443593
C       1.966360    3.686519   -1.388585
C       1.761103    2.724831   -0.380793
C       0.974274    3.968594   -3.781803
C       2.438766    2.644691    0.941614
C       0.638311    1.067804    3.425582
C       1.754762    0.048930    3.678943
C      -1.515384   -0.985667    3.051582
C      -2.132689   -0.707791    4.429507
C      -1.973947    1.980723    2.140070
C      -1.382948    3.325701    1.692491
H       1.304967   -0.392178    0.774115
H      -0.508745   -1.423413    0.499180
H      -0.511922    1.761553   -4.024678
H      -4.951602    0.391959   -2.222968
H      -2.805468    2.754135   -4.277775
H      -4.251486    1.737763   -4.477263
H      -2.669934    1.167840   -5.054933
H      -3.050290   -1.652803    0.371846
H      -4.693764   -1.066253    0.015164
H      -3.645851   -0.168839    1.132913
H       1.992721   -2.594379   -4.469563
H      -0.350285   -0.008037   -5.877770
H       1.169097   -0.804272   -6.342300
H       1.187628    0.856690   -5.709960
H       1.206079   -3.850580   -1.513910
H       1.790024   -2.562609   -0.435912
H       2.869590   -3.254767   -1.679353
H       2.643347    4.535157   -1.353489
H       1.327954    3.315897   -4.592951
H       1.557618    4.896327   -3.812623
H      -0.075668    4.214402   -3.991674
H       1.963074    3.311656    1.674803
H       3.487966    2.951678    0.844085
H       2.403363    1.623425    1.334111
H       1.063550    2.036967    3.130814
H       0.095105    1.263695    4.368224
H       1.351166   -0.907684    4.043410
H       2.479900    0.405754    4.426850
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H	2.314693	-0.174012	2.757091
H	-2.267330	-1.440086	2.391369
H	-0.716015	-1.741998	3.141920
H	-1.394441	-0.293441	5.132003
H	-2.537791	-1.623867	4.887639
H	-2.959821	0.015870	4.362149
H	-2.402882	2.074409	3.154339
H	-2.808875	1.714114	1.473208
H	-0.581172	3.658189	2.369294
H	-2.145294	4.119777	1.675401
H	-0.955852	3.251590	0.682180

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	146.609840662665675	3989.4567	91999.07	384924.08
Delta V^Pauli Coulomb:	-72.723210377373320	-1978.8992	-45634.51	-190934.76
Delta V^Pauli LDA-XC:	-19.308202867670413	-525.4029	-12116.08	-50693.68
Delta V^Pauli GGA-Exchange:	0.945027752692361	25.7155	593.01	2481.17
Delta V^Pauli GGA-Correlation:	-0.218367616568553	-5.9421	-137.03	-573.32
Total Pauli Repulsion:	55.305087553745750	1504.9280	34704.47	145203.49
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.305087553745750	1504.9280	34704.47	145203.49
Electrostatic Interaction:	-11.401454674417824	-310.2494	-7154.52	-29934.52
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	43.903632879327930	1194.6786	27549.95	115268.97
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-58.639137991004425	-1595.6521	-36796.62	-153957.04
Total Orbital Interactions:	-58.639137991004425	-1595.6521	-36796.62	-153957.04
Alternative Decomposition Orb.Int.				
Kinetic:	-131.641468148321195	-3582.1466	-82606.28	-345624.63
Coulomb:	67.815624003178840	1845.3570	42554.95	178049.90
XC:	5.186706154137949	141.1375	3254.71	13617.70
Total Orbital Interactions:	-58.639137991004404	-1595.6521	-36796.62	-153957.04
Residu (E=Steric+OrbInt+Res):	0.000001651679976	0.0000	0.00	0.00
Dispersion Energy:	-0.105369417631652	-2.8672	-66.12	-276.65
Total Bonding Energy:	-14.840872877628170	-403.8407	-9312.79	-38964.71

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.401454674417824	-310.2494	-7154.52	-29934.52
Kinetic Energy:	14.968372514344480	407.3101	9392.80	39299.46
Coulomb (Steric+OrbInt) Energy:	-4.907584722514500	-133.5422	-3079.56	-12884.86
XC Energy:	-13.394836577408658	-364.4920	-8405.39	-35168.14
Dispersion Energy:	-0.105369417631652	-2.8672	-66.12	-276.65
Total Bonding Energy:	-14.840872877628152	-403.8407	-9312.79	-38964.71

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LUWNAS  ZORA-PBE-D3(BJ)/all electron TZP
Ir     -0.527072    6.466499    3.094030
P      -1.718187    4.938936    1.823946
Si     -2.138534    6.350228    4.919010
N       0.374952    4.960497    4.013026
C      -0.633260    8.285982    1.791572
C      -0.519780    8.749553    3.160730
C       0.742544    8.287587    3.678178
C       1.440373    7.611660    2.594801
C       0.631481    7.648288    1.427861
C      -1.671732    8.728482    0.805844
C      -1.415896    9.726480    3.848063
C       1.359514    8.686791    4.978351
C       2.825248    7.057976    2.688976
C       1.080498    7.286059    0.047158
C       0.926587    4.088046    4.551207
C       1.558396    2.992926    5.261015
C      -1.132610    4.759752    0.089061
C      -1.617364    3.198508    2.382691
C      -3.503292    5.222142    1.529483
C      -1.345404    7.118801    6.471440
C      -1.922834    8.230293    7.116254
C      -1.351827    8.792313    8.262794
C      -0.185234    8.248874    8.806140
C       0.411987    7.148305    8.182383
C      -0.156960    6.604876    7.029307
C      -3.808339    7.215900    4.683000
C      -4.219439    7.853047    3.503816
C      -5.469635    8.470385    3.397485
C      -6.344447    8.458204    4.487639
C      -5.964349    7.815269    5.671289
C      -4.714781    7.198728    5.763211
C      -2.643968    4.582126    5.422414
C      -3.865425    4.040735    4.974019
C      -4.247747    2.731842    5.280612
C      -3.416186    1.923263    6.060346
C      -2.217025    2.448882    6.552697
C      -1.844714    3.759219    6.240332
H      -1.881129    7.962420    0.049154
H      -1.318309    9.625222    0.274988
H      -2.614916    8.992338    1.295024
H      -1.024875   10.740712    3.671732
H      -2.444639    9.690638    3.478531
H      -1.437178    9.563092    4.931399
H       1.990781    9.576173    4.824437
H       0.603878    8.933618    5.731843
H       1.997451    7.896635    5.391849
H       3.561225    7.856768    2.507802
H       3.000771    6.269145    1.947561
H       3.027801    6.651518    3.687998
H       1.706041    8.098471   -0.354905
H       0.241300    7.155195   -0.643145
H       1.686615    6.371972    0.030651
H       2.648989    3.022033    5.132886
H       1.321288    3.051529    6.333038
H       1.179308    2.035118    4.876887
H      -1.328403    5.675915   -0.481792
H      -1.673290    3.927973   -0.385483
H      -0.055606    4.549106    0.070019
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H	-0.576464	2.859324	2.290847
H	-1.945303	3.104114	3.425872
H	-2.254495	2.576819	1.737855
H	-3.633593	6.172960	0.996332
H	-3.905847	4.404916	0.914157
H	-4.052105	5.278591	2.474924
H	-2.841949	8.665840	6.721959
H	-1.826974	9.652992	8.736590
H	0.256263	8.679803	9.706604
H	1.329247	6.720557	8.592202
H	0.358864	5.778543	6.540056
H	-3.545300	7.854257	2.648094
H	-5.763731	8.958960	2.466068
H	-7.321174	8.939913	4.414579
H	-6.645799	7.790421	6.523342
H	-4.440697	6.690344	6.689666
H	-4.551576	4.662550	4.396504
H	-5.204409	2.348391	4.921548
H	-3.713557	0.903060	6.307877
H	-1.584649	1.842680	7.205200
H	-0.936240	4.162921	6.687422

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	176.032128829607785	4790.0779	110461.84	462172.29
Delta V^Pauli Coulomb:	-85.630102187358119	-2330.1136	-53733.71	-224821.80
Delta V^Pauli LDA-XC:	-22.949376085266778	-624.4843	-14400.95	-60253.58
Delta V^Pauli GGA-Exchange:	1.112501953862839	30.2727	698.11	2920.87
Delta V^Pauli GGA-Correlation:	-0.248852139426671	-6.7716	-156.16	-653.36
Total Pauli Repulsion:	68.316300371419061	1858.9811	42869.13	179364.42
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	68.316300371419061	1858.9811	42869.13	179364.42
Electrostatic Interaction:	-13.797645928545315	-375.4530	-8658.15	-36225.71
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	54.518654442873746	1483.5281	34210.98	143138.71
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-71.865981427079902	-1955.5729	-45096.59	-188684.11
Total Orbital Interactions:	-71.878837331858563	-1955.9227	-45104.66	-188717.86
Alternative Decomposition Orb.Int.				
Kinetic:	-158.814266899779426	-4321.5561	-99657.47	-416966.80
Coulomb:	80.618220123342383	2193.7334	50588.70	211663.11
XC:	6.317209444578475	171.9000	3964.11	16585.83
Total Orbital Interactions:	-71.878837331858563	-1955.9227	-45104.66	-188717.86
Residu (E=Steric+OrbInt+Res):	-0.000009898299832	-0.0003	-0.01	-0.03
Dispersion Energy:	-0.144606523595655	-3.9349	-90.74	-379.66
Total Bonding Energy:	-17.504799310880305	-476.3298	-10984.43	-45958.84

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.797645928545315	-375.4530	-8658.15	-36225.71
Kinetic Energy:	17.217861929828359	468.5219	10804.37	45205.49
Coulomb (Steric+OrbInt) Energy:	-5.011891962315573	-136.3805	-3145.01	-13158.72
XC Energy:	-15.768516826252132	-429.0832	-9894.89	-41400.24
Dispersion Energy:	-0.144606523595655	-3.9349	-90.74	-379.66
Total Bonding Energy:	-17.504799310880315	-476.3298	-10984.43	-45958.84

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COPLIC  ZORA-PBE-D3(BJ)/all electron TZP
Co     -0.011784    0.030227    0.009260
Si     -1.322446    1.595453   -1.286980
O       1.583874   -1.857519    1.599099
O       0.208754    2.199261    1.970230
O      -2.417659   -1.647042   -0.004454
O       1.778749   -0.019244   -2.314637
C       0.957064   -1.116716    0.971455
C       0.103144    1.376998    1.160613
C      -1.495000   -0.946271   -0.018243
C       1.038964    0.023682   -1.423513
C      -0.462390    3.272085   -1.300923
C       0.863933    3.425418   -1.750777
C       1.471873    4.681373   -1.786008
C       0.766954    5.813521   -1.361140
C      -0.548720    5.680485   -0.910927
C      -1.156851    4.421729   -0.883061
C      -3.033326    1.772120   -0.516838
C      -4.183167    1.513939   -1.284514
C      -5.461837    1.663720   -0.738929
C      -5.614438    2.080140    0.585859
C      -4.481436    2.346883    1.363453
C      -3.206386    2.189634    0.817746
C      -1.484802    0.953601   -3.051753
C      -1.037677    1.736972   -4.130903
C      -1.158276    1.283999   -5.448368
C      -1.735422    0.039340   -5.711747
C      -2.191533   -0.751709   -4.650742
C      -2.062414   -0.299855   -3.336346
H       1.434397    2.558656   -2.085380
H       2.499365    4.777177   -2.142052
H       1.243849    6.795643   -1.381011
H      -1.106983    6.558196   -0.580027
H      -2.187092    4.334169   -0.534674
H      -4.079664    1.194690   -2.322711
H      -6.339835    1.454386   -1.352939
H      -6.612410    2.196227    1.013370
H      -4.592060    2.675675    2.398440
H      -2.339326    2.403423    1.443250
H      -0.590124    2.713919   -3.940996
H      -0.800188    1.907739   -6.269576
H      -1.828670   -0.316256   -6.739894
H      -2.646210   -1.724262   -4.848475
H      -2.423353   -0.934844   -2.526732
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	116.956899543846035	3182.5592	73391.57	307070.30
Delta V^Pauli Coulomb:	-58.075956040034797	-1580.3272	-36443.22	-152478.40
Delta V^Pauli LDA-XC:	-14.660858655222032	-398.9423	-9199.83	-38492.08
Delta V^Pauli GGA-Exchange:	0.695514647418889	18.9259	436.44	1826.07
Delta V^Pauli GGA-Correlation:	-0.147020720771099	-4.0006	-92.26	-386.00
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	44.768578775237003	1218.2150	28092.71	117539.89
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	44.768578775237003	1218.2150	28092.71	117539.89
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-9.300388452074088	-253.0764	-5836.08	-24418.17
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	35.468190323162915	965.1386	22256.63	93121.72

Orbital Interactions

A:	-46.185714232191167	-1256.7772	-28981.98	-121260.58
Total Orbital Interactions:	-46.190492167065315	-1256.9072	-28984.97	-121273.12

Alternative Decomposition Orb.Int.

Kinetic:	-106.976811308624775	-2910.9871	-67128.97	-280867.58
Coulomb:	56.297632296119993	1531.9365	35327.30	147809.41
XC:	4.488686845439454	122.1434	2816.69	11785.05
Total Orbital Interactions:	-46.190492167065329	-1256.9072	-28984.97	-121273.12
Residu (E=Steric+OrbInt+Res):	-0.000027265729670	-0.0007	-0.02	-0.07
Dispersion Energy:	-0.073915736640053	-2.0113	-46.38	-194.07
Total Bonding Energy:	-10.796244846272124	-293.7808	-6774.75	-28345.54

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-9.300388452074088	-253.0764	-5836.08	-24418.17
Kinetic Energy:	9.980088235221260	271.5720	6262.60	26202.72
Coulomb (Steric+OrbInt) Energy:	-1.778351009644474	-48.3914	-1115.93	-4669.06
XC Energy:	-9.623677883134789	-261.8736	-6038.95	-25266.96
Dispersion Energy:	-0.073915736640053	-2.0113	-46.38	-194.07
Total Bonding Energy:	-10.796244846272145	-293.7808	-6774.75	-28345.54

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90
SOKROB  ZORA-PBE-D3(BJ)/all electron TZP
Ni      3.906499    8.354054    4.424376
H       4.187122    7.951223    5.857976
Si      5.611697    6.954093    4.757902
C       4.751891    5.277371    5.085913
C       4.511938    4.309950    4.093535
H       4.934272    4.447186    3.095972
C       3.756291    3.162041    4.358085
H       3.584052    2.430492    3.564666
C       3.231718    2.944265    5.636162
H       2.644033    2.047839    5.846787
C       3.481887    3.879937    6.647395
H       3.096006    3.710989    7.656078
C       4.225707    5.029040    6.370202
H       4.399337    5.759622    7.164611
C       6.764581    7.228195    6.248007
C       7.575409    6.197898    6.759326
H       7.529734    5.205362    6.303960
C       8.432648    6.416313    7.841755
H       9.047084    5.598090    8.224550
C       8.502693    7.681446    8.436553
H       9.170067    7.854107    9.283769
C       7.704955    8.720386    7.945588
H       7.747135    9.708155    8.410602
C       6.844111    8.487815    6.866841
H       6.199338    9.294143    6.502530
C       6.818497    6.629304    3.303803
C       8.217738    6.680496    3.450176
H       8.647213    6.886986    4.432422
C       9.076389    6.484401    2.362344
H      10.157761    6.538891    2.509499
C       8.556667    6.221046    1.091374
H       9.225636    6.067098    0.241955
C       7.168750    6.162208    0.919032
H       6.745540    5.964422   -0.068766
C       6.322282    6.373209    2.009823
H       5.244434    6.367940    1.845356
C       4.067755    8.696786    2.584170
N       4.923870    9.543532    1.915234
C       4.694655    9.525057    0.545284
H       5.273999   10.112684   -0.156661
C       3.673957    8.649759    0.327140
H       3.202515    8.340398   -0.598314
N       3.305898    8.153273    1.572407
C       5.982153   10.323530    2.582065
H       5.941651    9.965531    3.624234
C       7.355286   10.015263    1.989418
H       7.553300    8.936144    1.985935
H       8.130812   10.512151    2.589573
H       7.434456   10.397134    0.959125
C       5.681649   11.823380    2.531779
H       5.681418   12.185547    1.491892
H       6.459085   12.375005    3.079259
H       4.708890   12.063314    2.977111
C       2.229343    7.185540    1.827002
H       2.334364    6.971033    2.901164
C       2.439519    5.893853    1.038826
H       1.661843    5.166140    1.309933
H       3.415264    5.445688    1.265089
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H	2.376020	6.068568	-0.046307
C	0.863477	7.820442	1.567053
H	0.720364	8.702082	2.207043
H	0.061495	7.100565	1.785057
H	0.765103	8.127793	0.514319
C	2.145796	8.995003	4.848869
N	1.584660	10.237461	4.679857
C	0.244666	10.257370	5.052060
H	-0.375944	11.144293	4.995753
C	-0.057504	8.993738	5.463660
H	-0.990343	8.581711	5.829402
N	1.103310	8.243061	5.335112
C	2.354994	11.386467	4.194722
H	3.342175	10.946069	3.996352
C	1.774481	11.929047	2.889893
H	1.753069	11.144483	2.121156
H	2.391915	12.759548	2.518754
H	0.751965	12.310558	3.034784
C	2.491095	12.453014	5.280427
H	1.515282	12.897922	5.529650
H	3.150568	13.261566	4.932818
H	2.919626	12.019874	6.194293
C	1.253808	6.837870	5.751016
H	2.269478	6.571843	5.423802
C	0.244989	5.933207	5.047977
H	-0.787093	6.143666	5.370590
H	0.473403	4.885400	5.287752
H	0.298164	6.055710	3.957829
C	1.187756	6.730967	7.273068
H	0.207010	7.055990	7.654833
H	1.968802	7.354143	7.729604
H	1.351153	5.688426	7.577677

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	196.435124998368650	5345.2717	123264.91	515740.35
Delta V^Pauli Coulomb:	-93.904081063012285	-2555.2601	-58925.71	-246545.13
Delta V^Pauli LDA-XC:	-26.192223318223590	-712.7267	-16435.87	-68767.67
Delta V^Pauli GGA-Exchange:	1.231911716749792	33.5220	773.04	3234.38
Delta V^Pauli GGA-Correlation:	-0.258997129554563	-7.0477	-162.52	-680.00
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	77.311735204328002	2103.7594	48513.85	202981.93
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	77.311735204328002	2103.7594	48513.85	202981.93
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-15.517364482575665	-422.2490	-9737.29	-40740.83
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	61.794370721752337	1681.5104	38776.56	162241.10
Orbital Interactions				
A:	-81.679589414001896	-2222.6147	-51254.72	-214449.73
Total Orbital Interactions:	-81.679589414001910	-2222.6147	-51254.72	-214449.73
Alternative Decomposition Orb.Int.				
Kinetic:	-178.111716830836343	-4846.6664	-111766.80	-467632.25
Coulomb:	89.254604289290583	2428.7414	56008.12	234337.93
XC:	7.177523127544185	195.3103	4503.96	18844.58
Total Orbital Interactions:	-81.679589414001569	-2222.6147	-51254.72	-214449.73
Residu (E=Steric+OrbInt+Res):	-0.000058951908715	-0.0016	-0.04	-0.15
Dispersion Energy:	-0.151103909315485	-4.1117	-94.82	-396.72
Total Bonding Energy:	-20.036381553473774	-545.2177	-12573.02	-52605.51

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-15.517364482575665	-422.2490	-9737.29	-40740.83
Kinetic Energy:	18.323408167532307	498.6053	11498.11	48108.10
Coulomb (Steric+OrbInt) Energy:	-4.649535725630415	-126.5203	-2917.63	-12207.35

XC Energy:	-18.041785603484179	-490.9420	-11321.39	-47368.70
Dispersion Energy:	-0.151103909315485	-4.1117	-94.82	-396.72
Total Bonding Energy:	-20.036381553473436	-545.2177	-12573.02	-52605.51

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MSIHGB  ZORA-PBE-D3(BJ)/all electron TZP
Hg       0.000000    0.000000    0.000000
Si      -0.058076    1.688450    1.860329
C        0.843476    1.028501    3.379180
C        2.248739    0.071971    5.635574
C        2.196924    0.645677    3.283542
C        0.209534    0.909882    4.628910
C        2.896696    0.180301    4.399089
C        0.902639    0.432932    5.745510
C        0.789315    3.262187    1.254806
C        2.034325    5.608145    0.293931
C        0.363339    3.872176    0.057594
C        1.855485    3.852949    1.955970
C        0.972046    5.036045   -0.416883
C        2.474512    5.012993    1.480302
C       -1.853801    2.067034    2.298105
C       -4.551026    2.589195    2.951162
C       -2.711813    1.031209    2.720374
C       -2.381041    3.367413    2.204856
C       -4.043921    1.287828    3.051589
C       -3.717346    3.626867    2.523783
Si       0.058076   -1.688450   -1.860329
C       -0.843476   -1.028501   -3.379180
C       -0.789315   -3.262187   -1.254806
C        1.853801   -2.067034   -2.298105
C       -2.196924   -0.645677   -3.283542
C       -0.209534   -0.909882   -4.628910
C       -0.363339   -3.872176   -0.057594
C       -1.855485   -3.852949   -1.955970
C        2.711813   -1.031209   -2.720374
C        2.381041   -3.367413   -2.204856
C       -2.896696   -0.180301   -4.399089
C       -0.902639   -0.432932   -5.745510
C       -0.972046   -5.036045    0.416883
C       -2.474512   -5.012993   -1.480302
C        4.043921   -1.287828   -3.051589
C        3.717346   -3.626867   -2.523783
C       -2.248739   -0.071971   -5.635574
C       -2.034325   -5.608145   -0.293931
C        4.551026   -2.589195   -2.951162
H        2.518573    6.513621   -0.077024
H       -0.459727    3.432051   -0.511617
H        2.203894    3.401278    2.886776
H        0.624102    5.493303   -1.344306
H        3.300660    5.455373    2.040135
H       -5.593738    2.791357    3.203025
H       -2.331893    0.008898    2.794694
H       -1.736973    4.187635    1.882681
H       -4.690277    0.473076    3.382157
H       -4.106366    4.643699    2.442277
H        2.791223   -0.295610    6.508590
H        2.714168    0.720662    2.323617
H       -0.836754    1.202588    4.731904
H        3.946348   -0.102815    4.305153
H        0.390854    0.350145    6.706174
H       -2.714168   -0.720662   -2.323617
H        0.836754   -1.202588   -4.731904
H        0.459727   -3.432051    0.511617
H       -2.203894   -3.401278   -2.886776
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H	2.331893	-0.008898	-2.794694
H	1.736973	-4.187635	-1.882681
H	-3.946348	0.102815	-4.305153
H	-0.390854	-0.350145	-6.706174
H	-0.624102	-5.493303	1.344306
H	-3.300660	-5.455373	-2.040135
H	4.690277	-0.473076	-3.382157
H	4.106366	-4.643699	-2.442277
H	-2.791223	0.295610	-6.508590
H	-2.518573	-6.513621	0.077024
H	5.593738	-2.791357	-3.203025

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	169.749846293873134	4619.1283	106519.65	445678.16
Delta V^Pauli Coulomb:	-80.772600210420350	-2197.9343	-50685.58	-212068.43
Delta V^Pauli LDA-XC:	-21.868381053797673	-595.0689	-13722.62	-57415.43
Delta V^Pauli GGA-Exchange:	0.969242939693764	26.3744	608.21	2544.75
Delta V^Pauli GGA-Correlation:	-0.174242205245610	-4.7414	-109.34	-457.47
Total Pauli Repulsion:	67.903865764103259	1847.7582	42610.32	178281.57
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	67.903865764103259	1847.7582	42610.32	178281.57
Electrostatic Interaction:	-13.431820985543984	-365.4984	-8428.60	-35265.24
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	54.472044778559273	1482.2598	34181.73	143016.33
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A.g:	-35.390859881026088	-963.0343	-22208.10	-92918.69
A.u:	-35.305401189573239	-960.7088	-22154.48	-92694.32
Total Orbital Interactions:	-70.696261070599334	-1923.7431	-44362.58	-185613.01
Alternative Decomposition Orb.Int.				
Kinetic:	-154.146511523773540	-4194.5400	-96728.41	-404711.61
Coulomb:	77.239247022216816	2101.7869	48468.36	202791.61
XC:	6.211003430957269	169.0100	3897.46	16306.99
Total Orbital Interactions:	-70.696261070599462	-1923.7431	-44362.58	-185613.01
Residu (E=Steric+OrbInt+Res):	-0.000217895121244	-0.0059	-0.14	-0.57
Dispersion Energy:	-0.109721960575634	-2.9857	-68.85	-288.07
Total Bonding Energy:	-16.334156147736941	-444.4750	-10249.84	-42885.32

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.431820985543984	-365.4984	-8428.60	-35265.24
Kinetic Energy:	15.603334770099593	424.5883	9791.24	40966.55
Coulomb (Steric+OrbInt) Energy:	-3.533571083324773	-96.1534	-2217.35	-9277.39
XC Energy:	-14.862376888392252	-404.4259	-9326.28	-39021.16
Dispersion Energy:	-0.109721960575634	-2.9857	-68.85	-288.07
Total Bonding Energy:	-16.334156147737048	-444.4750	-10249.84	-42885.32

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109
EJOFUF  ZORA-PBE-D3(BJ)/all electron TZP
Rh       8.246526    1.460467    3.942828
H        8.089545    0.503903    2.683785
Si       9.614096    1.541311    2.058356
P        9.325932   -0.143397    5.189046
P        6.838695    3.183836    3.289127
N        7.866225    2.289532    5.822753
C        8.676407    1.857313    0.436238
C        9.170095    2.717547   -0.561021
H       10.075112    3.298747   -0.375361
C        8.513772    2.858065   -1.787368
H        8.915366    3.538919   -2.541226
C        7.343899    2.137177   -2.047448
H        6.830378    2.247750   -3.005230
C        6.829639    1.282787   -1.067041
H        5.909356    0.724863   -1.251584
C        7.489682    1.153201    0.157314
H        7.061839    0.497988    0.918947
C       10.652726   -0.008312    1.680266
C       11.974516   -0.165191    2.135638
H       12.446877    0.631414    2.712584
C       12.702366   -1.329434    1.866063
H       13.724404   -1.424505    2.238519
C       12.123848   -2.363446    1.122971
H       12.692594   -3.270715    0.907491
C       10.814526   -2.222316    0.648991
H       10.355461   -3.018832    0.059689
C       10.092163   -1.060286    0.929106
H        9.073945   -0.967909    0.546554
C       10.858566    2.954720    2.354870
C       11.954965    3.136303    1.491002
H       12.105326    2.447791    0.656924
C       12.871273    4.173790    1.691126
H       13.712855    4.295284    1.005796
C       12.717133    5.048446    2.772517
H       13.435484    5.855480    2.932600
C       11.641869    4.877561    3.651139
H       11.513819    5.549037    4.502825
C       10.726718    3.843555    3.437089
H        9.892984    3.712336    4.131778
C        6.896484    4.238648    4.771155
C        7.946459    1.457425    6.939892
C        8.665224    0.239240    6.834458
C        8.814686   -0.621396    7.927635
H        9.393564   -1.539328    7.799562
C        8.207108   -0.357486    9.157276
C        8.381911   -1.273507   10.342196
H        7.446692   -1.380352   10.910310
H        9.143142   -0.884669   11.037585
H        8.705815   -2.274724   10.027973
C        7.415980    0.804462    9.236510
H        6.874929    1.018112   10.162671
C        7.284205    1.688943    8.171592
H        6.633707    2.554928    8.274656
C        8.838402   -1.866819    4.847863
C        9.564962   -2.646223    3.932872
H       10.480168   -2.258703    3.484520
C        9.112713   -3.921032    3.586315
H        9.691661   -4.517095    2.878393
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C	7.926286	-4.422697	4.131311
H	7.575784	-5.420027	3.857701
C	7.188202	-3.639335	5.026455
H	6.257771	-4.019183	5.451929
C	7.639087	-2.367636	5.384277
H	7.064586	-1.759810	6.084519
C	11.145595	-0.131433	5.398087
C	11.768058	1.126110	5.355353
H	11.168199	2.015770	5.169870
C	13.147554	1.238231	5.521471
H	13.617345	2.221911	5.469358
C	13.920556	0.091068	5.734752
H	15.002876	0.173694	5.853850
C	13.302093	-1.161696	5.800004
H	13.898728	-2.058393	5.976080
C	11.918430	-1.276130	5.638865
H	11.446558	-2.257293	5.688295
C	7.458020	3.621549	5.917174
C	7.663267	4.448836	7.047288
H	8.169496	4.042645	7.921162
C	7.280610	5.786761	7.038108
H	7.481333	6.394550	7.924957
C	6.670655	6.383478	5.919763
C	6.504091	5.581729	4.786543
H	6.095849	6.024221	3.875999
C	6.231684	7.826523	5.937843
H	6.044171	8.197460	4.921475
H	6.991284	8.473235	6.400675
H	5.301954	7.955153	6.514647
C	5.118431	2.577954	3.108314
C	4.905573	1.201952	2.939668
H	5.768670	0.533388	2.942162
C	3.608830	0.702591	2.790179
H	3.452217	-0.369495	2.660623
C	2.517868	1.576344	2.814909
H	1.503672	1.188189	2.701130
C	2.724935	2.950200	2.993787
H	1.874053	3.633168	3.020950
C	4.019221	3.450510	3.140339
H	4.176994	4.520868	3.279685
C	7.030772	4.387764	1.921738
C	6.196982	4.362626	0.793673
H	5.397296	3.625715	0.720298
C	6.388990	5.281991	-0.241440
H	5.731949	5.253000	-1.112166
C	7.418881	6.223922	-0.167265
H	7.568319	6.939058	-0.979356
C	8.259777	6.245669	0.950943
H	9.069573	6.974381	1.020238
C	8.066149	5.336389	1.990260
H	8.716975	5.372232	2.861809

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	276.119935153897643	7513.6057	173267.89	724952.79
Delta V^Pauli Coulomb:	-132.463236766294216	-3604.5081	-83121.94	-347782.18
Delta V^Pauli LDA-XC:	-35.851392396139616	-975.5660	-22497.09	-94127.82
Delta V^Pauli GGA-Exchange:	1.666327295848717	45.3431	1045.64	4374.94
Delta V^Pauli GGA-Correlation:	-0.332841615691908	-9.0571	-208.86	-873.88
Total Pauli Repulsion:	109.138791671620623	2969.8176	68485.63	286543.86
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	109.138791671620623	2969.8176	68485.63	286543.86

Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-22.022600693326911	-599.2655	-13819.39	-57820.33
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	87.116190978293716	2370.5522	54666.24	228723.53

Orbital Interactions				
A:	-113.075824904259605	-3076.9498	-70956.16	-296880.54
Total Orbital Interactions:	-113.096810452996735	-3077.5208	-70969.33	-296935.63

Alternative Decomposition Orb.Int.				
Kinetic:	-251.732996524275421	-6850.0034	-157964.86	-660924.89
Coulomb:	127.976299889916916	3482.4123	80306.35	336001.73
XC:	10.659886181361811	290.0703	6689.18	27987.53
Total Orbital Interactions:	-113.096810452996692	-3077.5208	-70969.33	-296935.63
Residu (E=Steric+OrbInt+Res):	0.000019370182506	0.0005	0.01	0.05
Dispersion Energy:	-0.223177394380573	-6.0730	-140.05	-585.95
Total Bonding Energy:	-26.203777498901086	-713.0411	-16443.12	-68798.01

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-22.022600693326911	-599.2655	-13819.39	-57820.33
Kinetic Energy:	24.386938629622222	663.6024	15303.04	64027.90
Coulomb (Steric+OrbInt) Energy:	-4.486917506194800	-122.0952	-2815.58	-11780.40
XC Energy:	-23.858020534620998	-649.2098	-14971.14	-62639.22
Dispersion Energy:	-0.223177394380573	-6.0730	-140.05	-585.95
Total Bonding Energy:	-26.203777498901061	-713.0411	-16443.12	-68798.01

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50
PSICRE  ZORA-PBE-D3(BJ)/all electron TZP
C      -1.159243   -1.275700   -4.010511
C      -2.098894   -2.099748   -4.635802
Re      0.017955    0.045511   -0.014460
Si      1.009455   -0.659851   -2.215726
C       0.358918    1.870288    0.468562
O       0.574145    2.975091    0.793996
C      -1.210218    0.791245   -1.274753
O      -2.012953    1.224964   -2.010557
H       1.569378    0.393765   -0.555841
C      -2.104597   -3.475641   -4.384901
C      -1.162255   -4.021427   -3.506306
C      -0.224290   -3.191874   -2.886211
C      -0.200128   -1.803740   -3.125195
C       1.639851    2.079688   -2.903146
C       1.986841    3.119453   -3.769978
C       2.119625    2.872226   -5.139246
C       1.905883    1.580119   -5.632518
C       1.559276    0.545734   -4.759559
C       1.414899    0.775511   -3.377861
C       2.983506   -2.610818   -2.979510
C       4.156577   -3.361604   -2.862202
C       4.976917   -3.210992   -1.739393
C       4.617922   -2.298439   -0.742428
C       3.442491   -1.552168   -0.868733
C       2.594302   -1.694689   -1.982643
H      -1.169381   -0.204406   -4.216683
H      -2.829363   -1.664627   -5.320676
H      -2.836802   -4.120761   -4.874555
H      -1.153757   -5.095498   -3.309531
H       0.516280   -3.640217   -2.220852
H       1.536879    2.293994   -1.838738
H       2.148973    4.124280   -3.374325
H       2.388346    3.683256   -5.819604
H       2.009829    1.378066   -6.700481
H       1.389559   -0.455248   -5.162809
H       2.354934   -2.746616   -3.861837
H       4.431682   -4.065034   -3.650613
H       5.892523   -3.798235   -1.643657
H       5.256357   -2.166268    0.133724
H       3.182246   -0.840390   -0.082110
C      -0.315965   -0.691390    2.185087
C      -1.485960   -1.010137    1.427936
C      -1.100864   -1.936916    0.401022
C       0.302341   -2.187857    0.537676
C       0.787729   -1.421595    1.647901
H      -0.273922   -0.008525    3.029420
H      -2.486242   -0.627129    1.604247
H      -1.749273   -2.377835   -0.351064
H       0.896611   -2.863559   -0.067623
H       1.807875   -1.410220    2.017255
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	1.780321822220797	48.4450	1117.17	4674.23
Delta V^Pauli Coulomb:	-1.171112343345500	-31.8676	-734.88	-3074.76
Delta V^Pauli LDA-XC:	-0.329011640177626	-8.9529	-206.46	-863.82
Delta V^Pauli GGA-Exchange:	0.047314293226545	1.2875	29.69	124.22
Delta V^Pauli GGA-Correlation:	-0.021804284438112	-0.5933	-13.68	-57.25
Total Pauli Repulsion:	0.305707847486105	8.3187	191.83	802.64
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				

Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	0.305707847486105	8.3187	191.83	802.64
Electrostatic Interaction:	-0.329429776069079	-8.9642	-206.72	-864.92
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	-0.023721928582973	-0.6455	-14.89	-62.28
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-0.274150961733746	-7.4600	-172.03	-719.78
Total Orbital Interactions:	-0.274150961733746	-7.4600	-172.03	-719.78
Alternative Decomposition Orb.Int.				
Kinetic:	-1.107642064074351	-30.1405	-695.06	-2908.11
Coulomb:	0.703097246451038	19.1322	441.20	1845.98
XC:	0.130393855889567	3.5482	81.82	342.35
Total Orbital Interactions:	-0.274150961733746	-7.4600	-172.03	-719.78
Residu (E=Steric+OrbInt+Res):	0.000000696161826	0.0000	0.00	0.00
Dispersion Energy:	-0.018848570519768	-0.5129	-11.83	-49.49
Total Bonding Energy:	-0.316720764674661	-8.6184	-198.75	-831.55

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-0.329429776069079	-8.9642	-206.72	-864.92
Kinetic Energy:	0.672679758146446	18.3045	422.11	1766.12
Coulomb (Steric+OrbInt) Energy:	-0.468014400732636	-12.7353	-293.68	-1228.77
XC Energy:	-0.173107775499625	-4.7105	-108.63	-454.49
Dispersion Energy:	-0.018848570519768	-0.5129	-11.83	-49.49
Total Bonding Energy:	-0.316720764674661	-8.6184	-198.75	-831.55

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FACGIC  ZORA-PBE-D3(BJ)/all electron TZP
Ru      6.793111    3.907202   13.781735
H       5.392844    4.769329   14.092943
P       5.163080    2.146723   13.247323
Si      6.939708    6.316497   13.669174
P       7.256383    3.703795   16.093321
O       9.633172    2.977034   13.039985
N       6.416296    4.296634   10.529916
N       5.128932    2.982743   11.675036
C       4.789759    4.664677   16.997991
H       4.744083    5.120353   16.010703
C       5.904967    3.887364   17.329255
C       8.538708    3.293746   13.349086
C       3.756958    4.857996   17.918386
H       2.901592    5.477983   17.644050
C       3.826594    4.267517   19.182530
H       3.019444    4.414004   19.903457
C       4.940606    3.491874   19.525964
H       5.006109    3.031558   20.513587
C       5.976138    3.306344   18.608146
H       6.840007    2.700053   18.882721
C       8.593257    4.773846   16.790886
C       8.583227    5.253788   18.109563
H       7.763096    5.000879   18.780647
C       9.601127    6.097055   18.560587
H       9.568653    6.477867   19.583245
C      10.642527    6.470077   17.704477
H      11.428180    7.142523   18.055102
C      10.661580    5.992531   16.391273
H      11.451376    6.294500   15.701361
C       9.640010    5.154844   15.939486
H       9.633488    4.827751   14.903884
C       7.887564    2.010952   16.488876
C       9.257169    1.719503   16.400923
H       9.970721    2.516628   16.188958
C       9.717505    0.412873   16.587761
H      10.786324    0.204213   16.512896
C       8.819062   -0.618228   16.878222
H       9.180740   -1.636450   17.033746
C       7.452346   -0.334249   16.971381
H       6.740867   -1.130037   17.201126
C       6.990415    0.967594   16.767448
H       5.922397    1.178236   16.838567
C       5.658949    0.368583   12.708316
C       5.005380   -0.132583   11.409898
H       5.335285   -1.170851   11.238477
H       5.327860    0.458815   10.542702
H       3.909637   -0.138070   11.446964
C       5.356673   -0.608115   13.857980
H       4.281413   -0.791367   13.984128
H       5.776321   -0.257743   14.809801
H       5.833061   -1.574646   13.626991
C       7.181131    0.423993   12.496906
H       7.709290    0.684646   13.422536
H       7.458055    1.159379   11.729154
H       7.527296   -0.566798   12.160568
C       3.337832    2.174406   13.811847
C       3.331025    1.767017   15.298135
H       2.308151    1.873956   15.693808
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H	3.984952	2.419170	15.892200
H	3.640805	0.725307	15.449407
C	2.827897	3.621258	13.699674
H	2.780583	3.956721	12.654705
H	3.465814	4.315818	14.258016
H	1.810844	3.666834	14.120479
C	2.389200	1.270054	13.009198
H	2.632593	0.204695	13.106974
H	2.374239	1.532577	11.941246
H	1.364952	1.409665	13.393545
C	6.186668	3.854404	11.792623
C	5.480940	3.752456	9.646966
H	5.462384	4.024714	8.598012
C	4.674460	2.914459	10.358520
H	3.833718	2.312460	10.040728
C	7.485569	5.198094	10.129659
H	8.063955	5.459343	11.017945
H	7.065554	6.115162	9.700288
H	8.138340	4.697124	9.403022
C	8.642386	7.151854	13.368001
C	9.730816	6.464495	12.803402
H	9.635759	5.401025	12.580110
C	10.950766	7.097292	12.542546
H	11.776696	6.529415	12.107818
C	11.112547	8.452731	12.846538
H	12.063179	8.953314	12.649220
C	10.043818	9.161281	13.406619
H	10.156414	10.220623	13.647437
C	8.829400	8.517158	13.660327
H	8.008375	9.086210	14.099629
C	6.218170	7.278515	15.166126
C	7.008635	7.707661	16.247277
H	8.085160	7.526819	16.235219
C	6.450889	8.379276	17.341222
H	7.095477	8.695026	18.164945
C	5.080019	8.647789	17.379881
H	4.644195	9.176920	18.230659
C	4.273695	8.239801	16.311133
H	3.202365	8.456629	16.318119
C	4.839263	7.565684	15.226097
H	4.190330	7.270243	14.398911
C	5.855994	7.041353	12.248389
C	4.562878	6.541732	12.000178
H	4.210778	5.687317	12.577569
C	3.724438	7.097099	11.029777
H	2.724489	6.684243	10.872495
C	4.167133	8.178559	10.259954
H	3.519367	8.617052	9.497375
C	5.448482	8.692902	10.482175
H	5.807646	9.539141	9.891505
C	6.274128	8.133094	11.464570
H	7.269182	8.555395	11.617402

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	257.001391896786174	6993.3637	161270.83	674757.06
Delta V^Pauli Coulomb:	-124.143599231079506	-3378.1192	-77901.29	-325938.97
Delta V^Pauli LDA-XC:	-33.785800141523815	-919.3584	-21200.91	-88704.61
Delta V^Pauli GGA-Exchange:	1.624947983446432	44.2171	1019.67	4266.30
Delta V^Pauli GGA-Correlation:	-0.356303068215514	-9.6955	-223.58	-935.47
Total Pauli Repulsion:	100.340637439413783	2730.4077	62964.71	263444.31
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				

Steric Interaction

Pauli Repulsion (Delta E^Pauli):	100.340637439413783	2730.4077	62964.71	263444.31
Electrostatic Interaction:	-20.324422642458394	-553.0557	-12753.77	-53361.76
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	80.016214796955381	2177.3520	50210.94	210082.54
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-105.125349475144802	-2860.6063	-65967.16	-276006.57
Total Orbital Interactions:	-105.125349475144787	-2860.6063	-65967.16	-276006.57
Alternative Decomposition Orb.Int.				
Kinetic:	-233.609093491470844	-6356.8269	-146591.93	-613340.59
Coulomb:	118.816891442408078	3233.1721	74558.73	311953.70
XC:	9.666852573917982	263.0484	6066.04	25380.32
Total Orbital Interactions:	-105.125349475144787	-2860.6063	-65967.16	-276006.57
Residu (E=Steric+OrbInt+Res):	0.000001914732789	0.0001	0.00	0.01
Dispersion Energy:	-0.224529152345630	-6.1097	-140.89	-589.50
Total Bonding Energy:	-25.333661915802246	-689.3640	-15897.11	-66513.52

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-20.324422642458394	-553.0557	-12753.77	-53361.76
Kinetic Energy:	23.392298405315330	636.5368	14678.89	61416.47
Coulomb (Steric+OrbInt) Energy:	-5.326705873938636	-144.9470	-3342.56	-13985.26
XC Energy:	-22.850302652374911	-621.7884	-14338.78	-59993.46
Dispersion Energy:	-0.224529152345630	-6.1097	-140.89	-589.50
Total Bonding Energy:	-25.333661915802239	-689.3640	-15897.11	-66513.52

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89
QINZEU  ZORA-PBE-D3(BJ)/all electron TZP
Fe     10.396852    3.471361    2.989286
Si      8.201097    3.387379    2.096076
C      10.513576    5.012297    2.133635
O      10.624151    5.995589    1.520777
C      10.199086    1.724555    3.146137
O      10.134161    0.560928    3.171804
C       9.690523    4.044406    4.518005
O       9.126604    4.426271    5.464142
C      12.312153    3.362322    3.423455
N      12.941134    3.366204    4.645031
C      14.319498    3.203333    4.518459
H      14.973459    3.185698    5.381846
C      14.578494    3.095802    3.189873
H      15.506981    2.964958    2.648068
N      13.353618    3.190749    2.536072
C      12.322027    3.604054    5.925109
C      11.937584    2.509895    6.715364
C      11.380764    2.780494    7.970365
H      11.061788    1.940920    8.593166
C      11.222269    4.087586    8.444584
C      11.627882    5.146996    7.625852
H      11.497023    6.174757    7.973357
C      12.180757    4.932015    6.359886
C      12.106142    1.094093    6.232583
H      11.644635    3.636294   -3.360709
H      11.778216    0.383028    7.000441
H      13.155463    0.873918    5.986162
C      10.654270    4.348359    9.816806
H       9.959349    3.554518   10.119774
H      10.120789    5.307033    9.852728
H      11.457222    4.389311   10.569455
C      12.566130    6.087697    5.476053
H      13.602161    5.999474    5.117395
H      12.465320    7.037612    6.014095
H      11.917870    6.126139    4.587430
C      13.241081    3.231626    1.099221
C      13.404678    4.471239    0.456500
C      13.240359    4.512581   -0.931479
H      13.336150    5.474372   -1.441375
C      12.954030    3.364417   -1.677782
C      12.865562    2.141868   -1.005225
H      12.670506    1.228695   -1.573437
C      13.003746    2.046653    0.384551
C      13.768914    5.718567    1.219266
H      13.273728    5.764472    2.196308
H      13.486909    6.612624    0.651029
H      14.854885    5.759374    1.398945
C      12.711760    3.449583   -3.162129
H      11.518436    0.909575    5.323535
H      13.281637    4.270411   -3.616687
H      12.985753    2.514655   -3.668466
C      12.861910    0.712178    1.065315
H      13.427548    0.664588    2.003858
H      13.210196   -0.092170    0.405083
H      11.811036    0.507441    1.312571
C       7.273556    5.034380    2.298029
C       7.432589    6.056360    1.341517
H       8.051700    5.879442    0.460454
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C	6.806275	7.295796	1.490440
H	6.948043	8.069550	0.732687
C	5.999660	7.544623	2.606542
H	5.508369	8.513270	2.725953
C	5.821598	6.540924	3.563930
H	5.186046	6.720618	4.433968
C	6.452909	5.302602	3.409035
H	6.291486	4.530843	4.163212
C	7.135787	2.048634	2.929194
C	6.972169	1.987454	4.328229
H	7.471223	2.712037	4.971566
C	6.183198	1.002005	4.926144
H	6.068153	0.985442	6.012419
C	5.548176	0.036014	4.138253
H	4.935330	-0.738892	4.604335
C	5.707826	0.070884	2.750367
H	5.221717	-0.679621	2.123325
C	6.490892	1.066238	2.156828
H	6.603985	1.075522	1.071237
C	8.148505	3.023617	0.229208
C	9.209418	2.456534	-0.493752
H	10.151899	2.241245	0.012691
C	9.096458	2.173695	-1.859110
H	9.942524	1.735273	-2.394258
C	7.907208	2.456855	-2.536444
H	7.815769	2.242356	-3.603911
C	6.835195	3.022873	-1.836809
H	5.902631	3.253329	-2.355886
C	6.957499	3.300518	-0.472975
H	6.114285	3.747959	0.057300
H	10.803852	3.023524	1.602834

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	221.270112053818394	6021.0661	138849.11	580944.60
Delta V^Pauli Coulomb:	-107.103504349628849	-2914.4346	-67208.47	-281200.21
Delta V^Pauli LDA-XC:	-28.655219776627568	-779.7482	-17981.42	-75234.27
Delta V^Pauli GGA-Exchange:	1.333288379278944	36.2806	836.65	3500.55
Delta V^Pauli GGA-Correlation:	-0.271687137573011	-7.3930	-170.49	-713.31
Total Pauli Repulsion:	86.572989169267899	2355.7709	54325.38	227297.35
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	86.572989169267899	2355.7709	54325.38	227297.35
Electrostatic Interaction:	-17.550115683019065	-477.5629	-11012.87	-46077.82
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	69.022873486248841	1878.2080	43312.51	181219.53
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-90.080254224712803	-2451.2084	-56526.22	-236505.67
Total Orbital Interactions:	-90.097180668287010	-2451.6690	-56536.84	-236550.11
Alternative Decomposition Orb.Int.				
Kinetic:	-201.628480886228317	-5486.5901	-126523.80	-529375.50
Coulomb:	103.129644783766835	2806.3004	64714.84	270766.84
XC:	8.401655434174494	228.6207	5272.12	22058.54
Total Orbital Interactions:	-90.097180668286995	-2451.6690	-56536.84	-236550.11
Residu (E=Steric+OrbInt+Res):	-0.000039959691965	-0.0011	-0.03	-0.10
Dispersion Energy:	-0.157810345052852	-4.2942	-99.03	-414.33
Total Bonding Energy:	-21.232157486782985	-577.7564	-13323.38	-55745.02

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-17.550115683019065	-477.5629	-11012.87	-46077.82
Kinetic Energy:	19.641631167590077	534.4760	12325.31	51569.10
Coulomb (Steric+OrbInt) Energy:	-3.973899525553975	-108.1353	-2493.66	-10433.47

XC Energy:	-19.191963100747142	-522.2399	-12043.14	-50388.49
Dispersion Energy:	-0.157810345052852	-4.2942	-99.03	-414.33
Total Bonding Energy:	-21.232157486782956	-577.7564	-13323.38	-55745.02

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73
JAMZIH  ZORA-PBE-D3(BJ)/all electron TZP
Os       0.050612   -0.005581    0.020017
Br      -0.217562    0.948998    2.430340
P        0.920844    2.129007   -0.577490
Si       1.964192   -0.960196    1.141158
C       -2.289618   -0.499228    0.186961
C       -1.416194   -1.605927    0.572058
C       -0.666992   -1.994972   -0.594548
C       -1.019388   -1.064125   -1.660790
C       -2.077179   -0.202189   -1.181445
C       -3.333175    0.111864    1.063725
C       -1.501783   -2.347788    1.866424
C        0.115474   -3.260266   -0.757208
C       -0.633607   -1.248844   -3.097985
C       -2.952857    0.685672   -2.015796
C        2.712004    2.416868   -0.005160
C        2.771139    2.818680    1.473506
C        3.596187    3.361149   -0.835143
C       -0.035918    3.594491    0.127287
C       -1.554371    3.409384    0.041464
C        0.389268    4.975766   -0.384364
C        1.093915    2.505758   -2.417172
C       -0.233897    2.696807   -3.150836
C        1.952681    1.459366   -3.136238
C        3.147387   -1.949078    0.006340
C        3.762764   -3.119321    0.486572
C        4.608224   -3.888407   -0.320386
C        4.863007   -3.501814   -1.640299
C        4.270194   -2.337813   -2.139496
C        3.427403   -1.580463   -1.321662
H       -4.084793   -0.644631    1.338890
H       -2.886028    0.495811    1.993991
H       -3.850394    0.937250    0.559674
H       -2.355877   -3.043371    1.854573
H       -0.590206   -2.927296    2.051184
H       -1.629662   -1.652626    2.706308
H       -0.553693   -4.072537   -1.083062
H        0.586420   -3.566214    0.184305
H        0.914351   -3.156134   -1.501349
H       -1.323058   -1.959638   -3.581433
H        0.379841   -1.658289   -3.190095
H       -0.674348   -0.311437   -3.664869
H       -3.969366    0.262821   -2.049971
H       -3.033009    1.702571   -1.613897
H       -2.598480    0.754331   -3.050060
H        3.134121    1.401056   -0.088291
H        2.439600    3.858966    1.615020
H        2.153567    2.168904    2.104248
H        3.811709    2.751477    1.826078
H        3.714225    3.049958   -1.880626
H        3.225629    4.395945   -0.828690
H        4.601976    3.376115   -0.386800
H        1.631696    3.467089   -2.434910
H        0.225632    3.515707    1.194794
H       -1.840621    2.401503    0.365237
H       -2.050905    4.134775    0.704521
H       -1.933391    3.580924   -0.976340
H       -0.213474    5.749849    0.117742
H        0.223251    5.089365   -1.466513
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H	1.443951	5.196674	-0.175942
H	-0.853501	1.795794	-3.080855
H	-0.815824	3.539012	-2.756542
H	-0.043317	2.893969	-4.218443
H	3.564716	-3.443426	1.511814
H	5.066043	-4.796600	0.078545
H	5.516814	-4.103523	-2.275358
H	4.460697	-2.021415	-3.167918
H	2.964418	-0.685730	-1.740057
H	2.854816	-0.027378	1.910315
H	1.579259	-2.003140	2.160948
H	1.442919	0.487616	-3.163033
H	2.133479	1.776205	-4.175985
H	2.929958	1.310008	-2.659662
H	1.276596	-0.249080	-0.990224

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	141.514650038264961	3850.8096	88801.79	371546.66
Delta V^Pauli Coulomb:	-69.464170555034642	-1890.2163	-43589.43	-182378.15
Delta V^Pauli LDA-XC:	-18.898391673567804	-514.2514	-11858.92	-49617.72
Delta V^Pauli GGA-Exchange:	0.974453917322450	26.5162	611.48	2558.43
Delta V^Pauli GGA-Correlation:	-0.248864980352062	-6.7720	-156.17	-653.39
Total Pauli Repulsion:	53.877676746632908	1466.0862	33808.76	141455.82
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	53.877676746632908	1466.0862	33808.76	141455.82
Electrostatic Interaction:	-11.096660277789931	-301.9555	-6963.26	-29134.28
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	42.781016468842978	1164.1307	26845.50	112321.54
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-57.819452014641740	-1573.3473	-36282.26	-151804.95
Total Orbital Interactions:	-57.826810497009063	-1573.5476	-36286.88	-151824.27
Alternative Decomposition Orb.Int.				
Kinetic:	-126.386700615639839	-3439.1571	-79308.86	-331828.24
Coulomb:	64.050147217438862	1742.8932	40192.08	168163.64
XC:	4.509742901191942	122.7163	2829.91	11840.33
Total Orbital Interactions:	-57.826810497009035	-1573.5476	-36286.88	-151824.27
Residu (E=Steric+OrbInt+Res):	-0.000034346492759	-0.0009	-0.02	-0.09
Dispersion Energy:	-0.126996606909644	-3.4558	-79.69	-333.43
Total Bonding Energy:	-15.172824981568489	-412.8736	-9521.09	-39836.25

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.096660277789931	-301.9555	-6963.26	-29134.28
Kinetic Energy:	15.127949422625122	411.6524	9492.93	39718.43
Coulomb (Steric+OrbInt) Energy:	-5.414057684088533	-147.3240	-3397.37	-14214.61
XC Energy:	-13.663059835405477	-371.7908	-8573.70	-35872.36
Dispersion Energy:	-0.126996606909644	-3.4558	-79.69	-333.43
Total Bonding Energy:	-15.172824981568464	-412.8736	-9521.09	-39836.25

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92
AJUTIK  ZORA-PBE-D3(BJ)/all electron TZP
Ru      0.015086   -0.006227   -0.020118
H      -0.802140    1.075417   -0.895554
Si     -0.608166   -0.252233   -2.359157
H      -0.138591   -1.569263   -2.905287
H      -2.048580   -0.085437   -2.702760
Cl     -1.483708   -1.942235   -0.293332
N      -1.587909    0.425456    2.622496
N      -2.632526    1.303188    0.944924
C       1.779067    1.007222    0.862510
H       1.712998    1.946434    1.404158
C       1.968146    0.872300   -0.551675
H       2.043417    1.676997   -1.279467
C       2.070725   -0.530713   -0.845533
H       2.256228   -0.965609   -1.822645
C       1.961325   -1.244248    0.387815
H       1.961952   -2.327550    0.489455
C       1.797163   -0.315328    1.444008
H       1.737807   -0.557144    2.501023
C      -1.450798    0.646277    1.255747
C      -2.807318    0.894762    3.104453
H      -3.087726    0.783751    4.143602
C      -3.457605    1.449153    2.056035
H      -4.418791    1.941311    1.991913
C      -0.592035   -0.032860    3.559379
C       0.167051    0.939559    4.244257
C       1.087514    0.487857    5.199638
H       1.696703    1.212015    5.741878
C       1.235322   -0.871809    5.467673
H       1.957784   -1.202779    6.214900
C       0.453796   -1.806766    4.792127
H       0.566322   -2.867718    5.017854
C      -0.484078   -1.408357    3.828988
C      -1.375705   -2.422273    3.138756
H      -1.729708   -1.972866    2.202016
C      -0.630950   -3.703997    2.751311
H      -1.286812   -4.335562    2.136713
H       0.260212   -3.472335    2.153223
H      -0.325570   -4.290718    3.631473
C      -2.602972   -2.742113    4.011298
H      -3.263410   -3.448788    3.486939
H      -2.300984   -3.197355    4.967944
H      -3.186683   -1.837342    4.234801
C      -0.014308    2.432458    4.000310
H      -0.493354    2.551489    3.019010
C      -0.945989    3.057597    5.056758
H      -1.934401    2.580850    5.064079
H      -0.510271    2.955098    6.062642
H      -1.090136    4.129323    4.852363
C       1.312896    3.204799    3.971537
H       2.050396    2.736453    3.307429
H       1.137494    4.233840    3.625273
H       1.760469    3.272437    4.974075
C      -2.970140    1.974494   -0.286819
C      -2.377823    3.232464   -0.535655
C      -2.806869    3.933741   -1.667864
H      -2.365481    4.904121   -1.896752
C      -3.788527    3.408769   -2.509671
H      -4.107903    3.971611   -3.387716
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C	-4.357360	2.169038	-2.234515
H	-5.121530	1.767604	-2.901149
C	-3.965012	1.421212	-1.113464
C	-4.640401	0.095388	-0.788188
H	-3.994517	-0.437938	-0.076667
C	-4.806401	-0.814704	-2.012528
H	-5.238048	-1.775315	-1.696827
H	-5.485915	-0.375800	-2.758990
H	-3.839562	-1.015958	-2.488617
C	-6.013740	0.334852	-0.131194
H	-6.479434	-0.626513	0.132545
H	-5.940851	0.936396	0.784998
H	-6.688034	0.861269	-0.824790
C	-1.337143	3.822605	0.407167
H	-0.830034	2.974700	0.887116
C	-2.006332	4.674513	1.501874
H	-1.248817	5.063133	2.200449
H	-2.531765	5.533784	1.056783
H	-2.735056	4.091741	2.082523
C	-0.251419	4.629742	-0.313120
H	0.524248	4.928045	0.407786
H	0.226001	4.039587	-1.106607
H	-0.652053	5.553636	-0.757099
C	0.353472	1.010860	-3.408901
C	1.521289	0.648497	-4.102249
H	1.824116	-0.401792	-4.130064
C	2.311875	1.604050	-4.751913
H	3.220543	1.298469	-5.274930
C	1.940545	2.952593	-4.727451
H	2.558482	3.702926	-5.225240
C	0.767558	3.332037	-4.063891
H	0.463329	4.381993	-4.046758
C	-0.011009	2.369555	-3.416737
H	-0.916835	2.681443	-2.892082

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	201.343181245071008	5478.8267	126344.77	528626.45
Delta V^Pauli Coulomb:	-96.546096631530787	-2627.1530	-60583.60	-253481.74
Delta V^Pauli LDA-XC:	-26.833001582451612	-730.1631	-16837.96	-70450.04
Delta V^Pauli GGA-Exchange:	1.287335943531467	35.0302	807.82	3379.90
Delta V^Pauli GGA-Correlation:	-0.284198522953318	-7.7334	-178.34	-746.16
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	78.967220451666748	2148.8074	49552.68	207328.41
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	78.967220451666748	2148.8074	49552.68	207328.41
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-16.024506865190851	-436.0490	-10055.53	-42072.34
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	62.942713586475897	1712.7584	39497.15	165256.07
Orbital Interactions				
A:	-83.238264706130991	-2265.0284	-52232.81	-218542.03
Total Orbital Interactions:	-83.238264706130991	-2265.0284	-52232.81	-218542.03
Alternative Decomposition Orb.Int.				
Kinetic:	-182.463029401570509	-4965.0717	-114497.29	-479056.62
Coulomb:	91.851368516095945	2499.4029	57637.61	241155.73
XC:	7.373396179343586	200.6403	4626.88	19358.85
Total Orbital Interactions:	-83.238264706130977	-2265.0284	-52232.81	-218542.03
Residu (E=Steric+OrbInt+Res):	0.000027388593955	0.0007	0.02	0.07
Dispersion Energy:	-0.164984244006620	-4.4894	-103.53	-433.17
Total Bonding Energy:	-20.460507975067756	-556.7588	-12839.16	-53719.06

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-16.024506865190851	-436.0490	-10055.53	-42072.34
Kinetic Energy:	18.880151843500499	513.7551	11847.48	49569.83
Coulomb (Steric+OrbInt) Energy:	-4.694700726840892	-127.7493	-2945.97	-12325.94
XC Energy:	-18.456467982529880	-502.2260	-11581.61	-48457.45
Dispersion Energy:	-0.164984244006620	-4.4894	-103.53	-433.17
Total Bonding Energy:	-20.460507975067742	-556.7588	-12839.16	-53719.06

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92
CUTZOI  ZORA-PBE-D3(BJ)/all electron TZP
Ru      0.016525   -0.008277   -0.045354
Si     -1.249035    1.853132   -0.770873
C      -0.315833   -1.652783    1.538713
H      -0.002863   -1.557749    2.575199
C       0.419727   -2.269842    0.481999
H       1.406796   -2.715698    0.570162
C      -0.358941   -2.216788   -0.707790
H      -0.073295   -2.610561   -1.679918
C      -1.597125   -1.562214   -0.399939
H      -2.415680   -1.388971   -1.093160
C      -1.569728   -1.211656    0.989731
H      -2.371061   -0.728549    1.541175
N       2.516849    1.382657    1.054469
N       2.738366    1.021669   -1.071144
C       1.848143    0.811890   -0.022149
C       3.737171    1.934669    0.676242
H       4.383589    2.438644    1.382645
C       3.875931    1.707021   -0.653199
H       4.673836    1.964265   -1.336997
C       2.126404    1.246260    2.434422
C       1.290989    2.217017    3.014103
C       0.969126    2.067793    4.370553
H       0.318129    2.800130    4.849760
C       1.460868    0.996172    5.113658
H       1.197721    0.898449    6.167944
C       2.286605    0.047094    4.512672
H       2.665651   -0.788193    5.103374
C       2.636934    0.150923    3.159901
C       2.617106    0.460867   -2.395449
C       2.172698    1.279064   -3.451090
C       2.096597    0.704020   -4.728563
H       1.738002    1.306526   -5.562933
C       2.453674   -0.624137   -4.942847
H       2.383446   -1.053011   -5.943865
C       2.899611   -1.410427   -3.880286
H       3.176014   -2.449648   -4.060897
C       2.996022   -0.885990   -2.585826
C       0.765102    3.395102    2.210767
H       0.824896    3.119002    1.149921
C      -0.705398    3.702486    2.518158
H      -1.326122    2.803627    2.409496
H      -0.836068    4.100090    3.535799
H      -1.083164    4.456528    1.813928
C       1.642115    4.641023    2.421731
H       2.686565    4.452044    2.134891
H       1.266639    5.476130    1.811314
H       1.629465    4.953756    3.477451
C       3.563036   -0.872812    2.518434
H       3.425062   -0.800614    1.431462
C       5.037795   -0.554660    2.826006
H       5.699478   -1.277695    2.324790
H       5.314684    0.451243    2.483158
H       5.226841   -0.609136    3.909365
C       3.240267   -2.316446    2.928306
H       3.845327   -3.016756    2.333167
H       3.479076   -2.500990    3.986064
H       2.181416   -2.556899    2.771849
C       1.801489    2.737867   -3.233735
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H	1.499029	2.842914	-2.181689
C	0.621746	3.194370	-4.100674
H	0.301288	4.197744	-3.786373
H	0.901643	3.257837	-5.163463
H	-0.239220	2.520832	-4.006735
C	3.010913	3.658375	-3.483193
H	2.729449	4.706714	-3.302272
H	3.860260	3.418848	-2.830129
H	3.349374	3.571007	-4.527522
C	3.518811	-1.734621	-1.434787
H	2.996323	-1.390660	-0.531796
C	5.030807	-1.528034	-1.224995
H	5.382109	-2.124766	-0.368497
H	5.590588	-1.847966	-2.117631
H	5.274897	-0.476759	-1.024621
C	3.220443	-3.229755	-1.591595
H	3.491771	-3.761457	-0.667756
H	2.157967	-3.416178	-1.793564
H	3.809999	-3.678929	-2.404567
C	-2.274080	1.509189	-2.348791
C	-1.894658	0.543011	-3.299034
H	-0.974358	-0.024640	-3.141483
C	-2.671777	0.286329	-4.432304
H	-2.350481	-0.470986	-5.151479
C	-3.861776	0.991740	-4.639540
H	-4.477067	0.787695	-5.518743
C	-4.263154	1.953090	-3.705112
H	-5.196071	2.501373	-3.853201
C	-3.476842	2.202503	-2.575622
H	-3.808921	2.946766	-1.847307
H	-0.467289	3.121457	-1.025844
H	-2.331912	2.331297	0.173023
H	-0.182336	1.171501	1.018018
H	0.214143	0.477686	-1.565511

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	200.568875933069052	5457.7568	125858.88	526593.51
Delta V^Pauli Coulomb:	-95.869255950234731	-2608.7352	-60158.87	-251704.70
Delta V^Pauli LDA-XC:	-26.715023860419912	-726.9528	-16763.93	-70140.29
Delta V^Pauli GGA-Exchange:	1.264999280119977	34.4224	793.80	3321.26
Delta V^Pauli GGA-Correlation:	-0.276006215512004	-7.5105	-173.20	-724.65
Total Pauli Repulsion:	78.973589187022384	2148.9807	49556.68	207345.13
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	78.973589187022384	2148.9807	49556.68	207345.13
Electrostatic Interaction:	-16.013462660932827	-435.7485	-10048.60	-42043.34
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	62.960126526089553	1713.2322	39508.08	165301.79
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-83.265218250942127	-2265.7619	-52249.72	-218612.80
Total Orbital Interactions:	-83.284521408882668	-2266.2871	-52261.83	-218663.48
Alternative Decomposition Orb.Int.				
Kinetic:	-181.673398142870923	-4943.5847	-114001.79	-476983.44
Coulomb:	91.104995633167704	2479.0931	57169.25	239196.13
XC:	7.283881100820556	198.2045	4570.70	19123.83
Total Orbital Interactions:	-83.284521408882668	-2266.2871	-52261.83	-218663.48
Residu (E=Steric+OrbInt+Res):	-0.000034067377293	-0.0009	-0.02	-0.09
Dispersion Energy:	-0.158051800566116	-4.3008	-99.18	-414.96
Total Bonding Energy:	-20.482480750736524	-557.3567	-12852.95	-53776.75

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-16.013462660932827	-435.7485	-10048.60	-42043.34
Kinetic Energy:	18.895477790198129	514.1721	11857.09	49610.07
Coulomb (Steric+OrbInt) Energy:	-4.764294384444327	-129.6430	-2989.64	-12508.65
XC Energy:	-18.442149694991386	-501.8364	-11572.62	-48419.86
Dispersion Energy:	-0.158051800566116	-4.3008	-99.18	-414.96
Total Bonding Energy:	-20.482480750736528	-557.3567	-12852.95	-53776.75

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69
DVGGIN  ZORA-PBE-D3(BJ)/all electron TZP
Ru      8.950904    3.508264    8.916284
C      12.509185    2.590410    9.386491
C       7.187671    0.889907    8.740828
P       8.018102    4.100707   11.032222
C       8.164247    5.452620    7.954718
H       7.388901    6.078225    8.386482
C       7.938624    4.409568    7.024862
H       6.969213    4.090320    6.648180
C       9.203330    3.836841    6.674274
H       9.373420    3.029716    5.966730
C      10.215398    4.552964    7.390767
H      11.283708    4.396551    7.296036
C       9.581903    5.548044    8.201462
H      10.086124    6.300659    8.801956
N       7.860120    1.831437    8.890000
H      12.523266    2.809092   10.465075
Si     10.847202    1.838744    8.880762
C       5.453252    4.510816   12.306651
H       5.745216   -0.199127    7.664491
C       6.326445   -0.269008    8.594391
H       5.626844   -0.333406    9.440181
H       5.918740    5.188819   13.031710
H       5.309586    2.600405   10.267839
H       6.182590    5.529425   10.557955
H      12.732161    3.530070    8.862371
H      12.656484    2.532666    6.568693
H       6.921935   -1.192394    8.562842
H       5.411784    3.507306   12.754172
H      10.239968    2.120567   11.958375
C       6.170069    4.497563   10.948357
H      13.321832    1.880046    9.172335
H       9.599400   -0.221973    9.653327
C      10.555970    0.262456    9.891812
H      11.356365   -0.446197    9.626861
H      10.592097    0.418149   10.977954
C       5.397298    3.644275    9.934991
H       4.414523    4.845307   12.163648
H       5.875444    3.649301    8.949371
H       4.377169    4.042248    9.830019
C      10.986407    1.248373    7.090219
C      10.121119    0.255709    6.590589
C      10.208101   -0.185060    5.268676
C      11.170344    0.360994    4.411586
C      12.044617    1.341981    4.887414
C      11.951644    1.777728    6.213119
H       9.370900   -0.190116    7.247485
H       9.533486   -0.963250    4.905767
H      11.244114    0.013838    3.379641
H      12.805748    1.761162    4.227632
C       8.243953    2.863457   12.421136
H       7.747358    3.348196   13.277828
C       7.561969    1.513976   12.169348
H       6.496331    1.618887   11.925378
H       7.636670    0.896182   13.076823
H       8.056749    0.972679   11.354432
C       9.725948    2.660940   12.761652
H      10.267568    3.599494   12.930094
H       9.812909    2.055515   13.676080
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H	7.653882	6.020084	13.605431
C	8.799733	5.670667	11.763959
H	9.862173	5.535067	11.502073
C	8.301891	6.961280	11.097078
H	8.338119	6.933684	10.005100
H	8.929902	7.801823	11.426727
H	7.271248	7.194329	11.402479
C	8.690322	5.842571	13.289218
H	9.083597	4.996545	13.863413
H	9.269052	6.731738	13.581362
H	10.033281	3.141902	10.073237

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	133.464251272293978	3631.7471	83750.09	350410.34
Delta V^Pauli Coulomb:	-64.033126032535236	-1742.4300	-40181.40	-168118.95
Delta V^Pauli LDA-XC:	-17.969700569552295	-488.9804	-11276.16	-47179.44
Delta V^Pauli GGA-Exchange:	0.893253657933194	24.3067	560.53	2345.24
Delta V^Pauli GGA-Correlation:	-0.216162154820280	-5.8821	-135.64	-567.53
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	52.138516173319360	1418.7612	32717.42	136889.65
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	52.138516173319360	1418.7612	32717.42	136889.65
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-10.500293057259283	-285.7275	-6589.03	-27568.52
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	41.638223116060075	1133.0337	26128.38	109321.14
Orbital Interactions				
A:	-55.887367405872197	-1520.7726	-35069.86	-146732.26
Total Orbital Interactions:	-55.896601772405731	-1521.0239	-35075.65	-146756.51
Alternative Decomposition Orb.Int.				
Kinetic:	-120.423717626453822	-3276.8961	-75567.03	-316172.43
Coulomb:	59.920626709734464	1630.5232	37600.76	157321.58
XC:	4.606489144313612	125.3489	2890.62	12094.34
Total Orbital Interactions:	-55.896601772405745	-1521.0239	-35075.65	-146756.51
Residu (E=Steric+OrbInt+Res):	-0.000007775785563	-0.0002	-0.00	-0.02
Dispersion Energy:	-0.113220588110391	-3.0809	-71.05	-297.26
Total Bonding Energy:	-14.371607020241610	-391.0713	-9018.32	-37732.65

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-10.500293057259283	-285.7275	-6589.03	-27568.52
Kinetic Energy:	13.040533645840156	354.8510	8183.06	34237.92
Coulomb (Steric+OrbInt) Energy:	-4.112507098586335	-111.9070	-2580.64	-10797.39
XC Energy:	-12.686119922125767	-345.2069	-7960.66	-33307.40
Dispersion Energy:	-0.113220588110391	-3.0809	-71.05	-297.26
Total Bonding Energy:	-14.371607020241619	-391.0713	-9018.32	-37732.65

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Cl-DVGGIN ZORA-PBE-D3(BJ)/all electron TZP
Ru      8.996026    3.611128    8.908204
C      12.495395    2.603969    9.351045
H       7.291556    7.179618   11.448011
P       8.027423    4.069805   11.010127
C       8.113932    5.508991    7.882853
H       7.320626    6.125116    8.298703
C       7.924149    4.426373    6.995821
H       6.967389    4.038509    6.654623
C       9.205780    3.871702    6.672658
H       9.391283    3.034174    6.006538
C      10.196972    4.636816    7.370375
H      11.270451    4.508136    7.285945
C       9.524037    5.645016    8.141683
H      10.001693    6.435564    8.715643
Cl      7.654467    1.563017    8.752843
H      12.532472    2.835747   10.427578
Si     10.778731    1.903336    8.895144
C       5.477007    4.488781   12.326657
C       8.704428    5.804854   13.308015
H       9.079961    4.944432   13.873638
H       9.303719    6.680136   13.605330
H       5.964383    5.140462   13.062627
H       5.312126    2.610597   10.231941
H       6.200893    5.528474   10.590151
H      12.741358    3.531343    8.812692
H      12.722414    2.437916    6.640873
H      10.150959    3.475346   10.028357
H       5.422213    3.475914   12.751510
H      10.226544    2.122696   11.883004
C       6.179423    4.489068   10.960592
H      13.281231    1.863028    9.135625
H       9.581707   -0.108362    9.821268
C      10.583468    0.323955    9.935967
H      11.321571   -0.402649    9.560926
H      10.778318    0.474466   11.006190
C       5.382505    3.666704    9.941614
H       4.441907    4.844831   12.202156
H       5.847738    3.687382    8.950663
H       4.361403    4.074428    9.869017
C      10.963304    1.260391    7.112503
C      10.065368    0.306517    6.591964
C      10.194652   -0.173293    5.286393
C      11.228023    0.290963    4.463829
C      12.130681    1.236121    4.960249
C      11.997139    1.709304    6.270119
H       9.240270   -0.042392    7.214634
H       9.486969   -0.914537    4.907923
H      11.331114   -0.085485    3.444072
H      12.944208    1.600126    4.329160
C       8.239708    2.831507   12.406208
H       7.762307    3.322709   13.271051
C       7.538427    1.490646   12.161010
H       6.457819    1.607724   12.005185
H       7.684921    0.841054   13.039182
H       7.942107    0.988945   11.274224
C       9.725044    2.615942   12.722154
H      10.265380    3.548557   12.931468
H       9.823919    1.963679   13.603875
H       7.672756    6.000772   13.630976
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C	8.800522	5.633678	11.782748
H	9.861276	5.498197	11.514733
C	8.310424	6.927254	11.118042
H	8.311843	6.872167	10.026413
H	8.961678	7.764423	11.412997

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	120.965114655654787	3291.6282	75906.76	317593.86
Delta V^Pauli Coulomb:	-58.397264651517276	-1589.0704	-36644.84	-153322.00
Delta V^Pauli LDA-XC:	-16.389900232354304	-445.9919	-10284.82	-43031.68
Delta V^Pauli GGA-Exchange:	0.840660623162844	22.8755	527.52	2207.15
Delta V^Pauli GGA-Correlation:	-0.212634399574988	-5.7861	-133.43	-558.27
Total Pauli Repulsion:	46.805975995371057	1273.6554	29371.20	122889.07
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	46.805975995371057	1273.6554	29371.20	122889.07
Electrostatic Interaction:	-9.555593670040899	-260.0209	-5996.23	-25088.21
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	37.250382325330158	1013.6345	23374.97	97800.86
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-50.440759222274210	-1372.5629	-31652.06	-132432.19
Total Orbital Interactions:	-50.448525550146826	-1372.7742	-31656.93	-132452.59
Alternative Decomposition Orb.Int.				
Kinetic:	-108.851129851445975	-2961.9900	-68305.12	-285788.60
Coulomb:	54.489573639253507	1482.7367	34192.73	143062.36
XC:	3.913030662045649	106.4790	2455.46	10273.66
Total Orbital Interactions:	-50.448525550146819	-1372.7742	-31656.93	-132452.59
Residu (E=Steric+OrbInt+Res):	-0.000010393084005	-0.0003	-0.01	-0.03
Dispersion Energy:	-0.107641847641385	-2.9291	-67.55	-282.61
Total Bonding Energy:	-13.305795465542060	-362.0691	-8349.51	-34934.36

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-9.555593670040899	-260.0209	-5996.23	-25088.21
Kinetic Energy:	12.113984804208812	329.6383	7601.64	31805.26
Coulomb (Steric+OrbInt) Energy:	-3.907701405347773	-106.3340	-2452.12	-10259.67
XC Energy:	-11.848843346720798	-322.4234	-7435.26	-31109.13
Dispersion Energy:	-0.107641847641385	-2.9291	-67.55	-282.61
Total Bonding Energy:	-13.305795465542044	-362.0691	-8349.51	-34934.36

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69
DVGGIN ZORA-PBE0-dDsC/all electron TZP
Ru      8.862915    3.431624    8.870828
C      12.383353    2.476708    9.599173
C       7.114806    0.791414    8.865458
P       8.038114    4.090463   10.968845
C       8.084069    5.317677    7.916520
H       7.315344    5.943706    8.340472
C       7.859586    4.263667    7.014885
H       6.895787    3.934097    6.657738
C       9.116048    3.697363    6.665937
H       9.282569    2.881702    5.982588
C      10.121292    4.428869    7.353855
H      11.183556    4.264804    7.268004
C       9.493966    5.419906    8.149297
H       9.995718    6.172737    8.734301
N       7.762109    1.737460    8.925836
H      12.340117    2.567139   10.687026
Si     10.784647    1.779039    8.930533
C       5.602440    4.660570   12.326516
H       5.907582   -0.571034    7.841995
C       6.316356   -0.410832    8.840853
H       5.491342   -0.324556    9.551000
H       6.129307    5.364485   12.967336
H       5.316959    2.617618   10.456107
H       6.245941    5.517151   10.484403
H      12.602279    3.468347    9.197640
H      12.817810    2.512387    6.874464
H       6.933200   -1.269542    9.115306
H       5.555159    3.701107   12.843241
H      10.145266    1.977676   11.911736
C       6.236054    4.526981   10.949389
H      13.217236    1.814380    9.353929
H       9.574147   -0.363544    9.324158
C      10.384127    0.178712    9.811605
H      11.275888   -0.451593    9.756448
H      10.128513    0.299529   10.862976
C       5.401545    3.626818   10.051649
H       4.577629    5.021568   12.217764
H       5.819082    3.556650    9.047890
H       4.392236    4.035451    9.978118
C      11.034780    1.333167    7.128926
C      10.143602    0.483716    6.469661
C      10.286273    0.199979    5.122241
C      11.330526    0.762161    4.400309
C      12.236046    1.593137    5.039038
C      12.087690    1.871457    6.390799
H       9.316222    0.040948    7.014081
H       9.587322   -0.465612    4.629112
H      11.442920    0.542128    3.344963
H      13.064418    2.021066    4.485983
C       8.258585    2.922660   12.376565
H       7.833268    3.462511   13.226215
C       7.504171    1.614895   12.214162
H       6.443691    1.764626   12.016166
H       7.588021    1.035958   13.135246
H       7.931270    1.022828   11.406360
C       9.728413    2.649286   12.658969
H      10.343229    3.547915   12.675014
H       9.828596    2.161498   13.630432
H       7.909668    6.025680   13.526364
C       8.883273    5.627962   11.616306
H       9.913134    5.486337   11.274312
C       8.342317    6.907689   10.992374
H       8.279252    6.876860    9.909118
H       8.996626    7.739260   11.258396
H       7.353055    7.144333   11.386569
C       8.902751    5.816572   13.130868
H       9.317437    4.975658   13.679731
H       9.520822    6.687365   13.357846
H       9.950244    2.991634    9.991938
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	hartree	eV	kcal/mol	kJ/mol
pauli hf:	4.424013898706662	120.3835	2776.11	11615.25
elstat hf:	-7.279299519454710	-198.0798	-4567.83	-19111.80
Pauli Repulsion				
Kinetic (Delta T^0):	136.382272254716383	3711.1505	85581.18	358071.61
Delta V^Pauli Coulomb:	-64.747739463152442	-1761.8756	-40629.82	-169995.17
Delta V^Pauli Hybrid-X:	-12.297627840802534	-334.6355	-7716.88	-32287.42
Delta V^Pauli Hybrid-C:	-1.408972309450016	-38.3401	-884.14	-3699.26
Delta V^Pauli HF-Exchange:	-2.855285620748049	-77.6963	-1791.72	-7496.55
Total Pauli Repulsion:	55.072647020563345	1498.6030	34558.61	144593.21
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.072647020563345	1498.6030	34558.61	144593.21
Electrostatic Interaction:	-11.042652886242138	-300.4859	-6929.37	-28992.48
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	44.029994134321207	1198.1171	27629.24	115600.73
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-61.281163212240962	-1667.5453	-38454.51	-160893.67

Total Orbital Interactions:	-61.280816784752851	-1667.5359	-38454.30	-160892.76
Alternative Decomposition Orb.Int.				
Kinetic:	-119.597776296207456	-3254.4211	-75048.75	-314003.92
Coulomb:	58.490565973275004	1591.6093	36703.39	153566.96
XC+HF:	-0.173606461820387	-4.7241	-108.94	-455.80
XC only:	2.892448497177239	78.7075	1815.04	7594.12
HF Orbital:	-3.066054958997626	-83.4316	-1923.98	-8049.93
Total Orbital Interactions:	-61.280816784752837	-1667.5359	-38454.30	-160892.76
Residu (E=Steric+OrbInt+Res):	-0.000000996468374	-0.0000	-0.00	-0.00
Dispersion Energy:	-0.083844000739231	-2.2815	-52.61	-220.13
Total Bonding Energy:	-17.334667647639247	-471.7003	-10877.67	-45512.16

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Cl-DVGGIN ZORA-PBE0-dDsC/all electron TZP
Ru      8.979031    3.551930    8.898092
C      12.543732    2.795419    9.302184
H       7.435686    7.090834   11.546347
P       8.015497    4.051227   10.963904
C       8.092346    5.392202    7.933302
H       7.325052    6.001221    8.384632
C       7.857633    4.298431    7.082377
H       6.893818    3.899813    6.807624
C       9.115928    3.761233    6.693482
H       9.272639    2.909848    6.053191
C      10.127412    4.546485    7.309658
H      11.189104    4.411895    7.180502
C       9.503403    5.551505    8.097659
H      10.003036    6.343443    8.631156
Cl      7.768837    1.477374    8.882973
H      12.611755    2.987862   10.376440
Si     10.895714    1.968952    8.914267
C       5.578282    4.880944   12.187197
C       8.916835    5.594682   13.267236
H       9.377470    4.728894   13.739310
H       9.495133    6.473863   13.561901
H       6.103270    5.629056   12.779567
H       5.226116    2.744803   10.426774
H       6.345880    5.576097   10.331027
H      12.679201    3.751374    8.792152
H      12.664916    2.617778    6.588208
H      10.106459    3.204901   10.017827
H       5.494441    3.973233   12.785326
H       9.703966    1.615935   11.820884
C       6.252352    4.617355   10.848200
H      13.373864    2.138092    9.029802
H       9.801671    0.073356   10.128272
C      10.821017    0.432203    9.988256
H      11.391193   -0.350795    9.481927
H      11.288509    0.601956   10.959843
C       5.400369    3.716074    9.967205
H       4.564607    5.251030   12.013895
H       5.874464    3.524477    9.006113
H       4.430809    4.192228    9.802185
C      11.013631    1.350816    7.137334
C      10.147052    0.362053    6.664153
C      10.214697   -0.078766    5.352908
C      11.149465    0.460093    4.479798
C      12.025226    1.433900    4.932466
C      11.957240    1.867485    6.249802
H       9.394367   -0.049038    7.326633
H       9.532423   -0.847807    5.008385
H      11.199076    0.115361    3.452775
H      12.767412    1.852602    4.261300
C       8.029121    2.839144   12.357728
H       7.718892    3.438068   13.217518
C       7.070488    1.666411   12.229470
H       6.029257    1.982368   12.197865
H       7.189878    1.022818   13.104663
H       7.277464    1.085773   11.332664
C       9.442472    2.335015   12.592649
H      10.191603    3.128503   12.583241
H       9.499777    1.832198   13.560711
H       7.916742    5.715164   13.684389
C       8.903489    5.506567   11.745873
H       9.930877    5.348226   11.406247
C       8.426419    6.831899   11.169627
H       8.386887    6.826638   10.083048
H       9.106939    7.629967   11.472580
```

	hartree	eV	kcal/mol	kJ/mol
pauli hf:	4.424013898706662	120.3835	2776.11	11615.25
elstat hf:	-7.279299519454710	-198.0798	-4567.83	-19111.80
Pauli Repulsion				
Kinetic (Delta T^0):	136.382272254716383	3711.1505	85581.18	358071.61
Delta V^Pauli Coulomb:	-64.747739463152442	-1761.8756	-40629.82	-169995.17
Delta V^Pauli Hybrid-X:	-12.297627840802534	-334.6355	-7716.88	-32287.42
Delta V^Pauli Hybrid-C:	-1.408972309450016	-38.3401	-884.14	-3699.26
Delta V^Pauli HF-Exchange:	-2.855285620748049	-77.6963	-1791.72	-7496.55
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	55.072647020563345	1498.6030	34558.61	144593.21
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.072647020563345	1498.6030	34558.61	144593.21
Electrostatic Interaction:	-11.042652886242138	-300.4859	-6929.37	-28992.48
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	44.029994134321207	1198.1171	27629.24	115600.73
Orbital Interactions				
A:	-61.281163212240962	-1667.5453	-38454.51	-160893.67
Total Orbital Interactions:	-61.280816784752851	-1667.5359	-38454.30	-160892.76
Alternative Decomposition Orb.Int.				
Kinetic:	-119.597776296207456	-3254.4211	-75048.75	-314003.92
Coulomb:	58.490565973275004	1591.6093	36703.39	153566.96
XC+HF:	-0.173606461820387	-4.7241	-108.94	-455.80
XC only:	2.892448497177239	78.7075	1815.04	7594.12

HF Orbital:	-3.066054958997626	-83.4316	-1923.98	-8049.93
Total Orbital Interactions:	-61.280816784752837	-1667.5359	-38454.30	-160892.76
Residu (E=Steric+OrbInt+Res):	-0.000000996468374	-0.0000	-0.00	-0.00
Dispersion Energy:	-0.083844000739231	-2.2815	-52.61	-220.13
Total Bonding Energy:	-17.334667647639247	-471.7003	-10877.67	-45512.16

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.042652886242138	-300.4859	-6929.37	-28992.48
Kinetic Energy:	16.784495958508927	456.7294	10532.43	44067.69
Coulomb (Steric+OrbInt) Energy:	-6.257174486345811	-170.2664	-3926.44	-16428.21
XC Energy:	-16.735492232820985	-455.3959	-10501.68	-43939.03
Dispersion Energy:	-0.083844000739231	-2.2815	-52.61	-220.13
Total Bonding Energy:	-17.334667647639236	-471.7003	-10877.67	-45512.16