Symmetry and Magnetism in Ni_9Te_6 clusters ligated by CO and Phosphine Ligands.

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	CO			$P(Me)_3$		
Number of Ligands	Central	Ligated	Bare	Central	Ligated	Bare
8	0.92	0.4053	NA	0.86	0.44	NA
7	0	0	0	0	0	0
6	0.40	0.18	0.15	0.29	0.16	0.16
5	0	0	0	0	0	0
4	0	0	0	0.53	0.15	0.17
3	0	0	0	0	0	0
2	0.67	-0.02	0.20	0	0	0
1	0	0	0	0	0	0
0	1.05	NA	0.46	1.05	NA	0.46

Table S1. Average atomic magnetic moments on the Central Ni atom, the Ligated Ni atoms, and the bare Ni atoms in $Ni_9Te_6(CO)_x$, $Ni_9Te_6(PMe_3)_x$, x=0-8.

Ni9Te6-CO8
31
Energy = -190.48806055 eV
Ni 0. 0. 0.
Te 0. 0. 3.078473
Ni 1.432133 1.432133 1.432133
Ni 1.432133 -1.432133 1.432133
Ni -1.432133 -1.432133 1.432133
Ni -1.432133 1.432133 1.432133
Te -3.078473 0. 0.
Te 0. 3.078473 0.
Te 3.078473 0. 0.
Te 0. -3.078473 0.
Ni -1.432133 1.432133 -1.432133
Ni -1.432133 -1.432133 -1.432133
Ni 1.432133 -1.432133 -1.432133
Ni 1.432133 1.432133 -1.432133
Te 0. 0. -3.078473
C -2.473823 2.473823 -2.473823
O -3.138911 3.138911 -3.138911
C -2.473823 -2.473823 -2.473823
O -3.138911 -3.138911 -3.138911
C 2.473823 2.473823 -2.473823
O 3.138911 3.138911 -3.138911
C 2.473823 -2.473823 -2.473823
O 3.138911 -3.138911 -3.138911
C 2.473823 2.473823 2.473823
O 3.138911 3.138911 3.138911
C 2.473823 -2.473823 2.473823
O 3.138911 -3.138911 3.138911
C -2.473823 -2.473823 2.473823
O -3.138911 -3.138911 3.138911
C -2.473823 2.473823 2.473823
O -3.138911 3.138911 3.138911

Ni9Te6-CO7
29
Energy = -175.13946625 eV
Ni 0. 0. -0.003639
Ni 0. 0. 2.410447
Te 2.251022 0. 1.126553
Te -1.125511 -1.949442 1.126553
Te -1.125511 1.949442 1.126553
C 0. 0. 4.181951
O 0. 0. 5.335014
Ni 1.222326 -2.117131 -0.145941
Ni 1.222326 2.117131 -0.145941
Ni -2.444652 0. -0.145941
Ni 2.313753 0. -1.631605
Ni -1.156876 -2.003769 -1.631605

Ni -1.156876 2.003769 -1.631605
Te 1.215678 -2.105616 -2.772167
Te -2.431356 0. -2.772167
Te 1.215678 2.105616 -2.772167
C 2.071509 3.587959 0.449681
O 2.615614 4.530376 0.829242
C -2.050491 3.551554 -1.87689
O -2.616539 4.531979 -2.092234
C 4.100982 0. -1.87689
O 5.233078 0. -2.092234
C -2.050491 -3.551554 -1.87689
O -2.616539 -4.531979 -2.092234
C 2.071509 -3.587959 0.449681
O 2.615614 -4.530376 0.829242
C -4.143018 0. 0.449681
O -5.231228 0. 0.829242
Ni 0. 0. -2.451453

Ni9Te6-CO6
27
Energy = -158.86762113 eV
Ni 10.310717 9.999308 9.687327
Ni 11.342834 11.410487 11.512611
Ni 8.808358 11.211322 11.183605
Ni 8.805657 8.788481 11.181913
Ni 11.338827 8.583458 11.513418
Ni 11.422833 11.893791 8.601162
Ni 8.491517 11.41549 8.64829
Ni 8.491353 8.589378 8.644954
Ni 11.401745 8.10475 8.580172
Te 12.827203 9.988517 9.784019
Te 9.863879 13.21173 10.13614
Te 6.835767 10.001399 10.169781
Te 9.859306 6.787977 10.132663
Te 9.808023 9.999069 13.159997
Te 10.228811 10.009938 7.169518
C 12.527197 12.349271 12.492247
C 12.518653 7.637306 12.490744
C 12.429378 12.971417 7.605059
C 7.522408 12.362386 7.46228
C 7.519076 7.649344 7.455654
C 12.404835 7.024929 7.583095
O 13.27899 12.951721 13.124144
O 13.266383 7.029039 13.121858
O 13.08751 13.660317 6.955328
O 6.897439 12.971868 6.710275
O 6.892448 7.045582 6.700472
O 13.060285 6.334352 6.932526

Ni9Te6-CO5
25

Energy = -142.54351361 eV
Ni 10.377698 9.622592 9.620051
Ni 11.233653 11.31244 11.365638
Ni 8.889213 11.106521 11.092258
Ni 8.687621 8.76156 11.362916
Ni 11.329625 8.670878 11.747297
Ni 11.332695 11.721018 8.681868
Ni 8.518224 11.479654 8.688949
Ni 8.282107 8.664615 8.678408
Ni 11.791443 8.211536 8.292497
Te 12.881701 9.947267 9.977961
Te 9.882719 13.205734 10.239886
Te 6.792914 10.10983 10.236406
Te 10.057743 7.117381 9.976148
Te 9.802348 10.193057 13.236168
Te 10.102557 9.900051 7.162926
C 12.421988 7.582552 12.663811
C 12.319794 12.716981 7.574147
C 7.614404 12.381586 7.408866
C 7.291017 7.675398 7.568233
C 12.770894 7.239184 7.176294
O 13.129646 6.880495 13.243356
O 12.955245 13.356036 6.854579
O 7.014295 12.979697 6.626808
O 6.655765 7.038072 6.846981
O 13.3915 6.625 6.423333

Ni9Te6-CO4
23
Energy = -126.6328729
Ni 10.413586 10.411459 10.412699
Ni 11.78925 11.785544 11.787247
Ni 8.276436 11.34807 11.347189
Ni 8.682374 8.684478 11.210135
Ni 11.346375 8.273018 11.34756
Ni 11.349565 11.344409 8.274817
Ni 8.68525 11.21012 8.683248
Ni 8.858982 8.859836 8.860009
Ni 11.209007 8.681213 8.684092
Te 12.883223 10.04863 10.053294
Te 10.056299 12.881635 10.05159
Te 6.779972 9.84183 9.83906
Te 9.836406 6.779165 9.840271
Te 10.052598 10.052453 12.882694
Te 9.840125 9.837608 6.77995
C 12.815201 12.808385 12.809425
C 7.330691 12.42102 12.417129
C 12.41602 7.324531 12.418375
C 12.423781 12.410932 7.326657
O 13.48328 13.473773 13.473711

O 6.72842 13.118653 13.111044
O 13.109861 6.720214 13.114253
O 13.121424 13.102873 6.722165

Ni9Te6-CO3
21
Energy = -109.9821801
Ni 9.61371 10.428046 9.614499
Ni 11.336366 11.199414 11.337365
Ni 8.64684 11.343844 11.73897
Ni 8.791778 8.642857 11.350367
Ni 11.153758 8.844251 11.155592
Ni 11.738997 11.34233 8.647947
Ni 8.204092 11.729998 8.20437
Ni 8.812581 8.312807 8.81363
Ni 11.349275 8.641985 8.793729
Te 13.221568 9.839313 10.149323
Te 9.944463 12.879401 9.944119
Te 7.126426 10.008849 9.953962
Te 10.218276 6.720494 10.220538
Te 10.14688 9.840669 13.222551
Te 9.953927 10.008047 7.127472
C 7.548156 12.404528 12.666221
C 12.66799 12.402226 7.550025
C 7.159828 12.706887 7.157948
O 6.83079 13.094244 13.250446
O 13.253917 13.091536 6.833635
O 6.47436 13.330025 6.470329

Ni9Te6-CO2
19
Energy = -93.2123578
Ni 9.999993 10.361558 10.361254
Ni 11.818728 11.370139 11.606174
Ni 8.181988 11.606454 11.371221
Ni 8.724162 8.499757 11.229445
Ni 11.360501 8.616088 11.182965
Ni 11.275347 11.230129 8.499347
Ni 8.638957 11.184787 8.616835
Ni 8.781782 8.727614 8.772059
Ni 11.216823 8.772569 8.725881
Te 13.158486 10.026815 9.82604
Te 10.10249 12.917986 10.05083
Te 6.840962 9.827716 10.027469
Te 10.074405 6.778369 9.848905
Te 9.898362 10.049874 12.917605
Te 9.923616 9.851156 6.777858
C 12.813247 12.453643 12.600855
C 7.189735 12.601522 12.456413

O 13.464665 13.160082 13.240468
O 6.540404 13.241547 13.164328

Ni9Te6-CO
17
Energy = -76.7195425
Ni 9.538125 10.46017 10.460774
Ni 11.639802 11.23499 11.234009
Ni 8.172009 11.82766 11.833238
Ni 8.765452 8.359006 11.234444
Ni 11.341691 8.659415 11.259562
Ni 11.341336 11.262595 8.656893
Ni 8.764656 11.234844 8.360898
Ni 8.737778 8.658641 8.656558
Ni 11.106484 8.894415 8.890938
Te 13.2264 9.852561 9.855116
Te 9.923375 12.932778 10.081738
Te 7.066651 10.075946 10.080778
Te 10.149453 6.775891 9.853201
Te 9.92124 10.07927 12.934783
Te 10.144869 9.855178 6.772821
C 7.142504 12.867598 12.822647
O 6.466417 13.556639 13.457314

Ni9Te6
15
Energy = -60.42788293
Ni 0.000000 0.000000 0.000000
Te 0.000000 0.000000 3.157883
Ni 1.880090 0.000000 1.329941
Ni 0.000000 -1.880090 1.329941
Ni -1.880090 0.000000 1.329941
Ni 0.000000 1.880090 1.329941
Te -2.232720 2.232720 -0.000029
Ni 0.000000 1.880054 -1.329981
Ni -1.880054 0.000000 -1.329981
Te 0.000000 0.000000 -3.157938
Ni 0.000000 -1.880054 -1.329981
Te 2.232720 -2.232720 -0.000029
Ni 1.880054 0.000000 -1.329981
Te 2.232720 2.232720 -0.000029
Te -2.232720 -2.232720 -0.000029

Ni9Te6PMe8
119
Energy = -594.56005898

Ni 8.68201 10.397085 7.92264
Ni 11.546231 10.566988 8.132695
Ni 11.579456 8.121436 9.632433
Ni 8.725536 7.943283 9.419404
Ni 8.421761 11.89313 10.369819
Ni 8.454381 9.431629 11.860791
Ni 11.287736 12.04949 10.57846
Ni 11.310566 9.600988 12.069716
Ni 9.995117 10.006145 9.99513
Te 9.71065 11.596739 12.621967
Te 13.077181 10.177417 10.223655
Te 10.288753 8.404169 7.371702
Te 6.930709 9.822467 9.774573
Te 9.961448 12.632138 8.394939
Te 10.039813 7.364325 11.606835
P 7.050392 13.582754 10.695251
P 12.443041 13.852742 11.092503
P 12.452 9.242712 13.918893
P 7.064911 8.936323 13.495655
P 13.001658 6.46896 9.31054
P 12.887491 11.085078 6.46243
P 7.479337 10.741455 6.109434
P 7.621782 6.102978 8.923523
C 5.62479 13.32616 11.843199
C 7.762864 15.138416 11.394684
C 6.162078 14.265909 9.224822
C 13.174218 13.960941 12.787341
C 13.937588 14.227559 10.070304
C 11.579393 15.485478 11.006148
C 6.021357 10.303246 14.17389
C 7.781345 8.263793 15.061866
C 5.763687 7.666921 13.16205
C 11.506312 9.102413 15.501021
C 13.483764 7.71158 14.015625
C 13.707218 10.511129 14.403791
C 12.327255 4.748337 9.253284
C 13.987747 6.486396 7.747282
C 14.355277 6.244423 10.549768
C 12.155277 11.123349 4.765096
C 13.715053 12.737995 6.498551
C 14.350746 9.996148 6.163255
C 6.000636 11.841392 6.251169
C 6.709865 9.264618 5.306337
C 8.314297 11.507828 4.648394
C 6.320614 6.205809 7.613523
C 6.65816 5.287886 10.274487
C 8.596788 4.660329 8.302076
H 4.99519 14.225552 11.910427
H 6.00656 13.072148 12.839456
H 5.02285 12.483885 11.478547
H 6.988393 15.906271 11.537495

H 8.531022 15.518435 10.710283
H 8.238337 14.91234 12.357695
H 5.529046 15.122053 9.500573
H 5.538105 13.478286 8.785504
H 6.900207 14.581303 8.476162
H 13.69557 14.917557 12.938062
H 13.88244 13.135146 12.924925
H 12.373329 13.857053 13.530661
H 14.459123 15.125157 10.43369
H 13.627249 14.384016 9.030053
H 14.618639 13.367447 10.101338
H 12.263948 16.313982 11.239979
H 10.74564 15.490137 11.718442
H 11.171664 15.619508 9.99582
H 5.384009 9.951226 14.998284
H 5.390978 10.70417 13.371159
H 6.676118 11.107669 14.532711
H 6.995262 8.029898 15.794906
H 8.468071 9.004658 15.488681
H 8.352155 7.355035 14.831928
H 5.106745 7.526687 14.032998
H 6.248267 6.714874 12.914443
H 5.166563 7.986243 12.298244
H 12.178718 8.957591 16.359214
H 10.815174 8.253805 15.432133
H 10.917363 10.017309 15.645746
H 13.984793 7.625596 14.990858
H 14.238274 7.739272 13.220041
H 12.841262 6.836532 13.853623
H 14.238777 10.221789 15.322174
H 13.201408 11.471193 14.562806
H 14.427518 10.630882 13.584226
H 13.128814 4.007033 9.120176
H 11.617354 4.669583 8.421195
H 11.789071 4.544233 10.187889
H 14.644922 5.607393 7.67568
H 14.595488 7.398941 7.719334
H 13.300134 6.503407 6.891996
H 15.021671 5.415361 10.270086
H 13.911128 6.038772 11.531125
H 14.933809 7.17455 10.62021
H 12.913765 11.360166 4.004685
H 11.360786 11.878935 4.735788
H 11.709314 10.144333 4.547416
H 14.328115 12.899533 5.599731
H 14.352473 12.799067 7.38901
H 12.94824 13.520395 6.566343
H 14.957552 10.359465 5.32087
H 14.001644 8.978739 5.948836
H 14.964994 9.966411 7.072484
H 5.459775 11.911918 5.296128

H 6.326358 12.842104 6.559661
H 5.33175 11.441926 7.024272
H 6.154016 9.544067 4.399372
H 6.02807 8.785116 6.019043
H 7.499376 8.547343 5.047667
H 7.611601 11.650251 3.814334
H 9.137469 10.859654 4.324197
H 8.734362 12.477812 4.944103
H 5.817826 5.238309 7.468991
H 6.785922 6.518886 6.67106
H 5.582043 6.964173 7.903578
H 6.175969 4.363686 9.923478
H 5.891227 5.983367 10.63608
H 7.335291 5.056398 11.106639
H 7.943954 3.810158 8.055497
H 9.31471 4.356278 9.0734
H 9.156514 4.965885 7.408799

Ni9Te6PMe7
106
Energy = -528.37073827 eV
Ni 8.432969 10.367579 8.053881
Ni 11.931539 10.728116 7.692751
Ni 11.449085 7.954915 9.805752
Ni 8.645608 7.951347 9.501141
Ni 8.373312 11.827976 10.461506
Ni 8.888437 9.583972 11.32202
Ni 11.154913 12.069262 10.848152
Ni 11.210922 9.556998 12.124524
Ni 10.417228 10.162979 9.488485
Te 9.520263 11.466334 12.802519
Te 12.892155 10.187262 10.054434
Te 10.369264 8.637026 7.464543
Te 6.797983 9.757704 10.002452
Te 10.099316 12.440641 8.421172
Te 9.837112 7.338513 11.773257
P 7.049438 13.570325 10.661223
P 12.346312 13.865869 11.258296
P 12.522286 9.216034 13.854778
P 12.912629 6.385836 9.34837
P 13.277969 11.218532 6.097435
P 7.406559 10.723462 6.146675
P 7.577129 6.131924 8.879739
C 5.677865 13.321437 11.874415
C 7.742729 15.175994 11.261663
C 6.105134 14.157244 9.183156
C 13.072749 14.090364 12.944719
C 13.847992 14.12272 10.209331
C 11.523302 15.508283 11.04451
C 11.610921 8.97023 15.443242

C 13.632585 7.737085 13.87036
C 13.728082 10.528655 14.34826
C 12.327172 4.632957 9.276412
C 13.793417 6.516666 7.727339
C 14.361944 6.194472 10.481417
C 12.556339 11.339071 4.399003
C 14.165401 12.83692 6.209832
C 14.695202 10.071853 5.789746
C 5.831099 11.691467 6.154775
C 6.867945 9.238618 5.184214
C 8.353102 11.631449 4.84236
C 6.373592 6.212853 7.477104
C 6.497901 5.432206 10.207134
C 8.540246 4.63016 8.390755
H 5.033586 14.209681 11.949801
H 6.111634 13.094726 12.856737
H 5.079922 12.455438 11.563179
H 6.955549 15.935964 11.374849
H 8.495294 15.535566 10.549229
H 8.232744 15.010757 12.229527
H 5.471886 15.023586 9.424229
H 5.47744 13.336759 8.81453
H 6.814389 14.43294 8.391602
H 13.598773 15.052427 13.030589
H 13.776163 13.273907 13.147187
H 12.268869 14.04497 13.690907
H 14.36108 15.063809 10.456273
H 13.543082 14.134483 9.15509
H 14.535008 13.278918 10.352191
H 12.224486 16.333979 11.235566
H 10.677096 15.583519 11.737655
H 11.137512 15.584943 10.019913
H 12.298872 8.801214 16.284661
H 10.939294 8.108889 15.337063
H 10.993591 9.855626 15.641443
H 14.176563 7.653578 14.822649
H 14.352367 7.817721 13.046715
H 13.026769 6.835577 13.713836
H 14.315773 10.228928 15.228425
H 13.178284 11.450459 14.573782
H 14.406196 10.726517 13.507694
H 13.156434 3.93883 9.07576
H 11.572571 4.535529 8.486573
H 11.856767 4.373671 10.233752
H 14.529909 5.70988 7.598668
H 14.299833 7.489105 7.680038
H 13.058195 6.479007 6.913467
H 15.03677 5.398202 10.134489
H 14.005769 5.954378 11.490237
H 14.90912 7.144817 10.526076
H 13.321746 11.592725 3.650861

H 11.774093 12.108615 4.3969
H 12.094313 10.378342 4.138758
H 14.82945 12.994182 5.347121
H 14.756299 12.859026 7.134117
H 13.425891 13.646461 6.254834
H 15.315184 10.415504 4.948623
H 14.307129 9.069162 5.571388
H 15.310187 10.012976 6.696773
H 5.390702 11.754284 5.148971
H 6.029834 12.703655 6.527485
H 5.119041 11.209203 6.837119
H 6.397309 9.526942 4.232793
H 6.152996 8.660901 5.782009
H 7.741564 8.60493 4.985076
H 7.777557 11.720151 3.909259
H 9.290998 11.09578 4.647981
H 8.607012 12.63198 5.215282
H 5.861258 5.25042 7.331381
H 6.906676 6.483086 6.557321
H 5.631772 6.993129 7.690016
H 5.96995 4.528773 9.867985
H 5.768831 6.194658 10.509702
H 7.117027 5.19337 11.081159
H 7.878505 3.788577 8.138235
H 9.196585 4.342469 9.221053
H 9.166848 4.873226 7.522629

Ni9Te6PMe6
93
Energy = -461.88785646
Ni 8.715123 10.411877 7.941876
Ni 11.519498 10.570797 8.146357
Ni 11.992744 7.990306 9.631365
Ni 8.323438 7.795523 9.355071
Ni 8.676267 11.441045 10.272982
Ni 8.483439 9.453232 11.856943
Ni 11.099603 11.582633 10.452301
Ni 11.288194 9.616618 12.059771
Ni 10.044023 9.458259 9.867438
Te 9.712174 11.689288 12.574699
Te 13.192596 10.17793 10.228209
Te 10.276354 8.275847 7.629056
Te 6.803437 9.820453 9.77124
Te 9.958234 12.690156 8.475904
Te 10.052755 7.376294 11.323889
P 12.48364 9.331782 13.876663
P 7.088 8.993429 13.487709
P 13.309381 6.310279 9.287161
P 12.914344 11.08088 6.531836
P 7.534127 10.833525 6.140191
P 7.30174 5.959826 8.8541

C 5.934432 10.371468 13.908448
C 7.760301 8.571051 15.156678
C 5.897806 7.60212 13.238482
C 11.621368 9.077405 15.491242
C 13.689399 7.931036 13.909863
C 13.58345 10.754439 14.293752
C 12.528877 4.634082 9.292464
C 14.209071 6.260608 7.673998
C 14.705698 6.049881 10.468971
C 12.265044 11.325369 4.818379
C 13.834787 12.659739 6.789884
C 14.309466 9.914939 6.199206
C 6.246209 12.137162 6.363732
C 6.528817 9.459571 5.419738
C 8.393024 11.457946 4.627557
C 5.990929 6.03619 7.553857
C 6.394721 5.099422 10.214161
C 8.349724 4.577919 8.213483
H 5.240862 10.087267 14.713368
H 5.36748 10.645647 13.009817
H 6.521933 11.245431 14.217299
H 6.953845 8.406145 15.88622
H 8.40275 9.39015 15.502118
H 8.372245 7.663306 15.079126
H 5.211466 7.500014 14.091773
H 6.456966 6.66777 13.104017
H 5.321468 7.793318 12.324304
H 12.338852 8.988632 16.320067
H 11.010381 8.167767 15.438731
H 10.955075 9.929473 15.675817
H 14.268553 7.916844 14.844829
H 14.372006 8.033029 13.057131
H 13.143137 6.984923 13.803788
H 14.163166 10.561021 15.208173
H 12.966973 11.652034 14.429138
H 14.265405 10.935662 13.453372
H 13.269673 3.842076 9.108348
H 11.755325 4.601072 8.514751
H 12.045214 4.467894 10.263355
H 14.825765 5.353864 7.589795
H 14.849543 7.146772 7.588599
H 13.477931 6.283341 6.855949
H 15.306086 5.170552 10.193039
H 14.303778 5.913454 11.48049
H 15.342206 6.943844 10.470471
H 13.067576 11.605584 4.120592
H 11.501959 12.113088 4.832094
H 11.793391 10.395215 4.476671
H 14.535382 12.85886 5.965856
H 14.385471 12.597708 7.737064
H 13.114379 13.483587 6.870884

H 14.975667 10.298 5.41253
H 13.901871 8.943292 5.893357
H 14.878589 9.774209 7.126993
H 5.677646 12.30577 5.437543
H 6.736217 13.069523 6.67182
H 5.564764 11.831567 7.167689
H 5.933066 9.800815 4.560441
H 5.861543 9.064812 6.195973
H 7.201548 8.653061 5.100602
H 7.679144 11.659679 3.815559
H 9.127836 10.716091 4.291662
H 8.927038 12.382576 4.880631
H 5.543815 5.047542 7.374239
H 6.429769 6.412271 6.62144
H 5.211748 6.739263 7.87458
H 5.927128 4.170008 9.857685
H 5.622003 5.767572 10.61341
H 7.100036 4.867374 11.022181
H 7.749184 3.684658 7.986974
H 9.107452 4.32968 8.96745
H 8.867257 4.914183 7.306052

Ni9Te6PMe5
80
Energy = -395.2900713
Ni 8.384551 10.397881 7.339271
Ni 11.806544 10.532605 8.198384
Ni 11.618121 8.133913 9.697389
Ni 8.808938 7.730331 9.555072
Ni 8.493746 11.882951 10.540778
Ni 8.653509 9.48169 11.624423
Ni 11.127605 11.798247 10.485183
Ni 11.012166 9.66512 11.50999
Ni 9.666354 10.041228 9.335801
Te 9.84518 11.522478 12.753899
Te 13.167501 10.216662 10.381301
Te 10.219581 8.51978 7.413211
Te 7.118116 9.8241 9.593918
Te 9.858506 12.387938 8.322772
Te 10.111886 7.351913 11.764066
P 7.130453 13.552404 10.878452
P 12.947259 6.438797 9.194013
P 13.137052 11.172451 6.602885
P 7.241262 10.708692 5.543975
P 7.536817 6.01667 9.140509
C 5.909708 13.332576 12.244683
C 7.93088 15.147038 11.348901
C 6.032411 14.096694 9.495142
C 12.180267 4.812825 8.75812
C 14.147806 6.610212 7.797121
C 14.080733 5.92787 10.561374

C 12.432388 11.341802 4.902222
C 13.892862 12.839449 6.846545
C 14.640485 10.1582 6.253358
C 5.735163 11.769461 5.689429
C 6.546078 9.212155 4.712204
C 8.116396 11.5213 4.133589
C 6.600057 6.001407 7.547256
C 6.173416 5.76137 10.359107
C 8.29787 4.333146 9.112476
H 5.291911 14.231892 12.382858
H 6.451714 13.110694 13.172543
H 5.265056 12.475067 12.014309
H 7.184705 15.930704 11.545871
H 8.594593 15.467136 10.535903
H 8.543734 14.986359 12.244694
H 5.394518 14.942029 9.792171
H 5.402978 13.253166 9.18415
H 6.656068 14.390773 8.641211
H 12.940842 4.039868 8.57411
H 11.564686 4.938863 7.857704
H 11.525807 4.494039 9.578849
H 14.759769 5.70464 7.674188
H 14.801781 7.469703 7.9892
H 13.591899 6.801281 6.869735
H 14.721057 5.083212 10.267307
H 13.478522 5.646755 11.434863
H 14.706025 6.784061 10.844801
H 13.185076 11.70219 4.185746
H 11.589354 12.043435 4.934044
H 12.051919 10.365567 4.575476
H 14.559417 13.104969 6.013078
H 14.459443 12.839215 7.78624
H 13.093796 13.586322 6.933035
H 15.249693 10.607973 5.45585
H 14.337324 9.14737 5.954507
H 15.23906 10.080217 7.169872
H 5.228047 11.887555 4.720777
H 6.026669 12.755244 6.073223
H 5.04644 11.312625 6.411334
H 5.983243 9.481821 3.806708
H 5.883552 8.684571 5.409601
H 7.369198 8.537408 4.445744
H 7.454379 11.636998 3.263156
H 8.986939 10.915275 3.852886
H 8.474 12.507591 4.455283
H 5.958647 5.111894 7.461827
H 7.311274 6.023902 6.711988
H 5.981852 6.906509 7.493673
H 5.565682 4.880672 10.104409
H 5.538297 6.655854 10.377725
H 6.60776 5.633712 11.358578

H 7.540904 3.555512 8.933359
H 8.789866 4.148022 10.075681
H 9.059002 4.289559 8.323911

Ni9Te6PMe4
67
Energy = -328.17627815 eV
Ni 8.892065 10.250762 8.275583
Ni 11.359098 10.490459 8.301563
Ni 11.625435 7.817116 9.310317
Ni 8.664403 7.913527 9.37991
Ni 8.705203 11.533042 10.352298
Ni 8.435752 9.469814 11.917976
Ni 11.160197 11.816077 10.46522
Ni 11.338977 9.742936 12.414645
Ni 10.224298 9.596518 10.244881
Te 9.735862 11.724622 12.670877
Te 12.907106 9.877708 10.308029
Te 10.253098 8.374777 7.221818
Te 6.908293 9.822882 9.810707
Te 9.875807 12.643586 8.334496
Te 10.220447 7.458909 11.56509
P 12.596446 9.516721 14.164355
P 7.060022 9.04268 13.567629
P 13.059576 6.231173 8.951066
P 7.483424 6.16223 8.783439
C 5.777762 10.331602 13.876338
C 7.79138 8.848371 15.252387
C 6.024875 7.516601 13.456703
C 11.777828 9.248696 15.797438
C 13.81884 8.132768 14.147751
C 13.684813 10.959321 14.536529
C 12.434169 4.635534 8.264166
C 14.402443 6.642072 7.754221
C 14.034921 5.637316 10.402849
C 6.630135 6.324188 7.156042
C 6.084388 5.631246 9.866338
C 8.384571 4.565602 8.561633
H 5.131741 10.063667 14.72498
H 5.167501 10.452639 12.972359
H 6.275909 11.287967 14.079521
H 7.016142 8.665712 16.010749
H 8.344629 9.76119 15.506077
H 8.498649 8.009555 15.242406
H 5.350777 7.423691 14.320511
H 6.683219 6.63978 13.411437
H 5.432796 7.549872 12.533686
H 12.516596 9.169499 16.60823
H 11.182912 8.327634 15.757076
H 11.101083 10.08791 16.00062
H 14.417721 8.111317 15.070031

H 14.483208 8.256597 13.283088
H 13.283592 7.181461 14.035058
H 14.310282 10.773417 15.421726
H 13.059163 11.844423 14.706494
H 14.326686 11.156476 13.668762
H 13.250895 3.912462 8.1239
H 11.948542 4.828962 7.299337
H 11.687991 4.213038 8.948463
H 15.101933 5.802534 7.630786
H 14.947151 7.522736 8.117254
H 13.953973 6.893969 6.785158
H 14.747096 4.849851 10.116026
H 13.346401 5.250229 11.164655
H 14.580947 6.48561 10.834772
H 6.064888 5.415253 6.903858
H 7.379265 6.520575 6.37842
H 5.948842 7.183486 7.194005
H 5.563246 4.75761 9.44869
H 5.376117 6.463577 9.96605
H 6.468797 5.384758 10.863872
H 7.710409 3.76399 8.226314
H 8.849306 4.279265 9.513683
H 9.180294 4.708404 7.819992

Ni9Te6PMe3
54
Energy = -194.42062555
Ni 8.733168 10.459027 8.228028
Ni 11.236839 10.890342 8.240442
Ni 11.949702 7.693739 9.488889
Ni 8.425107 8.049737 9.482864
Ni 8.719765 11.518601 10.359708
Ni 8.585941 9.576056 11.705852
Ni 11.06273 11.907648 10.560265
Ni 11.211838 9.794347 12.280978
Ni 10.417418 9.454735 9.95465
Te 9.59587 11.764745 12.709705
Te 12.871994 10.093144 10.211643
Te 10.265247 8.479831 7.597017
Te 6.771705 9.990935 9.880096
Te 9.708925 12.908241 8.512016
Te 10.130849 7.477972 11.472091
P 12.335935 9.414028 14.110199
P 13.348269 6.103909 9.069021
P 7.270934 6.277906 8.962474
C 11.332167 8.883757 15.565216
C 13.634601 8.101174 14.074848
C 13.277023 10.84075 14.804076
C 12.637721 4.447613 8.669062
C 14.478569 6.377864 7.636885
C 14.543863 5.674671 10.408538

C 6.158283 6.439984 7.500462
C 6.101079 5.67617 10.256258
C 8.187156 4.727679 8.553343
H 11.962205 8.733232 16.453803
H 10.813933 7.948052 15.320182
H 10.573745 9.647573 15.777237
H 14.123078 7.991233 15.053984
H 14.38572 8.357221 13.317062
H 13.16975 7.149037 13.788856
H 13.790211 10.567676 15.737468
H 12.582804 11.668681 14.994562
H 14.014415 11.177825 14.064771
H 13.428621 3.711748 8.463627
H 11.98598 4.537532 7.791062
H 12.02925 4.102672 9.514459
H 15.161406 5.527267 7.498076
H 15.061196 7.291659 7.807537
H 13.879901 6.519392 6.728462
H 15.21955 4.864681 10.097752
H 13.987794 5.363331 11.301814
H 15.132516 6.564721 10.663491
H 5.599369 5.511062 7.316248
H 6.759173 6.688808 6.616819
H 5.455162 7.263741 7.67641
H 5.536282 4.798086 9.910511
H 5.40368 6.483531 10.512152
H 6.666606 5.415393 11.159664
H 7.498384 3.905883 8.308522
H 8.807907 4.441452 9.411679
H 8.849244 4.917407 7.699222

Ni9Te6PMe2
41
Energy = -194.42062555
Ni 8.917224 10.078337 7.878893
Ni 11.423258 10.407137 8.327065
Ni 11.226984 8.488432 9.726623
Ni 8.882877 8.067476 9.459203
Ni 7.989486 12.334277 10.399411
Ni 8.637229 9.141937 11.767422
Ni 11.531095 11.996945 10.593429
Ni 11.165249 9.556915 11.855935
Ni 9.571057 10.58085 10.113478
Te 9.599237 11.583971 12.415122
Te 13.153329 10.041669 10.23707
Te 10.465865 8.146038 7.350212
Te 7.080007 9.921277 9.780248
Te 9.889522 12.512479 8.528113
Te 10.163912 7.130895 11.563997
P 6.588884 13.956754 10.67985
P 12.642942 13.775798 11.192251

C 5.183727 13.631374 11.828639
C 7.278009 15.526529 11.362614
C 5.716535 14.553571 9.169055
C 13.537056 13.645243 12.80057
C 13.989845 14.33024 10.060798
C 11.692054 15.34065 11.428565
H 4.522833 14.506356 11.908855
H 5.579597 13.378656 12.820227
H 4.61084 12.771356 11.460138
H 6.496459 16.292441 11.470179
H 8.06408 15.898129 10.693446
H 7.727997 15.323868 12.342636
H 5.025888 15.375508 9.406503
H 5.156186 13.72209 8.723816
H 6.458207 14.897657 8.437458
H 14.086208 14.569785 13.030381
H 14.238964 12.803221 12.754988
H 12.812162 13.441511 13.59876
H 14.503252 15.219425 10.454067
H 13.56272 14.558773 9.076332
H 14.712774 13.513982 9.937702
H 12.345139 16.164432 11.75112
H 10.912162 15.173794 12.182326
H 11.203293 15.608482 10.483266

Ni9Te6PMe
28
Energy = -127.28153401 eV
Ni 8.807862 10.450585 8.044748
Ni 11.409575 10.497468 8.264121
Ni 11.419465 8.30472 9.667606
Ni 8.832295 8.103033 9.497346
Ni 8.414399 11.901886 10.37067
Ni 8.491571 9.477218 11.696428
Ni 11.174826 11.922345 10.616671
Ni 11.240635 9.647959 11.889895
Ni 9.924736 10.095526 10.016077
Te 9.670186 11.544349 12.73332
Te 13.132362 10.233526 10.167875
Te 10.211647 8.355155 7.331147
Te 6.87201 9.804583 9.651974
Te 10.071076 12.725518 8.406531
Te 10.048209 7.366965 11.707704
P 6.97745 13.561239 10.707166
C 5.657196 13.231999 11.949369
C 7.684732 15.153182 11.306671
C 6.001913 14.098897 9.239479
H 4.988596 14.09714 12.062488
H 6.121823 12.998508 12.915667
H 5.074457 12.358607 11.630075

H 6.901805 15.914012 11.435851
H 8.42947 15.51272 10.585477
H 8.190263 14.9828 12.265614
H 5.304172 14.907899 9.498216
H 5.439852 13.241603 8.847887
H 6.689067 14.444664 8.45698728