Cycle no: 43 Heat of formation = 130.156 rmsG = 0.0003 rmsD = 0.0108

Cycle no: 44 Heat of formation = 130.146 rmsG = 0.0002 rmsD = 0.0035

Cycle no: 45 Heat of formation = 130.138 rmsG = 0.0001 rmsD = 0.0111

Cycle no: 46 Heat of formation = 130.129 rmsG = 0.0003 rmsD = 0.0084

Cycle no: 47 Heat of formation = 130.121 rmsG = 0.0003 rmsD = 0.0024

Cycle no: 48 Heat of formation = 130.112 rmsG = 0.0002 rmsD = 0.0111

Cycle no: 49 Heat of formation = 130.098 rmsG = 0.0002 rmsD = 0.0104

Cycle no: 50 Heat of formation = 130.085 rmsG = 0.0003 rmsD = 0.0067

Cycle no: 51 Heat of formation = 130.072 rmsG = 0.0003 rmsD = 0.0058

Cycle no: 52 Heat of formation = 130.060 rmsG = 0.0003 rmsD = 0.0112

Cycle no: 53 Heat of formation = 130.059 rmsG = 0.0006 rmsD = 0.0121

Cycle no: 54 Heat of formation = 130.056 rmsG = 0.0008 rmsD = 0.0109

Cycle no: 55 Heat of formation = 130.019 rmsG = 0.0002 rmsD = 0.0058

Cycle no: 56 Heat of formation = 130.005 rmsG = 0.0003 rmsD = 0.0072

Cycle no: 57 Heat of formation = 129.985 rmsG = 0.0003 rmsD = 0.0105

Cycle no: 58 Heat of formation = 129.970 rmsG = 0.0006 rmsD = 0.0045

Cycle no: 59 Heat of formation = 129.936 rmsG = 0.0003 rmsD = 0.0106

Cycle no: 60 Heat of formation = 129.903 rmsG = 0.0003 rmsD = 0.0121

Cycle no: 61 Heat of formation = 129.876 rmsG = 0.0004 rmsD = 0.0121

Cycle no: 62 Heat of formation = 129.844 rmsG = 0.0004 rmsD = 0.0121

Cycle no: 63 Heat of formation = 129.815 rmsG = 0.0005 rmsD = 0.0120

Cycle no: 64 Heat of formation = 129.782 rmsG = 0.0005 rmsD = 0.0065

Cycle no: 65 Heat of formation = 129.854 rmsG = 0.0010 rmsD = 0.0084

Cycle no: 66 Heat of formation = 129.739 rmsG = 0.0004 rmsD = 0.0072

Cycle no: 67 Heat of formation = 129.721 rmsG = 0.0004 rmsD = 0.0079

Cycle no: 68 Heat of formation = 129.697 rmsG = 0.0003 rmsD = 0.0072

Cycle no: 69 Heat of formation = 129.673 rmsG = 0.0004 rmsD = 0.0121

Cycle no: 70 Heat of formation = 129.658 rmsG = 0.0004 rmsD = 0.0061

Cycle no: 71 Heat of formation = 129.646 rmsG = 0.0004 rmsD = 0.0076

Cycle no: 72 Heat of formation = 129.628 rmsG = 0.0003 rmsD = 0.0032

Cycle no: 73 Heat of formation = 129.619 rmsG = 0.0002 rmsD = 0.0027

Cycle no: 74 Heat of formation = 129.614 rmsG = 0.0002 rmsD = 0.0021

Cycle no: 75 Heat of formation = 129.611 rmsG = 0.0001 rmsD = 0.0017

Cycle no: 76 Heat of formation = 129.608 rmsG = 0.0001 rmsD = 0.0019

Cycle no: 77 Heat of formation = 129.606 rmsG = 0.0001 rmsD = 0.0017

Cycle no: 78 Heat of formation = 129.605 rmsG = 0.0001 rmsD = 0.0009

Cycle no: 79 Heat of formation = 129.604 rmsG = 0.0001 rmsD = 0.0019

Cycle no: 80 Heat of formation = 129.603 rmsG = 0.0001 rmsD = 0.0019

Cycle no: 81 Heat of formation = 129.601 rmsG = 0.0001 rmsD = 0.0025

Cycle no: 82 Heat of formation = 129.598 rmsG = 0.0001 rmsD = 0.0023

Cycle no: 83 Heat of formation = 129.595 rmsG = 0.0001 rmsD = 0.0043

Cycle no: 84 Heat of formation = 129.592 rmsG = 0.0001 rmsD = 0.0028

Cycle no: 85 Heat of formation = 129.589 rmsG = 0.0001 rmsD = 0.0020

Cycle no: 86 Heat of formation = 129.586 rmsG = 0.0001 rmsD = 0.0043

Cycle no: 87 Heat of formation = 129.583 rmsG = 0.0001 rmsD = 0.0012

Cycle no: 88 Heat of formation = 129.582 rmsG = 0.0001 rmsD = 0.0032

Cycle no: 89 Heat of formation = 129.580 rmsG = 0.0001 rmsD = 0.0014

Cycle no: 90 Heat of formation = 129.579 rmsG = 0.0001 rmsD = 0.0011

Cycle no: 91 Heat of formation = 129.577 rmsG = 0.0001 rmsD = 0.0026

Cycle no: 92 Heat of formation = 129.576 rmsG = 0.0001 rmsD = 0.0013

Cycle no: 93 Heat of formation = 129.575 rmsG = 0.0001 rmsD = 0.0038

Cycle no: 94 Heat of formation = 129.573 rmsG = 0.0001 rmsD = 0.0012

Cycle no: 95 Heat of formation = 129.572 rmsG = 0.0001 rmsD = 0.0019

Cycle no: 96 Heat of formation = 129.571 rmsG = 0.0001 rmsD = 0.0025

Cycle no: 97 Heat of formation = 129.570 rmsG = 0.0001 rmsD = 0.0007

Cycle no: 98 Heat of formation = 129.569 rmsG = 0.0001 rmsD = 0.0034

Cycle no: 99 Heat of formation = 129.568 rmsG = 0.0001 rmsD = 0.0008

Cycle no: 100 Heat of formation = 129.567 rmsG = 0.0001 rmsD = 0.0013

Cycle no: 101 Heat of formation = 129.567 rmsG = 0.0001 rmsD = 0.0007

Cycle no: 102 Heat of formation = 129.567 rmsG = 0.0000 rmsD = 0.0019

Cycle no: 103 Heat of formation = 129.566 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 104 Heat of formation = 129.566 rmsG = 0.0000 rmsD = 0.0011

Cycle no: 105 Heat of formation = 129.565 rmsG = 0.0000 rmsD = 0.0009

Cycle no: 106 Heat of formation = 129.565 rmsG = 0.0000 rmsD = 0.0015

Cycle no: 107 Heat of formation = 129.565 rmsG = 0.0000 rmsD = 0.0009

Cycle no: 108 Heat of formation = 129.565 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 109 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0004

Cycle no: 110 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 111 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0005

Cycle no: 112 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0005

Cycle no: 113 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 114 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0001

Cycle no: 115 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0009

Cycle no: 116 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 117 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0004

Cycle no: 118 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0001

Convergence on Energy - difference below 0.5000D-03 kcal/mol

Cycle no: 119 Heat of formation = 129.564 rmsG = 0.0000 rmsD = 0.0001

GEMEPH/GEOOPTAM1

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

C 1	-1.1216513	1.1697037	-0.3550179
Ge 2	-1.7845588	0.6058521	1.4109143
C 3	-1.7252057	2.0080657	2.7970069
C 4	1.6070551	-1.3727322	0.0425184
C 5	-3.5698268	-0.2279927	1.3672045
C 6	-0.0296798	0.4325722	-0.6535227
C 7	-1.7616798	2.1973809	-1.1392369
C 8	-0.3015915	-0.6867676	1.4794858
C 9	0.4131869	-0.5732528	0.3389415
C 10	0.7479122	0.5878223	-1.8878226
C 11	-0.0924612	-1.5828431	2.5906058
H 12	-0.7374180	2.5073539	2.7755431
H 13	-1.8891101	1.5490031	3.7914517
H 14	-2.5226058	2.7509740	2.5998120
H 15	-3.7765845	-0.7000893	2.3469982
H 16	-3.5971730	-0.9968923	0.5712820
H 17	-4.3306416	0.5489452	1.1595068
C 18	3.8834638	-2.9106110	-0.5002175
C 19	1.5069021	-2.5366296	-0.7320381
C 20	2.8569310	-0.9874557	0.5449120
C 21	3.9885961	-1.7545239	0.2721858
C 22	2.6414201	-3.2999308	-1.0012106
H 23	0.5292081	-2.8421798	-1.1331559
H 24	2.9429896	-0.0777576	1.1571375
H 25	4.9664330	-1.4451011	0.6692492
H 26	2.5554489	-4.2106401	-1.6116065
H 27	4.7774494	-3.5137923	-0.7142982
C 28	0.2364529	-3.3066338	4.7814343
C 29	0.1170433	-2.9563113	2.3930383
C 30	-0.1326529	-1.0852642	3.9042596
C 31	0.0354633	-1.9417064	4.9888122
C 32	0.2757074	-3.8106658	3.4820266
H 33	0.1647520	-3.3521306	1.3663041
H 34	-0.2903918	-0.0083994	4.0746525
H 35	0.0097321	-1.5397191	6.0122911
H 36	0.4369746	-4.8856010	3.3135891
H 37	0.3652179	-3.9814973	5.6397226
C 38	2.2187902	0.9017658	-4.2500163
C 39	1.7245158	1.5877489	-1.9851341
C 40	0.5127784	-0.2520301	-2.9851183
C 41	1.2464179	-0.0940107	-4.1594134
C 42	2.4559138	1.7409199	-3.1620242
H 43	1.9120202	2.2534909	-1.1299154
H 44	-0.2491540	-1.0422598	-2.9133951
H 45	1.0579384	-0.7582361	-5.0153535
H 46	3.2215839	2.5274502	-3.2303884
H 47	2.7971753	1.0241639	-5.1770299
C 48	-3.0750303	4.1944895	-2.6116154
C 49	-2.1539283	3.3986915	-0.5240230
C 50	-2.0372068	2.0144242	-2.5029787
C 51	-2.6926461	3.0052979	-3.2308038
C 52	-2.8007273	4.3892723	-1.2575855
H 53	-1.9402122	3.5585716	0.5449798
H 54	-1.7215314	1.0816444	-2.9964429

H 55	-2.9042770	2.8483114	-4.2987085
H 56	-3.0961855	5.3283032	-0.7670056
H 57	-3.5893560	4.9768104	-3.1879202

Heat of Formation: 129.564 kcal/mol

Mulliken and electrostatic fit charges (electrons)

atom	Mulliken	electro fit
C 1	-0.327298	-0.295088
Ge 2	1.114511	0.817896
C 3	-0.493426	-0.296690
C 4	-0.032476	0.045025
C 5	-0.485329	-0.374454
C 6	-0.010029	-0.025857
C 7	-0.020973	0.090516
C 8	-0.327553	-0.315381
C 9	-0.009704	-0.004555
C 10	-0.032543	0.090830
C 11	-0.020903	0.113082
H 12	0.086410	0.050509
H 13	0.083536	0.040245
H 14	0.083294	0.044623
H 15	0.084675	0.062446
H 16	0.087679	0.072280
H 17	0.084396	0.063416
C 18	-0.127601	-0.088610
C 19	-0.118294	-0.073652
C 20	-0.106797	-0.101656
C 21	-0.129528	-0.100505
C 22	-0.131851	-0.131897
H 23	0.131172	0.088352
H 24	0.135409	0.099935
H 25	0.130645	0.095760
H 26	0.129409	0.102869
H 27	0.129576	0.096431
C 28	-0.130937	-0.116236
C 29	-0.113630	-0.130404
C 30	-0.132544	-0.155286
C 31	-0.129634	-0.088684
C 32	-0.128331	-0.084886
H 33	0.139329	0.109692
H 34	0.130399	0.107906
H 35	0.129658	0.095891
H 36	0.131089	0.096016
H 37	0.130112	0.100765
C 38	-0.127655	-0.099092
C 39	-0.106932	-0.117787
C 40	-0.118438	-0.112894
C 41	-0.131881	-0.108206

C 42	-0.129555	-0.103015
H 43	0.135470	0.102446
H 44	0.131386	0.096710
H 45	0.129484	0.097564
H 46	0.130680	0.102291
H 47	0.129614	0.097433
C 48	-0.130757	-0.113561
C 49	-0.132864	-0.157610
C 50	-0.113482	-0.124655
C 51	-0.128461	-0.084307
C 52	-0.129699	-0.088803
H 53	0.130410	0.110363
H 54	0.139838	0.110869
H 55	0.131137	0.095490
H 56	0.129662	0.096000
H 57	0.130121	0.100122

Dipole moments from Mulliken and electrostatic fit charges and from wavefunction (debyes)

comp	Mulliken	electro fit	actual
X	-0.6932	-0.2941	-0.2615
Y	0.1352	0.0516	0.0510
Z	0.4441	0.1681	0.1649
Total	0.8343	0.3426	0.3133

Graphics requests:

surface=homo resolution=med pending
surface=lumo resolution=med pending

Graphics files written:
surface=homo resolution=med completed
surface=lumo resolution=med completed

Time for Semi Empirical Engine CPU: 000:44:57.38 Wall: 000:56:09.57
Time for Properties Engine CPU: 000:01:30.07 Wall: 000:01:48.39
Time for Graphics Engine CPU: 000:01:02.35 Wall: 000:01:19.06

Time for GeMe2Ph4semiAM1 CPU: 000:47:30.20 Wall: 000:59:17.42

GePh
MacSPARTAN semi-empirical program: Release 1.0

GEPH6/GEOOPTAM1
Geometry Optimization
AM1
Number of basis functions: 194
Number of electrons: 194
Total molecular charge: 0
Multiplicity: 1
Point group: C1
Number of independent degrees of freedom: 207
No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	-1.1647899	-0.2990153	-1.1522332
Ge 2	-1.8873003	1.2847793	-0.5522828
H 3	-4.3250176	-3.3134373	-2.7189114
C 4	1.6328164	0.1266457	1.3001331
C 5	-1.9062842	-1.7426679	-4.5381782
C 6	-0.0197929	-0.6075166	-0.4992908
C 7	-1.7795533	-1.0859050	-2.2043342
C 8	-0.4129708	1.4287892	0.7081295
C 9	0.4057468	0.3629333	0.5417212
C 10	0.7774169	-1.8113445	-0.7395392
C 11	-0.2248965	2.5085464	1.6575609
H 12	-1.5217233	-1.6729095	-5.5662445
H 13	-3.4676258	-3.1514888	-5.0576599
C 14	-1.8482030	2.6021283	-1.6856557
H 15	-0.4369474	-0.3643973	-3.7477811
H 16	-3.2548545	-2.0001057	-0.8995406
C 17	-3.3731471	1.1144386	0.3410588
C 18	3.9842645	-0.2851480	2.7665677
C 19	1.5880101	0.0206146	2.6974384
C 20	2.8682908	0.0273396	0.6454990
C 21	4.0368500	-0.1740402	1.3773432
C 22	2.7582905	-0.1890135	3.4242137
H 23	0.6227547	0.1173003	3.2177454
H 24	2.9086995	0.0987069	-0.4522709
H 25	5.0020288	-0.2479780	0.8554243
H 26	2.7130870	-0.2739622	4.5197048
H 27	4.9071543	-0.4472794	3.3417729
C 28	0.0963904	4.6255883	3.4714668
C 29	-0.8877509	2.4939341	2.8948562
C 30	0.6081773	3.5942752	1.3458103
C 31	0.7648267	4.6446211	2.2479144
C 32	-0.7285895	3.5479785	3.7919678
H 33	-1.5372502	1.6455508	3.1569931
H 34	1.1444996	3.6107098	0.3853000
H 35	1.4224665	5.4887931	1.9936374
H 36	-1.2549182	3.5267943	4.7575232

H 37	0.2217281	5.4550595	4.1819311
C 38	2.2703475	-4.1297608	-1.2259382
C 39	1.6441987	-1.8773318	-1.8391256
C 40	0.6636320	-2.9174322	0.1131233
C 41	1.4080893	-4.0701962	-0.1316512
C 42	2.3867590	-3.0321518	-2.0784044
H 43	1.7308855	-1.0151834	-2.5170455
H 44	-0.0141252	-2.8737427	0.9781606
H 45	1.3135552	-4.9343332	0.5420415
H 46	3.0640689	-3.0769257	-2.9436496
H 47	2.8562525	-5.0403287	-1.4170151
C 48	-2.9924380	-2.5699990	-4.2548005
C 49	-1.3009426	-1.0070289	-3.5216797
C 50	-2.8703652	-1.9243853	-1.9281183
C 51	-3.4709665	-2.6592872	-2.9481367
C 52	-5.8265163	0.8540824	1.6677315
C 53	-3.6668240	-0.0413870	1.0652071
C 54	-4.3187221	2.1384682	0.2873486
C 55	-5.5419538	2.0134266	0.9463352
C 56	-4.8870567	-0.1755453	1.7274930
H 57	-2.9293333	-0.8590078	1.1153650
H 58	-4.0976334	3.0560799	-0.2833080
H 59	-6.2802268	2.8268661	0.8966833
H 60	-5.1088575	-1.0906689	2.2952564
H 61	-6.7899826	0.7513839	2.1883305
C 62	-1.9691545	4.6741474	-3.5668533
C 63	-1.5782560	3.9176813	-1.3075513
C 64	-2.1732755	2.3323162	-3.0149657
C 65	-2.2357520	3.3612704	-3.9550132
C 66	-1.6376550	4.9526750	-2.2406993
H 67	-1.3033810	4.1420629	-0.2622036
H 68	-2.3762713	1.2938682	-3.3299354
H 69	-2.4949294	3.1372934	-4.9999068
H 70	-1.4228026	5.9858879	-1.9317724
H 71	-2.0184722	5.4880604	-4.3050438

Hessian calculated using X forcefield

Cycle no: 1 Heat of formation = 210.287 rmsG = 0.0084 rmsD = 0.0109

Cycle no: 2 Heat of formation = 201.209 rmsG = 0.0058 rmsD = 0.0109

Cycle no: 3 Heat of formation = 195.185 rmsG = 0.0031 rmsD = 0.0109

Cycle no: 4 Heat of formation = 192.236 rmsG = 0.0017 rmsD = 0.0109

Cycle no: 5 Heat of formation = 190.536 rmsG = 0.0009 rmsD = 0.0109

Cycle no: 6 Heat of formation = 189.764 rmsG = 0.0006 rmsD = 0.0109

Cycle no: 7 Heat of formation = 189.418 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 8 Heat of formation = 189.421 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 9 Heat of formation = 189.432 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 10 Heat of formation = 189.438 rmsG = 0.0005 rmsD = 0.0109

Cycle no: 11 Heat of formation = 189.199 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 12 Heat of formation = 189.112 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 13 Heat of formation = 189.115 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 14 Heat of formation = 189.084 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 15 Heat of formation = 189.045 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 16 Heat of formation = 189.052 rmsG = 0.0002 rmsD = 0.0101

Cycle no: 17 Heat of formation = 189.028 rmsG = 0.0001 rmsD = 0.0060

Cycle no: 18 Heat of formation = 189.018 rmsG = 0.0001 rmsD = 0.0109

Cycle no: 19 Heat of formation = 189.011 rmsG = 0.0002 rmsD = 0.0045

Cycle no: 20 Heat of formation = 189.004 rmsG = 0.0001 rmsD = 0.0060

Cycle no: 21 Heat of formation = 189.000 rmsG = 0.0001 rmsD = 0.0047

Cycle no: 22 Heat of formation = 188.995 rmsG = 0.0001 rmsD = 0.0047

Cycle no: 23 Heat of formation = 188.991 rmsG = 0.0001 rmsD = 0.0062

Cycle no: 24 Heat of formation = 188.988 rmsG = 0.0001 rmsD = 0.0040

Cycle no: 25 Heat of formation = 188.986 rmsG = 0.0001 rmsD = 0.0044

Cycle no: 26 Heat of formation = 188.985 rmsG = 0.0001 rmsD = 0.0010

Cycle no: 27 Heat of formation = 188.984 rmsG = 0.0000 rmsD = 0.0052

Cycle no: 28 Heat of formation = 188.983 rmsG = 0.0001 rmsD = 0.0018

Cycle no: 29 Heat of formation = 188.983 rmsG = 0.0000 rmsD = 0.0022

Cycle no: 30 Heat of formation = 188.982 rmsG = 0.0000 rmsD = 0.0007

Cycle no: 31 Heat of formation = 188.982 rmsG = 0.0000 rmsD = 0.0018

Cycle no: 32 Heat of formation = 188.981 rmsG = 0.0000 rmsD = 0.0009

Cycle no: 33 Heat of formation = 188.981 rmsG = 0.0000 rmsD = 0.0029

Cycle no: 34 Heat of formation = 188.980 rmsG = 0.0000 rmsD = 0.0015

Cycle no: 35 Heat of formation = 188.980 rmsG = 0.0000 rmsD = 0.0022

Cycle no: 36 Heat of formation = 188.979 rmsG = 0.0000 rmsD = 0.0031

Cycle no: 37 Heat of formation = 188.978 rmsG = 0.0000 rmsD = 0.0011

Cycle no: 38 Heat of formation = 188.977 rmsG = 0.0000 rmsD = 0.0018

Cycle no: 39 Heat of formation = 188.977 rmsG = 0.0000 rmsD = 0.0016

Cycle no: 40 Heat of formation = 188.976 rmsG = 0.0000 rmsD = 0.0021

Cycle no: 41 Heat of formation = 188.976 rmsG = 0.0000 rmsD = 0.0007

Cycle no: 42 Heat of formation = 188.975 rmsG = 0.0000 rmsD = 0.0019

Cycle no: 43 Heat of formation = 188.975 rmsG = 0.0000 rmsD = 0.0019

Cycle no: 44 Heat of formation = 188.974 rmsG = 0.0000 rmsD = 0.0025

Cycle no: 45 Heat of formation = 188.973 rmsG = 0.0000 rmsD = 0.0032

Cycle no: 46 Heat of formation = 188.972 rmsG = 0.0000 rmsD = 0.0037

Cycle no: 47 Heat of formation = 188.971 rmsG = 0.0000 rmsD = 0.0035

Cycle no: 48 Heat of formation = 188.969 rmsG = 0.0000 rmsD = 0.0041

Cycle no: 49 Heat of formation = 188.967 rmsG = 0.0000 rmsD = 0.0034

Cycle no: 50 Heat of formation = 188.965 rmsG = 0.0000 rmsD = 0.0051

Cycle no: 51 Heat of formation = 188.963 rmsG = 0.0000 rmsD = 0.0058

Cycle no: 52 Heat of formation = 188.960 rmsG = 0.0001 rmsD = 0.0079

Cycle no: 53 Heat of formation = 188.955 rmsG = 0.0001 rmsD = 0.0067

Cycle no: 54 Heat of formation = 188.951 rmsG = 0.0001 rmsD = 0.0034

Cycle no: 55 Heat of formation = 188.951 rmsG = 0.0002 rmsD = 0.0075

Cycle no: 56 Heat of formation = 188.944 rmsG = 0.0001 rmsD = 0.0032

Cycle no: 57 Heat of formation = 188.943 rmsG = 0.0001 rmsD = 0.0063

Cycle no: 58 Heat of formation = 188.937 rmsG = 0.0001 rmsD = 0.0059

Cycle no: 59 Heat of formation = 188.960 rmsG = 0.0004 rmsD = 0.0079

Cycle no: 60 Heat of formation = 188.928 rmsG = 0.0001 rmsD = 0.0102

Cycle no: 61 Heat of formation = 188.921 rmsG = 0.0002 rmsD = 0.0083

Cycle no: 62 Heat of formation = 188.912 rmsG = 0.0002 rmsD = 0.0087

Cycle no: 63 Heat of formation = 188.895 rmsG = 0.0001 rmsD = 0.0109

Cycle no: 64 Heat of formation = 188.882 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 65 Heat of formation = 188.867 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 66 Heat of formation = 188.850 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 67 Heat of formation = 188.839 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 68 Heat of formation = 188.820 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 69 Heat of formation = 188.811 rmsG = 0.0004 rmsD = 0.0036

Cycle no: 70 Heat of formation = 188.791 rmsG = 0.0002 rmsD = 0.0068

Cycle no: 71 Heat of formation = 188.776 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 72 Heat of formation = 188.757 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 73 Heat of formation = 188.751 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 74 Heat of formation = 188.729 rmsG = 0.0004 rmsD = 0.0101

Cycle no: 75 Heat of formation = 188.790 rmsG = 0.0007 rmsD = 0.0086

Cycle no: 76 Heat of formation = 188.714 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 77 Heat of formation = 188.708 rmsG = 0.0003 rmsD = 0.0106

Cycle no: 78 Heat of formation = 188.696 rmsG = 0.0004 rmsD = 0.0055

Cycle no: 79 Heat of formation = 188.689 rmsG = 0.0003 rmsD = 0.0108

Cycle no: 80 Heat of formation = 188.668 rmsG = 0.0003 rmsD = 0.0095

Cycle no: 81 Heat of formation = 188.659 rmsG = 0.0003 rmsD = 0.0071

Cycle no: 82 Heat of formation = 188.639 rmsG = 0.0002 rmsD = 0.0097

Cycle no: 83 Heat of formation = 188.626 rmsG = 0.0003 rmsD = 0.0103

Cycle no: 84 Heat of formation = 188.609 rmsG = 0.0003 rmsD = 0.0109

Cycle no: 85 Heat of formation = 188.594 rmsG = 0.0002 rmsD = 0.0042

Cycle no: 86 Heat of formation = 188.603 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 87 Heat of formation = 188.575 rmsG = 0.0002 rmsD = 0.0084

Cycle no: 88 Heat of formation = 188.570 rmsG = 0.0003 rmsD = 0.0035

Cycle no: 89 Heat of formation = 188.569 rmsG = 0.0003 rmsD = 0.0050

Cycle no: 90 Heat of formation = 188.558 rmsG = 0.0001 rmsD = 0.0052

Cycle no: 91 Heat of formation = 188.554 rmsG = 0.0002 rmsD = 0.0046

Cycle no: 92 Heat of formation = 188.550 rmsG = 0.0001 rmsD = 0.0057

Cycle no: 93 Heat of formation = 188.545 rmsG = 0.0001 rmsD = 0.0049

Cycle no: 94 Heat of formation = 188.543 rmsG = 0.0002 rmsD = 0.0082

Cycle no: 95 Heat of formation = 188.537 rmsG = 0.0001 rmsD = 0.0032

Cycle no: 96 Heat of formation = 188.536 rmsG = 0.0002 rmsD = 0.0049

Cycle no: 97 Heat of formation = 188.532 rmsG = 0.0001 rmsD = 0.0018

Cycle no: 98 Heat of formation = 188.530 rmsG = 0.0001 rmsD = 0.0050

Cycle no: 99 Heat of formation = 188.526 rmsG = 0.0001 rmsD = 0.0075

Cycle no: 100 Heat of formation = 188.519 rmsG = 0.0002 rmsD = 0.0022

Cycle no: 101 Heat of formation = 188.515 rmsG = 0.0002 rmsD = 0.0079

Cycle no: 102 Heat of formation = 188.506 rmsG = 0.0001 rmsD = 0.0060

Cycle no: 103 Heat of formation = 188.499 rmsG = 0.0002 rmsD = 0.0046

Cycle no: 104 Heat of formation = 188.493 rmsG = 0.0002 rmsD = 0.0048

Cycle no: 105 Heat of formation = 188.487 rmsG = 0.0001 rmsD = 0.0023

Cycle no: 106 Heat of formation = 188.484 rmsG = 0.0001 rmsD = 0.0059

Cycle no: 107 Heat of formation = 188.482 rmsG = 0.0002 rmsD = 0.0038

Cycle no: 108 Heat of formation = 188.479 rmsG = 0.0001 rmsD = 0.0027

Cycle no: 109 Heat of formation = 188.476 rmsG = 0.0001 rmsD = 0.0013

Cycle no: 110 Heat of formation = 188.474 rmsG = 0.0001 rmsD = 0.0041

Cycle no: 111 Heat of formation = 188.471 rmsG = 0.0001 rmsD = 0.0032

Cycle no: 112 Heat of formation = 188.469 rmsG = 0.0001 rmsD = 0.0034

Cycle no: 113 Heat of formation = 188.467 rmsG = 0.0001 rmsD = 0.0020

Cycle no: 114 Heat of formation = 188.465 rmsG = 0.0001 rmsD = 0.0011

Cycle no: 115 Heat of formation = 188.464 rmsG = 0.0001 rmsD = 0.0012

Cycle no: 116 Heat of formation = 188.463 rmsG = 0.0001 rmsD = 0.0006

Cycle no: 117 Heat of formation = 188.463 rmsG = 0.0000 rmsD = 0.0025

Cycle no: 118 Heat of formation = 188.462 rmsG = 0.0001 rmsD = 0.0013

Cycle no: 119 Heat of formation = 188.462 rmsG = 0.0000 rmsD = 0.0010

Cycle no: 120 Heat of formation = 188.462 rmsG = 0.0000 rmsD = 0.0004

Cycle no: 121 Heat of formation = 188.462 rmsG = 0.0000 rmsD = 0.0009

Cycle no: 122 Heat of formation = 188.461 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 123 Heat of formation = 188.461 rmsG = 0.0000 rmsD = 0.0003

Cycle no: 124 Heat of formation = 188.461 rmsG = 0.0000 rmsD = 0.0012

Cycle no: 125 Heat of formation = 188.460 rmsG = 0.0000 rmsD = 0.0003

Cycle no: 126 Heat of formation = 188.460 rmsG = 0.0000 rmsD = 0.0031

Cycle no: 127 Heat of formation = 188.460 rmsG = 0.0001 rmsD = 0.0012

Cycle no: 128 Heat of formation = 188.459 rmsG = 0.0001 rmsD = 0.0011

Cycle no: 129 Heat of formation = 188.458 rmsG = 0.0001 rmsD = 0.0008

Cycle no: 130 Heat of formation = 188.458 rmsG = 0.0000 rmsD = 0.0013

Cycle no: 131 Heat of formation = 188.457 rmsG = 0.0001 rmsD = 0.0017

Cycle no: 132 Heat of formation = 188.456 rmsG = 0.0001 rmsD = 0.0044

Cycle no: 133 Heat of formation = 188.454 rmsG = 0.0001 rmsD = 0.0008

Cycle no: 134 Heat of formation = 188.454 rmsG = 0.0001 rmsD = 0.0030

Cycle no: 135 Heat of formation = 188.454 rmsG = 0.0001 rmsD = 0.0010

Cycle no: 136 Heat of formation = 188.452 rmsG = 0.0001 rmsD = 0.0012

Cycle no: 137 Heat of formation = 188.451 rmsG = 0.0000 rmsD = 0.0007

Cycle no: 138 Heat of formation = 188.451 rmsG = 0.0000 rmsD = 0.0020

Cycle no: 139 Heat of formation = 188.449 rmsG = 0.0001 rmsD = 0.0035

Cycle no: 140 Heat of formation = 188.447 rmsG = 0.0001 rmsD = 0.0037

Cycle no: 141 Heat of formation = 188.445 rmsG = 0.0001 rmsD = 0.0046

Cycle no: 142 Heat of formation = 188.443 rmsG = 0.0001 rmsD = 0.0039

Cycle no: 143 Heat of formation = 188.439 rmsG = 0.0001 rmsD = 0.0057

Cycle no: 144 Heat of formation = 188.436 rmsG = 0.0001 rmsD = 0.0055

Cycle no: 145 Heat of formation = 188.432 rmsG = 0.0001 rmsD = 0.0047

Cycle no: 146 Heat of formation = 188.429 rmsG = 0.0001 rmsD = 0.0026

Cycle no: 147 Heat of formation = 188.429 rmsG = 0.0001 rmsD = 0.0049

Cycle no: 148 Heat of formation = 188.426 rmsG = 0.0001 rmsD = 0.0024

Cycle no: 149 Heat of formation = 188.425 rmsG = 0.0001 rmsD = 0.0008

Cycle no: 150 Heat of formation = 188.424 rmsG = 0.0000 rmsD = 0.0040

Cycle no: 151 Heat of formation = 188.423 rmsG = 0.0001 rmsD = 0.0009

Cycle no: 152 Heat of formation = 188.422 rmsG = 0.0000 rmsD = 0.0031

Cycle no: 153 Heat of formation = 188.421 rmsG = 0.0000 rmsD = 0.0015

Cycle no: 154 Heat of formation = 188.420 rmsG = 0.0000 rmsD = 0.0024

Cycle no: 155 Heat of formation = 188.420 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 156 Heat of formation = 188.420 rmsG = 0.0000 rmsD = 0.0027

Cycle no: 157 Heat of formation = 188.420 rmsG = 0.0001 rmsD = 0.0014

Cycle no: 158 Heat of formation = 188.419 rmsG = 0.0000 rmsD = 0.0010

Cycle no: 159 Heat of formation = 188.419 rmsG = 0.0000 rmsD = 0.0003

Cycle no: 160 Heat of formation = 188.419 rmsG = 0.0000 rmsD = 0.0005

Cycle no: 161 Heat of formation = 188.418 rmsG = 0.0000 rmsD = 0.0017

Cycle no: 162 Heat of formation = 188.418 rmsG = 0.0000 rmsD = 0.0012

Cycle no: 163 Heat of formation = 188.418 rmsG = 0.0000 rmsD = 0.0002

Cycle no: 164 Heat of formation = 188.417 rmsG = 0.0000 rmsD = 0.0015

Cycle no: 165 Heat of formation = 188.417 rmsG = 0.0000 rmsD = 0.0015

Cycle no: 166 Heat of formation = 188.417 rmsG = 0.0000 rmsD = 0.0016

Cycle no: 167 Heat of formation = 188.416 rmsG = 0.0000 rmsD = 0.0014

Cycle no: 168 Heat of formation = 188.416 rmsG = 0.0000 rmsD = 0.0016

Cycle no: 169 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0004

Cycle no: 170 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0015

Cycle no: 171 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0005

Cycle no: 172 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0004

Cycle no: 173 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0006

Cycle no: 174 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0002

Cycle no: 175 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0002

Cycle no: 176 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0002

Cycle no: 177 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0002

Cycle no: 178 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0003

Convergence on Energy - difference below 0.5000D-03 kcal/mol

Cycle no: 179 Heat of formation = 188.415 rmsG = 0.0000 rmsD = 0.0001

GEPH6/GEOOPTAM1

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	-1.1537190	-0.3660476	-1.1249845
Ge 2	-1.8617520	1.3458624	-0.4687618
H 3	-4.9259534	-2.2158813	-3.0496386
C 4	1.6876538	0.0649050	1.2833136
C 5	-1.7385422	-2.3584372	-4.2553597
C 6	-0.0039536	-0.6397416	-0.4705311
C 7	-1.8024053	-1.1337599	-2.1605356
C 8	-0.3137135	1.4352725	0.7412457
C 9	0.4476953	0.3364542	0.5483577
C 10	0.8073817	-1.8392022	-0.7019995
C 11	-0.0958549	2.5089458	1.6822566
H 12	-1.1638425	-2.7594587	-5.1031216
H 13	-3.6312040	-3.1212921	-4.9820086
C 14	-1.8959739	2.7185024	-1.8454703
H 15	0.0072534	-1.5066942	-3.2921545
H 16	-3.7673269	-0.9418530	-1.2515272
C 17	-3.5652428	1.1930959	0.4563279
C 18	4.0508613	-0.4261913	2.7024130
C 19	1.6703114	-0.7429017	2.4283002
C 20	2.8980158	0.6281360	0.8577141
C 21	4.0730375	0.3814293	1.5658664
C 22	2.8484214	-0.9871359	3.1318343
H 23	0.7236299	-1.1873376	2.7689684
H 24	2.9179131	1.2676917	-0.0369577
H 25	5.0192389	0.8272042	1.2260393
H 26	2.8277482	-1.6246012	4.0277022
H 27	4.9790230	-0.6200012	3.2590156
C 28	0.2555480	4.6161877	3.5009569

C 29	0.0365355	2.2510461	3.0553970
C 30	-0.0450347	3.8381936	1.2321831
C 31	0.1341083	4.8816083	2.1370052
C 32	0.2054583	3.2993746	3.9570943
H 33	0.0158095	1.2100500	3.4132982
H 34	-0.1392108	4.0540722	0.1558510
H 35	0.1812731	5.9183609	1.7728067
H 36	0.3045314	3.0852089	5.0313577
H 37	0.3928697	5.4421847	4.2133477
C 38	2.3435229	-4.1350815	-1.1611404
C 39	1.9495985	-1.7762810	-1.5120137
C 40	0.4397792	-3.0628233	-0.1267955
C 41	1.2069795	-4.2038901	-0.3563323
C 42	2.7127756	-2.9201969	-1.7381849
H 43	2.2460779	-0.8176229	-1.9628538
H 44	-0.4583375	-3.1216033	0.5053046
H 45	0.9123283	-5.1605946	0.0990949
H 46	3.6094640	-2.8623324	-2.3722684
H 47	2.9476768	-5.0361288	-1.3400736
C 48	-3.1161761	-2.5618378	-4.1879595
C 49	-1.0836160	-1.6528765	-3.2480426
C 50	-3.1914650	-1.3418575	-2.1030423
C 51	-3.8394953	-2.0543207	-3.1080400
C 52	-6.0074184	0.9803080	1.8042555
C 53	-3.8314191	0.0849902	1.2583070
C 54	-4.5277466	2.1922921	0.3298384
C 55	-5.7473651	2.0900407	1.0003669
C 56	-5.0482180	-0.0242190	1.9330782
H 57	-3.0808648	-0.7143507	1.3653974
H 58	-4.3300711	3.0708671	-0.3067311
H 59	-6.5019219	2.8829767	0.8951903
H 60	-5.2503387	-0.9005043	2.5658666
H 61	-6.9668143	0.8973325	2.3354987
C 62	-1.9491321	4.6586520	-3.8595258
C 63	-2.1713603	4.0479527	-1.5330354
C 64	-1.6474673	2.3636466	-3.1699337
C 65	-1.6732146	3.3289409	-4.1775856
C 66	-2.1985805	5.0189481	-2.5352903
H 67	-2.3682614	4.3445943	-0.4898615
H 68	-1.4314190	1.3126130	-3.4275648
H 69	-1.4773295	3.0410954	-5.2207172
H 70	-2.4165693	6.0664353	-2.2815525
H 71	-1.9704128	5.4217776	-4.6512067

Heat of Formation: 188.415 kcal/mol

Mulliken and electrostatic fit
charges (electrons)

atom	Mulliken	electro fit
C 1	-0.377623	-0.224620

Ge 2	1.425619	0.954295
H 3	0.131504	0.092864
C 4	-0.032758	0.083188
C 5	-0.130146	-0.111328
C 6	-0.003807	-0.119922
C 7	-0.025685	0.072675
C 8	-0.366761	-0.332952
C 9	-0.008450	0.026777
C 10	-0.034306	0.100755
C 11	-0.019977	0.061111
H 12	0.130891	0.101033
H 13	0.130091	0.101369
C 14	-0.404124	-0.287411
H 15	0.139806	0.085941
H 16	0.138565	0.122713
C 17	-0.405289	-0.246889
C 18	-0.127379	-0.099464
C 19	-0.114720	-0.102259
C 20	-0.108374	-0.114597
C 21	-0.130118	-0.101569
C 22	-0.131132	-0.115164
H 23	0.131467	0.095122
H 24	0.134658	0.101693
H 25	0.130217	0.098265
H 26	0.129567	0.101061
H 27	0.129379	0.098321
C 28	-0.131646	-0.092573
C 29	-0.112812	-0.121595
C 30	-0.134743	-0.096139
C 31	-0.129923	-0.125199
C 32	-0.127797	-0.096916
H 33	0.136587	0.110315
H 34	0.136557	0.092141
H 35	0.129193	0.101986
H 36	0.130495	0.098694
H 37	0.129475	0.095207
C 38	-0.127487	-0.093956
C 39	-0.116004	-0.085661
C 40	-0.108405	-0.155685
C 41	-0.130093	-0.089790
C 42	-0.131317	-0.121365
H 43	0.133718	0.092457
H 44	0.133784	0.121089
H 45	0.130519	0.096384
H 46	0.130230	0.100677
H 47	0.129773	0.096202
C 48	-0.130745	-0.117277
C 49	-0.117583	-0.068720
C 50	-0.131910	-0.199335
C 51	-0.127802	-0.061771
C 52	-0.116633	-0.077452
C 53	-0.102458	-0.062739
C 54	-0.103270	-0.086796
C 55	-0.136733	-0.095733

C 56	-0.138723	-0.123097
H 57	0.129815	0.088635
H 58	0.131720	0.086829
H 59	0.130462	0.093111
H 60	0.130159	0.100438
H 61	0.129828	0.095354
C 62	-0.117593	-0.055576
C 63	-0.113105	0.015164
C 64	-0.100388	-0.065242
C 65	-0.135411	-0.120912
C 66	-0.138562	-0.167994
H 67	0.128597	0.069590
H 68	0.138022	0.086631
H 69	0.131413	0.100468
H 70	0.129748	0.105022
H 71	0.129932	0.094117

Dipole moments from Mulliken and electrostatic fit charges and from wavefunction (debyes)

comp	Mulliken	electro fit	actual
X	-0.6327	-0.4398	-0.4210
Y	0.3306	0.1716	0.1759
Z	-0.2457	-0.1871	-0.1843
Total	0.7550	0.5078	0.4921

Graphics requests:

surface=homo resolution=med pending
surface=lumo resolution=med pending

Graphics files written:
surface=homo resolution=med completed
surface=lumo resolution=med completed

Time for Semi Empirical Engine CPU: 002:06:37.15 Wall: 002:32:21.13
Time for Properties Engine CPU: 000:02:29.47 Wall: 000:02:56.02
Time for Graphics Engine CPU: 000:01:31.29 Wall: 000:01:53.24

Time for GePh6semiAM1 CPU: 002:10:38.31 Wall: 002:37:10.39

SnMe
MacSPARTAN semi-empirical program: Release 1.0

SNMEPH/GEOOPTAM1
Geometry Optimization
AM1
Number of basis functions: 150
Number of electrons: 150
Total molecular charge: 0
Multiplicity: 1
Point group: C1
Number of independent degrees of freedom: 165
No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	-1.1216513	1.1697037	-0.3550179
Sn 2	-1.8287604	0.5682554	1.5286638
C 3	-1.7252058	2.0080657	2.7970069
C 4	1.6070551	-1.3727322	0.0425184
C 5	-3.5698268	-0.2279927	1.3672045
C 6	-0.0296798	0.4325722	-0.6535227
C 7	-1.7616798	2.1973809	-1.1392369
C 8	-0.3015915	-0.6867676	1.4794858
C 9	0.4131869	-0.5732528	0.3389415
C 10	0.7479122	0.5878223	-1.8878225
C 11	-0.0924612	-1.5828431	2.5906058
H 12	-0.7374180	2.5073539	2.7755432
H 13	-1.8891101	1.5490032	3.7914518
H 14	-2.5226058	2.7509740	2.5998120
H 15	-3.7765845	-0.7000893	2.3469982
H 16	-3.5971730	-0.9968923	0.5712820
H 17	-4.3306416	0.5489452	1.1595068
C 18	3.8834638	-2.9106110	-0.5002175
C 19	1.5069020	-2.5366296	-0.7320381
C 20	2.8569311	-0.9874557	0.5449120
C 21	3.9885961	-1.7545239	0.2721857
C 22	2.6414201	-3.2999308	-1.0012106
H 23	0.5292081	-2.8421798	-1.1331559
H 24	2.9429896	-0.0777576	1.1571375
H 25	4.9664330	-1.4451011	0.6692492
H 26	2.5554489	-4.2106402	-1.6116065
H 27	4.7774494	-3.5137923	-0.7142982
C 28	0.2364529	-3.3066338	4.7814343
C 29	0.1170433	-2.9563113	2.3930383
C 30	-0.1326529	-1.0852642	3.9042597
C 31	0.0354633	-1.9417065	4.9888122
C 32	0.2757074	-3.8106658	3.4820266
H 33	0.1647520	-3.3521306	1.3663042
H 34	-0.2903919	-0.0083994	4.0746525
H 35	0.0097321	-1.5397191	6.0122911
H 36	0.4369746	-4.8856010	3.3135891

H 37	0.3652179	-3.9814973	5.6397226
C 38	2.2187902	0.9017658	-4.2500163
C 39	1.7245158	1.5877489	-1.9851341
C 40	0.5127784	-0.2520301	-2.9851183
C 41	1.2464179	-0.0940107	-4.1594133
C 42	2.4559138	1.7409199	-3.1620242
H 43	1.9120202	2.2534909	-1.1299154
H 44	-0.2491540	-1.0422598	-2.9133951
H 45	1.0579384	-0.7582360	-5.0153535
H 46	3.2215839	2.5274502	-3.2303884
H 47	2.7971753	1.0241639	-5.1770299
C 48	-3.0750303	4.1944895	-2.6116154
C 49	-2.1539282	3.3986916	-0.5240230
C 50	-2.0372068	2.0144242	-2.5029787
C 51	-2.6926461	3.0052979	-3.2308038
C 52	-2.8007273	4.3892723	-1.2575855
H 53	-1.9402122	3.5585715	0.5449798
H 54	-1.7215314	1.0816444	-2.9964429
H 55	-2.9042769	2.8483114	-4.2987085
H 56	-3.0961855	5.3283032	-0.7670056
H 57	-3.5893560	4.9768104	-3.1879202

Hessian calculated using X forcefield

Cycle no: 1 Heat of formation = 178.753 rmsG = 0.0069 rmsD = 0.0121

Cycle no: 2 Heat of formation = 172.759 rmsG = 0.0057 rmsD = 0.0121

Cycle no: 3 Heat of formation = 167.601 rmsG = 0.0039 rmsD = 0.0121

Cycle no: 4 Heat of formation = 165.493 rmsG = 0.0022 rmsD = 0.0121

Cycle no: 5 Heat of formation = 163.085 rmsG = 0.0012 rmsD = 0.0121

Cycle no: 6 Heat of formation = 162.989 rmsG = 0.0011 rmsD = 0.0121

Cycle no: 7 Heat of formation = 162.875 rmsG = 0.0011 rmsD = 0.0121

Cycle no: 8 Heat of formation = 161.896 rmsG = 0.0007 rmsD = 0.0121

Cycle no: 9 Heat of formation = 161.635 rmsG = 0.0005 rmsD = 0.0121

Cycle no: 10 Heat of formation = 161.610 rmsG = 0.0005 rmsD = 0.0121

Cycle no: 11 Heat of formation = 161.622 rmsG = 0.0006 rmsD = 0.0121

Cycle no: 12 Heat of formation = 161.401 rmsG = 0.0005 rmsD = 0.0121

Cycle no: 13 Heat of formation = 161.199 rmsG = 0.0004 rmsD = 0.0121

Cycle no: 14 Heat of formation = 161.076 rmsG = 0.0004 rmsD = 0.0121
Lambda correction applied

Cycle no: 15 Heat of formation = 160.977 rmsG = ****** rmsD = 0.0121

Cycle no: 16 Heat of formation = 163.983 rmsG = 0.0081 rmsD = 0.0121

Cycle no: 17 Heat of formation = 171.837 rmsG = 0.0152 rmsD = 0.0121

Cycle no: 18 Heat of formation = 171.413 rmsG = 0.0140 rmsD = 0.0121

Cycle no: 19 Heat of formation = 174.255 rmsG = 0.0143 rmsD = 0.0091

Cycle no: 20 Heat of formation = 163.212 rmsG = 0.0047 rmsD = 0.0083

Cycle no: 21 Heat of formation = 162.015 rmsG = 0.0032 rmsD = 0.0097
Lambda correction applied

Cycle no: 22 Heat of formation = 161.394 rmsG = ****** rmsD = 0.0121

Cycle no: 23 Heat of formation = 161.349 rmsG = 0.0016 rmsD = 0.0121

Cycle no: 24 Heat of formation = 175.240 rmsG = 0.0183 rmsD = 0.0121

Cycle no: 25 Heat of formation = 169.480 rmsG = 0.0111 rmsD = 0.0072

Cycle no: 26 Heat of formation = 164.286 rmsG = 0.0069 rmsD = 0.0064

Cycle no: 27 Heat of formation = 161.914 rmsG = 0.0033 rmsD = 0.0073

Cycle no: 28 Heat of formation = 161.384 rmsG = 0.0018 rmsD = 0.0068

Cycle no: 29 Heat of formation = 161.141 rmsG = 0.0011 rmsD = 0.0087

Cycle no: 30 Heat of formation = 161.059 rmsG = 0.0007 rmsD = 0.0121

Cycle no: 31 Heat of formation = 161.013 rmsG = 0.0006 rmsD = 0.0121

Cycle no: 32 Heat of formation = 161.041 rmsG = 0.0007 rmsD = 0.0065
Lambda correction applied

Cycle no: 33 Heat of formation = 161.003 rmsG = ****** rmsD = 0.0121
Lambda correction applied

Cycle no: 34 Heat of formation = 161.038 rmsG = nan0x8 rmsD = 0.0000
Lambda correction applied

Cycle no: 35 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 36 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 37 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 38 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 39 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 40 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 41 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 42 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 43 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 44 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 45 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000
Lambda correction applied

Cycle no: 46 Heat of formation = 161.038 rmsG = inf rmsD = 0.0000

ERROR Error in SEDIIS. Matrix cannot be inverted

DIIS error- matrix cannot be inverted

Time for Semi Empirical Engine CPU: 000:15:27.42 Wall: 000:18:50.21

Time for SnMe2Ph4semiAM1 CPU: 000:15:27.42 Wall: 000:18:50.21

Mulliken and electrostatic fit
charges (electrons)

atom	Mulliken	electro fit
C 1	-0.346016	-0.305621
Sn 2	1.089730	0.776721
C 3	-0.488056	-0.308470
C 4	-0.031374	0.081366
C 5	-0.478988	-0.378024
C 6	0.002404	-0.039012
C 7	-0.009615	0.112900
C 8	-0.347997	-0.352567
C 9	0.002087	0.020576
C 10	-0.032416	0.104382
C 11	-0.008868	0.136728
H 12	0.095683	0.065310
H 13	0.093186	0.053812
H 14	0.091793	0.057439

H 15	0.093381	0.078032
H 16	0.097903	0.086294
H 17	0.092755	0.075698
C 18	-0.128897	-0.091375
C 19	-0.118836	-0.103603
C 20	-0.107412	-0.137073
C 21	-0.129477	-0.090132
C 22	-0.131991	-0.127268
H 23	0.130004	0.096889
H 24	0.134795	0.109226
H 25	0.129994	0.095937
H 26	0.128513	0.103545
H 27	0.128614	0.093477
C 28	-0.135696	-0.112000
C 29	-0.119940	-0.130917
C 30	-0.135425	-0.168884
C 31	-0.128888	-0.090012
C 32	-0.127068	-0.091185
H 33	0.136907	0.106530
H 34	0.128236	0.113920
H 35	0.128431	0.095184
H 36	0.129652	0.096832
H 37	0.129177	0.096912
C 38	-0.129054	-0.103703
C 39	-0.107477	-0.131994
C 40	-0.119348	-0.095933
C 41	-0.131892	-0.118589
C 42	-0.129206	-0.089200
H 43	0.134974	0.105347
H 44	0.130658	0.089707
H 45	0.128679	0.098009
H 46	0.129714	0.094943
H 47	0.128751	0.098674
C 48	-0.134835	-0.124610
C 49	-0.135995	-0.158199
C 50	-0.119211	-0.143774
C 51	-0.127298	-0.074870
C 52	-0.129453	-0.083063
H 53	0.127551	0.104941
H 54	0.139232	0.113454
H 55	0.130125	0.093244
H 56	0.128467	0.093810
H 57	0.129334	0.100238

Dipole moments from Mulliken and electrostatic fit charges and from wavefunction (debyes)

comp	Mulliken	electro fit	actual
X	-1.7057	-1.1845	-1.1500
Y	0.3138	0.1836	0.1832
Z	0.9260	0.5920	0.5822

Total 1.9660 1.3369 1.3019

Graphics requests:

surface=homo resolution=med pending
surface=lumo resolution=med pending

Graphics files written:
surface=homo resolution=med completed
surface=lumo resolution=med completed

Time for Properties Engine CPU: 000:01:29.46 Wall: 000:01:47.48
Time for Graphics Engine CPU: 000:01:05.10 Wall: 000:01:22.18

Time for SnMe2Ph4semiAM1 CPU: 000:02:34.56 Wall: 000:03:10.06

SnPh
MacSPARTAN semi-empirical program: Release 1.0

SNPH6/GEOOPTAM1
Geometry Optimization
AM1
Number of basis functions: 194
Number of electrons: 194
Total molecular charge: 0
Multiplicity: 1
Point group: C1
Number of independent degrees of freedom: 207
No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	-1.1537190	-0.3660476	-1.1249845
Sn 2	-1.9102632	1.4631548	-0.4238003
H 3	-4.9259534	-2.2158813	-3.0496386
C 4	1.6876538	0.0649050	1.2833137
C 5	-1.7385422	-2.3584372	-4.2553598
C 6	-0.0039536	-0.6397416	-0.4705311
C 7	-1.8024053	-1.1337599	-2.1605356
C 8	-0.3137135	1.4352725	0.7412457
C 9	0.4476953	0.3364542	0.5483578
C 10	0.8073817	-1.8392022	-0.7019995
C 11	-0.0958550	2.5089457	1.6822566
H 12	-1.1638425	-2.7594587	-5.1031216
H 13	-3.6312040	-3.1212921	-4.9820086
C 14	-1.8959739	2.7185024	-1.8454703
H 15	0.0072534	-1.5066942	-3.2921545
H 16	-3.7673269	-0.9418530	-1.2515272
C 17	-3.5652428	1.1930959	0.4563280
C 18	4.0508613	-0.4261913	2.7024130
C 19	1.6703114	-0.7429017	2.4283002
C 20	2.8980158	0.6281360	0.8577141
C 21	4.0730375	0.3814293	1.5658664
C 22	2.8484214	-0.9871359	3.1318343
H 23	0.7236299	-1.1873376	2.7689684
H 24	2.9179131	1.2676918	-0.0369577
H 25	5.0192389	0.8272042	1.2260393
H 26	2.8277483	-1.6246012	4.0277021
H 27	4.9790230	-0.6200012	3.2590156
C 28	0.2555480	4.6161877	3.5009569
C 29	0.0365355	2.2510460	3.0553970
C 30	-0.0450347	3.8381936	1.2321831
C 31	0.1341083	4.8816083	2.1370052
C 32	0.2054583	3.2993746	3.9570943
H 33	0.0158095	1.2100500	3.4132982
H 34	-0.1392108	4.0540722	0.1558510
H 35	0.1812731	5.9183609	1.7728067
H 36	0.3045314	3.0852089	5.0313577

H 37	0.3928697	5.4421847	4.2133477
C 38	2.3435229	-4.1350815	-1.1611404
C 39	1.9495985	-1.7762810	-1.5120137
C 40	0.4397792	-3.0628233	-0.1267955
C 41	1.2069796	-4.2038901	-0.3563323
C 42	2.7127756	-2.9201969	-1.7381848
H 43	2.2460779	-0.8176229	-1.9628538
H 44	-0.4583375	-3.1216033	0.5053046
H 45	0.9123283	-5.1605946	0.0990949
H 46	3.6094640	-2.8623324	-2.3722684
H 47	2.9476768	-5.0361288	-1.3400736
C 48	-3.1161761	-2.5618378	-4.1879595
C 49	-1.0836160	-1.6528765	-3.2480427
C 50	-3.1914651	-1.3418575	-2.1030423
C 51	-3.8394953	-2.0543207	-3.1080400
C 52	-6.0074183	0.9803080	1.8042554
C 53	-3.8314191	0.0849902	1.2583070
C 54	-4.5277466	2.1922921	0.3298385
C 55	-5.7473651	2.0900407	1.0003669
C 56	-5.0482180	-0.0242190	1.9330782
H 57	-3.0808648	-0.7143507	1.3653974
H 58	-4.3300711	3.0708670	-0.3067310
H 59	-6.5019219	2.8829767	0.8951903
H 60	-5.2503387	-0.9005043	2.5658666
H 61	-6.9668143	0.8973325	2.3354987
C 62	-1.9491321	4.6586521	-3.8595258
C 63	-2.1713603	4.0479527	-1.5330354
C 64	-1.6474673	2.3636466	-3.1699337
C 65	-1.6732145	3.3289409	-4.1775857
C 66	-2.1985805	5.0189480	-2.5352903
H 67	-2.3682614	4.3445943	-0.4898615
H 68	-1.4314190	1.3126130	-3.4275648
H 69	-1.4773295	3.0410954	-5.2207172
H 70	-2.4165693	6.0664353	-2.2815526
H 71	-1.9704128	5.4217776	-4.6512067

Hessian calculated using X forcefield

Cycle no: 1 Heat of formation = 247.087 rmsG = 0.0071 rmsD = 0.0109

Cycle no: 2 Heat of formation = 239.814 rmsG = 0.0055 rmsD = 0.0109

Cycle no: 3 Heat of formation = 233.933 rmsG = 0.0031 rmsD = 0.0109

Cycle no: 4 Heat of formation = 230.848 rmsG = 0.0017 rmsD = 0.0109

Cycle no: 5 Heat of formation = 229.045 rmsG = 0.0009 rmsD = 0.0109

Cycle no: 6 Heat of formation = 228.135 rmsG = 0.0006 rmsD = 0.0109

Cycle no: 7 Heat of formation = 227.759 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 8 Heat of formation = 227.747 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 9 Heat of formation = 227.736 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 10 Heat of formation = 227.339 rmsG = 0.0063 rmsD = 0.0109

Cycle no: 11 Heat of formation = 227.954 rmsG = 0.0014 rmsD = 0.0109

Cycle no: 12 Heat of formation = 227.403 rmsG = 0.0009 rmsD = 0.0109

Cycle no: 13 Heat of formation = 227.160 rmsG = 0.0007 rmsD = 0.0109

Cycle no: 14 Heat of formation = 227.104 rmsG = 0.0007 rmsD = 0.0109

Cycle no: 15 Heat of formation = 226.953 rmsG = 0.0006 rmsD = 0.0109

Cycle no: 16 Heat of formation = 226.823 rmsG = 0.0005 rmsD = 0.0109

Cycle no: 17 Heat of formation = 226.750 rmsG = 0.0004 rmsD = 0.0109

Cycle no: 18 Heat of formation = 227.042 rmsG = 0.0013 rmsD = 0.0105

Cycle no: 19 Heat of formation = 226.661 rmsG = 0.0002 rmsD = 0.0109

Cycle no: 20 Heat of formation = 226.621 rmsG = 0.0003 rmsD = 0.0109
Matrix diagonalization failure - SSQEIG
Matrix diagonalization failure

Time for Semi Empirical Engine CPU: 000:14:11.44 Wall: 000:17:07.32

Time for SnPh6semiAM1 CPU: 000:14:11.44 Wall: 000:17:07.32

Mulliken and electrostatic fit
charges (electrons)

atom	Mulliken	electro fit
C 1	-0.342625	-0.271605
Sn 2	1.208799	0.806187
H 3	0.130491	0.098418
C 4	-0.033015	0.103295
C 5	-0.129381	-0.097803
C 6	0.003604	-0.040161
C 7	-0.015900	0.128527
C 8	-0.332287	-0.322690
C 9	-0.000272	0.009662
C 10	-0.033942	0.052344
C 11	-0.012262	0.099523
H 12	0.130347	0.097342
H 13	0.129628	0.098786
C 14	-0.350855	-0.251538
H 15	0.139134	0.093201
H 16	0.134331	0.117866

C 17	-0.350807	-0.231392
C 18	-0.128135	-0.098554
C 19	-0.115935	-0.102032
C 20	-0.109067	-0.136464
C 21	-0.129881	-0.101411
C 22	-0.130977	-0.120982
H 23	0.131372	0.093697
H 24	0.134558	0.106993
H 25	0.129783	0.101310
H 26	0.129234	0.103328
H 27	0.128987	0.097511
C 28	-0.133429	-0.093718
C 29	-0.115957	-0.131827
C 30	-0.133577	-0.114426
C 31	-0.130480	-0.120303
C 32	-0.127579	-0.093488
H 33	0.136766	0.112387
H 34	0.133386	0.095266
H 35	0.128499	0.100611
H 36	0.130114	0.095764
H 37	0.129158	0.093606
C 38	-0.128240	-0.094404
C 39	-0.116370	-0.074283
C 40	-0.109376	-0.138576
C 41	-0.129867	-0.095296
C 42	-0.131050	-0.113490
H 43	0.133296	0.092069
H 44	0.133194	0.114321
H 45	0.129932	0.097578
H 46	0.129678	0.095827
H 47	0.129274	0.095720
C 48	-0.133343	-0.117360
C 49	-0.120017	-0.103626
C 50	-0.132107	-0.190177
C 51	-0.128729	-0.079024
C 52	-0.115155	-0.063633
C 53	-0.096557	-0.048997
C 54	-0.094175	-0.057617
C 55	-0.138237	-0.117909
C 56	-0.139460	-0.129615
H 57	0.131790	0.092835
H 58	0.131580	0.081869
H 59	0.131159	0.100651
H 60	0.131116	0.101644
H 61	0.130471	0.092867
C 62	-0.116437	-0.042212
C 63	-0.103983	0.013732
C 64	-0.093845	-0.058013
C 65	-0.136849	-0.128030
C 66	-0.139278	-0.170511
H 67	0.128386	0.076254
H 68	0.137750	0.092831
H 69	0.132286	0.101222
H 70	0.130682	0.105525

H 71 0.130652 0.090600

Dipole moments from Mulliken and electrostatic fit charges and from wavefunction (debyes)

comp	Mulliken	electro fit	actual
X	-0.9957	-0.7726	-0.7567
Y	0.6299	0.4534	0.4555
Z	-0.3319	-0.2676	-0.2608
Total	1.2241	0.9349	0.9209

Graphics requests:

surface=homo resolution=med pending
surface=lumo resolution=med pending

Graphics files written:
surface=homo resolution=med completed
surface=lumo resolution=med completed

Time for Properties Engine CPU: 000:02:32.15 Wall: 000:03:03.26
Time for Graphics Engine CPU: 000:01:34.35 Wall: 000:01:58.21

Time for SnPh6semiAM1 CPU: 000:04:06.50 Wall: 000:05:01.47