

Microsolvation of Methlymercury: Structures, Energies, Bonding and NMR Constants (^{199}Hg , ^{13}C and ^{17}O)

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Scalar HF clusters

W_1S_1

C	-2.17876253	-0.00063507	0.00086803
H	-2.48761726	1.02093998	-0.15566917
H	-2.48795632	-0.64631883	-0.80593347
H	-2.48788238	-0.37580687	0.96369086
Hg	-0.05934593	-0.00038742	0.00020613
O	2.22523702	-0.00060450	0.00002926
H	2.78159929	-0.75778354	-0.12457806
H	2.78184112	0.75639926	0.12462442

W_2S_1

C	-2.43168352	0.67912878	-0.02402979
H	-2.93291570	0.15011345	-0.81999880
H	-2.89915424	0.49325396	0.93073668
H	-2.36545531	1.73602085	-0.23245710
Hg	-0.46229010	-0.06429687	0.08369772
O	1.61392365	-0.84284158	0.19628691
H	2.40754178	-0.30432394	0.07821519
H	1.86673732	-1.73846308	0.36427627
O	3.76348571	0.73642660	-0.14678953
H	4.24456013	0.85269693	-0.95111656
H	4.27136229	1.14006191	0.53952902

W₂S₂

C	-2.30996789	0.49142454	-0.00056692
H	-2.30422768	1.57013366	-0.02725115
H	-2.77715263	0.07442002	-0.87920129
H	-2.76402482	0.11848487	0.90438140
Hg	-0.26666898	-0.15216382	0.00043219
O	1.78675954	-1.18082959	0.00187703
H	2.55080284	-0.61742429	0.00059494
H	2.04655917	-2.09195878	0.00285459
O	1.92685635	1.61459591	-0.00318585
H	2.14191792	2.14269333	0.75350087
H	2.14161117	2.14010014	-0.76176180

W₃S₁

C	-2.77469551	0.00106269	0.00027833
H	-3.10608304	0.90026778	-0.49719894
H	-3.10640112	-0.87884315	-0.53039436
H	-3.10651846	-0.01805220	1.02752102
Hg	-0.67394211	0.00068520	-0.00086868
O	2.88571110	-2.35641500	-0.07442537
H	3.24097718	-2.76877837	-0.84565801
H	3.24016039	-2.81612125	0.66995203
O	1.50332373	0.00009761	-0.00184779
H	2.04711113	-0.79113130	-0.02606441
H	2.04755920	0.79100710	0.02268031
O	2.88713477	2.35578394	0.07074065
H	3.24264378	2.81464167	-0.67365166
H	3.24177295	2.76864827	0.84199688

W₃S₂

C	2.71418146	1.04674559	0.28265307
H	3.46090812	0.35506138	0.64200124
H	3.01514846	1.49875852	-0.65021529
H	2.48603149	1.79648616	1.02508955
Hg	0.95284838	-0.04697070	-0.07708136
O	-0.89175771	-1.18769922	-0.44462993
H	-1.00314613	-1.90995043	-1.04362772
H	-1.74108431	-0.98269693	-0.01088417
O	-5.16723982	1.07325905	-0.26773945
H	-5.39501530	1.94537961	0.01014619
H	-5.85817481	0.78097918	-0.83953882
O	-3.09800756	-0.52939139	0.78765406
H	-3.44433476	-0.94658876	1.55921532
H	-3.79039250	0.01909594	0.42605931

W_3S_4

C	-2.68069420	0.06223298	0.01549486
H	-3.11238753	-0.37344059	-0.87253065
H	-3.11909409	-0.35781481	0.90770261
H	-2.77115972	1.13781816	0.00575136
Hg	-0.61487103	-0.40516072	0.02673980
O	1.23851299	1.44100891	-0.07035831
H	2.17830998	1.32216908	-0.06940353
H	1.06720029	2.36813147	-0.11408575
O	1.39545682	-1.51493576	0.06846222
H	2.25477740	-1.09889104	0.04484387
H	1.50712172	-2.45210078	0.11119466
O	3.81989184	-0.02084775	-0.01395180
H	4.39022930	0.03091070	0.73845462
H	4.38279724	-0.04056584	-0.77344297

 W_3S_5

C	2.27973768	-1.37741930	0.42888330
H	2.28532835	-1.88253442	1.38291659
H	2.37339420	-2.08194811	-0.38365677
H	3.05210928	-0.62446922	0.38239209
Hg	0.40133766	-0.38952177	0.22371446
O	-4.06210410	-0.85511183	0.05726505
H	-4.61553489	-0.98492254	0.81294837
H	-4.54116631	-1.15739522	-0.69991279
O	0.29105228	2.47917323	-0.10892470
H	0.49996318	3.07531116	0.59645484
H	0.57389323	2.90385297	-0.90656679
O	-1.66512899	0.43522521	0.02791666
H	-1.75177767	1.37239675	-0.08316235
H	-2.52398790	-0.00118992	0.03548703

W_3S_6

C	2.48793901	-0.00869590	0.00204452
H	2.81956396	0.99486002	-0.21672713
H	2.81682567	-0.32114097	0.98141805
H	2.81858341	-0.70076631	-0.75734616
Hg	0.33094898	-0.00661124	-0.00059559
O	-1.54931106	-1.46907781	-0.90313499
H	-2.16398661	-1.03842270	-1.48112836
H	-1.47041851	-2.36922394	-1.18613192
O	-1.54674698	1.50652766	-0.82066921
H	-1.46616256	2.20175059	-1.45843518
H	-2.16324257	1.79162915	-0.16035387
O	-1.55149359	-0.05258400	1.71472722
H	-2.16774929	-0.76699853	1.62982906
H	-1.47334386	0.15208698	2.63590955

Scalar MP2 clusters

W_1S_1

C	-2.1253323304	-0.0011206442	0.0035138742
H	-2.4453040957	1.0365750503	-0.0899418217
H	-2.4532852020	-0.6020766344	-0.8444261736
H	-2.4364672955	-0.4356187254	0.9530480417
Hg	-0.0636694620	-0.0000215432	-0.0210648643
O	2.1665142117	-0.0003098953	-0.0915318555
H	2.7218852684	-0.7785122527	0.0457672748
H	2.7227719056	0.7768876448	0.0478735245

W_2S_1

C	-2.3294528462	0.6711496650	-0.0279110754
H	-2.8720140889	0.0635011149	-0.7520876439
H	-2.7806755213	0.6010092817	0.9617794187
H	-2.2640225685	1.7081892740	-0.3574191446
Hg	-0.4155473387	-0.0654627207	0.1041379666
O	1.6102827126	-0.8259304764	0.2939713742
H	2.4137620658	-0.2609405575	0.1110284133
H	1.8428218528	-1.7542375063	0.1825465569
O	3.5921203643	0.7720927983	-0.1262984056
H	4.0844543403	0.8851235259	-0.9460470212
H	4.1943830278	1.0432826012	0.5746495610

W_2S_2

C	-2.2695655678	0.5050008278	0.0028685842
H	-2.2487326918	1.5896641161	-0.0408752228
H	-2.7560664590	0.0737663495	-0.8667866258
H	-2.7067585123	0.1452401044	0.9293528368
Hg	-0.2534577141	-0.1536264192	-0.0278989877
O	1.7829127640	-1.1578687616	-0.1031875734
H	2.5342715686	-0.5586483130	0.0320355642
H	2.0541504829	-2.0748182406	0.0457590180
O	1.8816789282	1.5418317720	0.0142855865
H	2.0396872468	2.1278636415	0.7695536952
H	2.1143449546	2.0710709230	-0.7634328750

W_3S_1

C	-2.6348749475	0.0021524101	-0.0351364415
H	-2.9360874932	0.9146303051	-0.5502308513
H	-2.9365207073	-0.8772016246	-0.6047090788
H	-3.0532116814	-0.0283391791	0.9711190804
Hg	-0.5890162282	-0.0030816972	0.1209120203
O	2.7343772566	-2.3036978537	-0.1319149942
H	3.1250642848	-2.6216969167	-0.9518962098
H	3.1695273274	-2.8054928859	0.5648732235
O	1.5352875056	-0.0102180016	0.3395570967
H	2.0603095907	-0.8211364974	0.1328399679
H	2.060749792	0.8113598072	0.1818599655
O	2.7356225651	2.3067708230	0.0065271037
H	3.1264950308	2.6731859011	-0.7929024221
H	3.1710317046	2.7656184100	0.7321615396

W_3S_2

C	2.6603558665	1.0528277494	0.2734723503
H	3.4156214803	0.3463814686	0.6054493732
H	2.9351198285	1.5184013886	-0.6685285666
H	2.4447844521	1.7945780844	1.0371476850
Hg	0.8872187877	-0.0369334246	-0.0576880896
O	-0.9536145104	-1.1860566050	-0.3704231868
H	-1.0984431486	-1.7836025128	-1.1163615300
H	-1.8439198068	-0.9456651112	0.0779914583
O	-4.9851216540	1.0332114548	-0.3053246373
H	-5.2421881677	1.9020251465	0.0287516686
H	-5.7036842202	0.7424986219	-0.8811623559
O	-3.0563679889	-0.5113569186	0.8218059267
H	-3.4429819948	-1.0440467680	1.5278923681
H	-3.7768139236	0.0302054260	0.4260795361

W_3S_3

C	2.3359601485	0.7870440740	-0.3476968887
H	2.5542532469	1.5862297733	0.3608841619
H	3.1002843645	0.0116482926	-0.3009765702
H	2.2484463061	1.1792409230	-1.3612245245
Hg	0.5301566541	-0.0522506316	0.1715620136
O	-3.1356292767	-0.0667696309	-0.7829165962
H	-3.2029126664	0.8765435240	-0.5977043913
H	-4.0000860039	-0.3496192295	-1.0968183006
O	-1.4786990281	1.9507430634	0.5317096151
H	-1.2627029532	2.8200187490	0.1746334358
H	-1.7515668890	2.1417969183	1.4367420136
O	-1.3199033266	-1.0489113238	0.7509956705
H	-1.3455571789	-2.0060251789	0.8644460607
H	-2.1069063974	-0.7778643228	0.1970043003

W_3S_4

C	-2.5666535345	0.0675760553	0.0517095851
H	-3.0402341391	-0.2807977488	-0.8658153254
H	-3.0235140497	-0.3975914129	0.9246704179
H	-2.6077494194	1.1542632796	0.1237991049
Hg	-0.5784450059	-0.4870666226	-0.0074873701
O	1.1838687290	1.4082158681	-0.1165567730
H	2.1469416487	1.3335625434	-0.1093893481
H	0.9940094183	2.3432835857	-0.2401321846
O	1.4030893576	-1.5012315165	-0.1023606307
H	2.2614126695	-1.0358567624	-0.0037342786
H	1.5272938401	-2.4206757274	0.1555818307
O	3.6848722822	-0.0225985967	0.0454740430
H	4.2389582730	0.0264689563	0.8336258526
H	4.3122409303	-0.0890379011	-0.6845139237

W_3S_5

C	2.2444479932	-1.3339339789	0.4120815760
H	2.2751679299	-1.8695519555	1.3564055059
H	2.3237076324	-2.0150610084	-0.4301403223
H	3.0072665453	-0.5619328096	0.3699672423
Hg	0.3664275201	-0.3748292878	0.2848471528
O	-3.9624804260	-0.8430754644	0.0271246887
H	-4.5921462613	-0.9222264321	0.7555579314
H	-4.4209735456	-1.1408349393	-0.7691659047
O	0.2543104067	2.3685430483	-0.1391543671
H	0.4701020289	2.9957877555	0.5664020721
H	0.6000910994	2.7752786097	-0.9469772825
O	-1.6821768043	0.4542767900	0.2152753174
H	-1.7290685718	1.3846930799	-0.0502917402
H	-2.5575595471	-0.0056864074	0.1138231301

W₃S₆

C	2.4843285621	-0.0098476847	0.0011321481
H	2.8134273084	0.9986589909	-0.2297933229
H	2.8066369157	-0.3165814337	0.9914641141
H	2.8046671690	-0.7165865112	-0.7582363263
Hg	0.3420364634	0.0009356788	0.0009444603
O	-1.5616301172	-1.4182637726	-0.8051347152
H	-2.1227037377	-0.9279582422	-1.4252533434
H	-1.4835021322	-2.3178021236	-1.1555629281
O	-1.5618811195	1.3991731053	-0.8232385264
H	-1.4859459421	2.1551211190	-1.4239534896
H	-2.1257440661	1.6849973348	-0.0882652634
O	-1.5671760931	0.0077477710	1.6210165782
H	-2.1259031373	-0.7748599552	1.4977317788
H	-1.4952040735	0.1485987235	2.5765548359

Full relativistic DHF clusters

W_1S_1

C	-0.0010186264	-0.0000570530	2.1390088316
H	0.8390742452	0.6033966265	2.4563482992
H	-0.9433920814	0.4261627652	2.4563112643
H	0.1019660018	-1.0290889643	2.4566932031
H	-0.5971329616	-0.4810373484	-2.7655332590
H	0.5987892060	0.4812462416	-2.7653078662
O	0.0008080412	0.0000000000	-2.2083749231
Hg	0.0000000000	0.0000000000	0.0386282189

W_2S_1

C	1.0423768935	0.0006042384	2.1471651195
H	2.0998822058	0.0313781147	1.9178537960
H	0.7374459371	0.8781926995	2.7025692692
H	0.7837089416	-0.9073325579	2.6766419087
H	-0.6633584747	-0.0005965941	-2.4361582243
H	-2.0233719215	-0.0021606951	-1.6688086080
H	0.3570550799	-0.7578774049	-4.4601433406
H	0.3549395247	0.7580902503	-4.4604709920
O	-1.0831156283	-0.0004248544	-1.5643468452
O	0.1973632459	0.0000000000	-3.9181610696
Hg	0.0000000000	0.0000000000	0.3351953343

W_3S_1

C	0.0000000000	-0.0090563348	2.5822512529
H	-0.8907922459	-0.5256350713	2.9175184738
H	0.8909040071	-0.5254511998	2.9175164703
H	-0.0001035541	1.0180288860	2.9252660776
H	2.7866379394	-0.7574127274	-3.3775879126
H	2.7917444116	0.7562848060	-3.3741476768
H	0.7929759815	0.0061496441	-2.1923350068
H	-0.7929755077	0.0053576741	-2.1923370754
H	-2.7859832362	-0.7601469005	-3.3774274026
H	-2.7923991253	0.7535459850	-3.3742897019
O	2.3666734764	0.0000000000	-2.9996758343
O	-0.0000027307	0.0109349705	-1.6491128137
O	-2.3666722715	-0.0022957231	-2.9996688116
Hg	0.0000000000	0.0000000000	0.4978380637

W_3S_2

C	0.7329335949	1.0318931137	2.3606021666
H	0.0660524690	0.8423785368	3.1921534888
H	1.7290910273	0.6636239497	2.5705069311
H	0.7536413729	2.0859418730	2.1138288990
H	-0.9153455456	-1.9897217758	-1.0913724755
H	-0.8409911096	-0.6491708519	-1.9111358230
H	1.5844977735	0.7119277476	-5.6547810407
H	1.0813563534	-0.6612318954	-6.0342007119
H	-1.7003481656	0.5045893033	-3.7050432766
H	-0.2548794765	0.1214456762	-4.0140646492
O	-0.7783639664	-1.0566223916	-1.0254315655
O	1.0378136735	0.0000000000	-5.3614243885
O	-0.9040320258	0.1797654045	-3.3158133274
Hg	0.0000000000	0.0000000000	0.7006661889

W_3S_3

C	-0.7434166596	1.2499522028	1.8772949591
H	-1.8252429522	1.1207293537	1.9145783311
H	-0.2897827656	0.9750230494	2.8292629865
H	-0.4832285361	2.2743601293	1.6097023593
H	0.3989266911	0.3182179116	-3.4684087102
H	1.8231814024	-0.0703527003	-3.9251213483
H	-1.9796592400	1.0944805634	-2.0980947506
H	-2.0337138014	-0.4069761881	-2.2840961038
H	1.5636046231	-1.9835058298	-0.7772289822
H	1.0861532887	-0.9595027616	-1.8983748590
O	1.2523782522	0.0000000000	-3.1537214286
O	-1.4311968783	0.3038567831	-2.0356370628
O	0.8461791490	-1.3904762692	-1.0286502135
Hg	0.0000000000	0.0000000000	0.4212995369

W_3S_4

C	-1.1133097747	-0.0015116033	2.2381087323
H	-0.8663528344	-0.8997904074	2.7891362725
H	-0.8469036953	0.8823294147	2.8032114489
H	-2.1626497437	0.0120619679	1.9719171745
H	-1.0645669289	0.0019970503	-2.7245648668
H	-2.3365076257	0.0022703199	-1.8922188976
H	1.3426921507	-0.0008122934	-2.1151942693
H	2.4681197378	-0.0002590351	-1.0498965829
H	0.9529972434	0.7555106032	-4.4424505583
H	0.9513376589	-0.7557649774	-4.4425765117
O	-1.3935114910	0.0019689745	-1.8365608869
O	1.5312953865	-0.0006707978	-1.1763343902
O	0.7958680873	0.0000000000	-3.8947592119
Hg	0.0000000000	0.0000000000	0.4594921178